Discontinuous Phase Transitions in Quantum Lattice Systems

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par

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acceptée sur proposition du jury :

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à mes parents,
André et Madeleine Ueltschi

Résumé

Une classe de systèmes de Physique Statistique Quantique sur réseau est étudiée mathématiquement de manière rigoureuse. Les modèles que nous considérons ont un hamiltonien composé de deux termes : $H = V + T$; typiquement, V représente une interaction entre les particules, et T est l'énergie cinétique. Nous supposons que pour une base judicieusement choisie de l'espace de Hilbert, V est un opérateur diagonal, pouvant être représenté par une interaction classique. T n'est pas nécessairement diagonal dans cette base; sa norme est petite devant V.

Dans la première partie de ce travail, nous admettons que V satisfait une "condition de Peierls"; en gros, cela signifie que les excitations de V sont séparées par un gap. À l'aide d'une extension de la théorie de Pirogov-Sinai, nous pouvons montrer que le diagramme de phases de $V + T$, à basse température, est proche de celui de V à température nulle. Cela signifie que ce dernier est stable par rapport aux fluctuations quantiques et thermiques. Certaines propriétés des phases à basse température peuvent alors être établies, concernant la valeur des paramètres d'ordre et la décroissance des fonctions de corrélation.

La deuxième partie de ce travail consiste à mieux comprendre les effets quantiques. Nous montrons que les fluctuations quantiques créent une nouvelle "interaction effective" qui s'ajoute à l'interaction V. Une formule est proposée, qui permet de calculer explicitement cette interaction pour des modèles précis. Sous certaines hypothèses — notamment une condition de Peierls pour cette nouvelle interaction, et une condition assurant que les autres effets quantiques sont faibles — nous prouvons que le diagramme de phases à basse température est proche de celui, à température nulle, de cette nouvelle interaction. Dans ce cas aussi, certaines caractéristiques des phases peuvent être précisées.

Ces résultats sont illustrés en considérant deux modèles simples. Un modèle de Hubbard modifié, "asymétrique", dans lequel les électrons de spin "up" ont une masse plus faible que ceux de spin "down". Les déplacements des électrons, combinés à la répulsion coulombienne, sont responsables d'une interaction antiferromagnétique effective. Les phases à basse température brisent une symétrie de l'hamiltonien (l'invariance sous les translations). Le second modèle est celui de Bose-Hubbard, qui décrit un système de bosons sur réseau, avec interactions locales et entre proches voisins. Lorsque les interactions sont fortes, le caractère isolant des phases à basse température peut être démontré.

Abstract

A class of lattice systems of Quantum Statistical Physics is mathematically and rigorously studied. The models we are considering have Hamiltonian formed by two terms: $H = V + T$; typically, V represents an interaction between the particles and T is the kinetic energy. We suppose that, in a judiciously chosen basis of the Hilbert space, V is a diagonal operator that can be represented by a classical interaction. T is not necessarily diagonal in this basis; its norm is small compared to that of V.

In the first part of this work, we assume that V satisfies a "Peierls condition"; roughly speaking, this means that excitations of V are separated by a gap. With the help of an extension of the Pirogov-Sinai theory, we can show that the low temperature phase diagram of $V + T$ is close to that of V at temperature zero. This means that the latter is stable with respect to quantum and thermal fluctuations. Some properties of the low temperature phases can be established, concerning values of order parameters and decay of correlation functions.

The second part of this work consists in better understanding the quantum effects. We show that quantum fluctuations create a new "effective interaction", which adds to the interaction V. A formula is proposed, allowing to compute explicitely this interaction in concrete models. Under some assumptions — in particular, a Peierls condition for this new interaction, and a condition ensuring that other quantum effects are small — we prove that the low temperature phase diagram is close to that of this new interaction at temperature zero. In this case also, several features of the phases can be precised.

These results are illustrated by considering two simple models. A modified, "asymmetric" Hubbard model in which spin "up" electrons have a smaller mass than spin "down" electrons. The moves of electrons, combined with Coulomb repulsion, is responsible for an effective antiferromagnetic interaction. Low temperature phases break a symmetry of the Hamiltonian, namely the invariance under translations. The second model is the Bose-Hubbard one, which describes a system of bosons on a lattice, with local and neighbour interactions. When the interactions are strong, the insulating behaviour of the low temperature phases can be proven.

Remerciements

Je suis particulièrement reconnaissant envers le Prof. Christian Gruber. Dans son cours de "Mécanique Générale", il écrivit un jour sur le tableau noir

"La Mécanique, c'est beau et c'est simple
(conceptuellement)"

Je fus très impressionné par la confiance mêlée d'humour qui ressort de ces quelques mots. Pour ses cours, pour la possibilité qu'il m'a accordée de faire une thèse sous sa direction — à un moment où j'envisageais d'abandonner la Physique — et pour les nombreuses discussions que nous avons eues, notamment lors de nos travaux sur le modèle de Falicov-Kimball, je remercie cordialement le professeur Gruber.

Ma gratitude va également au Prof. Roman Kotecký, qui m'a accueilli lors de mon séjour à Prague. C'est lui qui m'a suggéré d'étudier des systèmes quantiques avec des techniques géométriques, ce qui débouche, cinq années plus tard, sur ce travail. J'ai beaucoup bénéficié de ses connaissances et de son intuition sur les systèmes classiques sur réseaux, tout au long d'une collaboration extrêmement plaisante. Tě moc děkuji, Romane; a na zdraví!

L'enthousiasme — contagieux — d'Yvan Velenik pour la Physique Statistique Classique, et les nombreuses et longues discussions que nous avons eues, m'ont énormément apporté, tant au niveau des connaissances que de la motivation.

Je remercie les Prof. Roberto Fernández, Xenophon Zotos et Jean Buttet pour avoir bien voulu accepter de consacrer quelque temps à ce travail, en étant membres du jury.

De nombreuses discussions, réponses à des questions, ... , de la part de Nils Berglund, Nicolas Macris, Charles-Édouard Pfister et Claude-Alain Piguet, m'ont été très utiles. Je tiens à leur exprimer ma reconnaissance, ainsi qu'à tous les membres de l'Institut de Physique Théorique qui conservent leur motivation pour cette formidable aventure humaine qu'est la Physique.

La qualité rédactionnelle de cet ouvrage s'est beaucoup améliorée grâce aux commentaires de Ch. Gruber, R. Fernández et R. Kotecký.

Enfin, je n'aurais pu *commencer* cette thèse sans le soutien de mes parents, avant et pendant mes études. Je leur suis d'autant plus reconnaissant qu'ils me comprennent peu, et donc qu'ils durent me faire doublement confiance. Comme modeste marque de ma gratitude, je leur dédie cette thèse.

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CHAPTER 0

Prolog

La légende... C'est ce qui nous reste
des vérités d'hier, quand elles passent
par le crible des vérités du jourd'hui...
François Bourgeon,
Le Dernier Chant des Malaterre

– NON ! Mais enfin, vous voulez décrire *deux* phases, aux propriétés physiques différentes, avec les mêmes équations ? Regardez-la, notre fonction de partition

[il désigne le tableau noir, sur lequel la main nerveuse de Max Born avait tracé

$$\begin{aligned} Z &= \mathrm{e}^{-NF/kT} \\ &= \int_V \mathrm{d}q_1 ... \int_V \mathrm{d}q_N \, \mathrm{e}^{-U(q_1,...,q_N)/kT} \end{aligned} \quad]$$

Vous voudriez que pour une valeur de la température, on ait un gaz, et pour une autre valeur de la température, même proche, on ait un liquide ? Et au point de transition, que *tous les deux* découlent de cette équation ? Si votre père vous entendait... vous êtes complétement dépourvu de sa clairvoyance !

Bouillonnant, la moustache agressive, Arnold Sommerfeld parvenait à se faire entendre malgré le brouhaha dû à de nombreuses autres discussions, tout aussi animées. Sa réplique laissa van der Waals Jr sans voix. Il n'est pas facile de se créer une personnalité scientifique lorsque toute réflexion s'accompagne d'une pensée à ce père prestigieux, et Sommerfeld, sans doute involontairement, avait touché un point douloureux. Mal à l'aise, van der Waals se tourna en direction de Sommerfeld, et je ne l'eus pas entendu si je ne fus assis à proximité.

– Monsieur, je me permets d'insister, il n'existe pas deux descriptions possibles pour un système de physique statistique; et l'intégrale contient toutes les positions possibles des particules du système. Celles qui correspondent à un gaz, et celles qui correspondent à un liquide.

Je ne sais pas si Sommerfeld comprit les mots de van der Waals. Les débats étaient vifs. Afin de mieux saisir le sujet de la discussion, je revins à la fonction de partition sur le tableau noir. Celui-ci était caché par un groupe dans lequel je reconnus notre orateur, Max Born, qui détaillait certains passages de cette théorie de Mayer qu'il venait de nous expliquer. Un de ses auditeurs, les cheveux noirs et les lèvres proéminentes, contrastait singulièrement avec le visage fin au front dégarni, et les cheveux grisonnants, de Born. C'était George Uhlenbeck, qui justement prenait la parole :

– D'où vient la grande similitude des propriétés macroscopiques ? Par exemple, toutes les substances apparaissent dans des phases solide, liquide ou gaz. Cela indique, je

crois, que ces propriétés ne dépendent que de certaines caractéristiques qualitatives des forces interatomiques.

Cette session matinale de la conférence à l'occasion du centenaire de Johannes van der Waals, commençait à me lasser. Il était certes distrayant d'assister à ces empoignades intellectuelles — qui par ailleurs menaçaient de ne pas en rester là — mais tout cela me dépassait, et je peinais à saisir les subtilités de cette controverse sur les transitions de phases.

La fenêtre laissait voir des nuages au-dessus d'Amsterdam, en ce jour de novembre 1937. Mon voisin, moins rêveur, prenait part à la discussion :

– Une fonction de partition, ce sont des intégrales de fonctions continues. Comment obtenir les discontinuités associées aux transitions de phases ?

Revenant à l'assemblée, je vis Hendrik Kramers, le chairman, qui rajustait ses lunettes; et d'une voix autoritaire qui contredisait l'aspect juvénile de son visage,

– Mes chers collègues, s'il vous plaît, un peu de retenue. Arnold, s'il vous plaît. L'heure du repas approche. Puisqu'aucun consensus ne se dégage, je propose de voter. Que ceux qui soutiennent l'idée que la fonction de partition contient la possibilité d'une transition de phases, lèvent la main.

Je regardai autour de moi, quelque peu apeuré. Un vote sur un sujet scientifique, quelle idée incongrue ! Et surtout, quelle position devais-je prendre ? J'aperçus Sommerfeld croisant fermement les bras, alors que Born, Uhlenbeck et van der Waals levaient la main. De nombreuses personnes soutenaient le même point de vue. Puis le chairman demanda à ceux jugeant qu'une et une seule phase pouvait être décrite par la même équation, de se manifester. Sommerfeld ne fut pas le seul à exprimer cet avis, et un nombre semblable de mains se levèrent. Kramers, dépité, décida que ce vote n'était pas concluant, et refusa d'en faire un acte officiel du colloque.

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The legend... This is what remains
from yesterday truths, when they go
through the riddle of today truths...
François Bourgeon,
Le Dernier Chant des Malaterre

– NO! How dare you describe two phases, with different physical features, with the same equations? Look at it, our partition function

[he pointed towards the blackboard, on which Max Born's nervous hand had drawn

$$Z = \mathrm{e}^{-NF/kT} = \int_V \mathrm{d}q_1 ... \int_V \mathrm{d}q_N \, \mathrm{e}^{-U(q_1,...,q_N)/kT} \quad]$$

You'd like that for a temperature value we get a gas, and for another temperature value, even close, we get a liquid? And at the transition point, that both of them result from this equation? If your father could hear you... you're totally devoid of his cleverness!

Boiling, with agressive moustache, Arnold Sommerfeld succeeded in making himself heard despite the hubbub due to numerous animated discussions. His respons let van der Waals Jr speechless. It is not easy to create oneself a scientific personality, when each reflection comes with a thought to his pretigious father, and Sommerfeld, doubtless unintentionally, had touched a sensible point. Ill at ease, van der Waals turned to Sommerfeld. I would not have heard him if I had not been seated nearby.

– Sir, allow me to insist, there aren't two possible descriptions for a system of statistical physics, and the integral contains all possible positions of particles of the system. Those that correspond to a gas, and those that correspond to a liquid.

I do not know whether Sommerfeld understood the words of van der Waals. The debates were spirited. In order to catch better the subject of the discussion, I looked again at the partition function on the blackboard. But it was hidden by some people among whom I recognised our speaker, Max Born, who was explaining in detail some parts of Mayer's theory that he had just been talking about. One of his listener, with black hair and prominent lips, singularly contrasted with the fine and bald foreheaded face, and the grey hair of Born. This was George Uhlenbeck, who started to speak:

– Where does the great similarity of the macroscopic properties come from? For example, all substances appear in solid, liquid, or gas phases. This means, I believe, that these properties only depend on certain qualitative characteristics of interatomic forces.

This morning session of the conference of Johannes van der Waals' centenary was boring me. It was certainly piece of entertainment to assist to such intellectual fights —

which moreover threatened to go further — but all of this was well beyond me and I was smuggling to grasp the subtleties of this controversy about the phase transitions.

Clouds above Amsterdam could be seen through the window, on this November day of 1937. My neighbour, less daydreamer, was taking part in the discussion:

– Partition functions, they are integrals of continuous functions. How to obtain the discontinuities associated to phase transitions?

Coming back to the meeting, I saw Hendrik Kramers, the chairman, readjusting his glasses; and with an autoritative voice, that contradicted his youthful face,

– My dear collegues, please, have some restraint. Arnold, please. It will soon be lunch time. As no consensus is being drawn, I suggest to vote. Those who uphold the idea that the partition function contains the possibility of a phase transition, please lift up your hands.

I looked around me, somehow scared. A vote on a scientific subject, what a peculiar idea! And moreover what position should I support? I noticed Sommerfeld crossing resolutely his arms, while Born, Uhlenbeck and van der Waals were raising their hands. Numerous people were approving the same point of view. Then the chairman requested to those that reckon that one and only one phase could be described by the same equation, to express themselves. Sommerfeld was not the only one to agree with this idea, and a similar number of hands were uplifted. Kramers, destressed, decided that this vote was not conclusive, and refused to make of it an official deed of the colloquium.

References: see page 2. The translation of this prolog was achieved by Anne-Lise Ueltschi; merci, petite sœur !

CHAPTER 1

Introduction

1. Generalities

Many physical systems consist of particles in interaction, and share two characteristics:

- the particles are described by the rules of Quantum Mechanics;
- the number of particles is enormous.

Some phenomena are closely related to these systems, as for instance magnetization, long-range order, superfluidity, superconductivity. Varying the thermodynamic parameters may result in changing the properties of the phases. Sometimes the change is sudden, there is *phase transition*.

A key role is played by the number of particles. First, it is a limitation to attempts of solving explicitely the Schrödinger equation associated with interacting particles. Second, a sufficient description of the system involves only a small number of relevant (macroscopic) quantities — the system is governed by the laws of Thermodynamics.

Thermodynamics is at the same time a powerful tool that applies to a wide class of systems, and a semi-phenomenological theory that requires a few inputs — for instance, a state equation. We cannot content ourselves with this theory for several reasons. First, we would like to derive the state equation. Second, the description provided by bare Quantum Mechanics, although inconvenient, is correct and we have to check that it does not bring predictions that contradict those of Thermodynamics.

A third motivation comes from the progress of Experimental Physics. Atomic scales are now under observation, and natural questions are what are the electronic properties of a given material, knowing its atomic structure. In particular, what are the mechanisms favouring magnetism or superconductivity?

The link between the "true" microscopic description — here Quantum Mechanics — and macroscopic observation — thermodynamic quantities — is the subject of Statistical Physics. It provides recepies for the computation of thermodynamic potentials from the basic laws. Actually, the creation of Statistical Physics was far from easy; strong resistance arose from the scientific community. Its main figure, Ludwig Boltzmann, eventually committed suicide, partly because of numerous misunderstandings met by his ideas. Two main phenomena of Thermodynamics, namely irreversibility and phase transitions, seem incompatible with a microscopic description. Newton equations are reversible, therefore a classical gas should obey a reversible equation of motion? And the withstanding to phase transitions was illustrated in the prolog.

It is now commonly accepted that phase transitions occur in the limit of infinite systems, although this can be proven only in models quite far from reality. Irreversibility is still a subject of debate; see Lebowitz [Leb 1993] and Bricmont [Bri 1995] for two excellent discussions.

Since it is in general mathematically not easy to obtain some information on the macroscopic properties of a system, we have to look at caricatures. A very useful simplification is to consider lattice models; many mathematical techniques exist that apply only in this case. Going back to a physical justification for this assumption, we can invoke applications to condensed matter systems. The lattice is due to a periodic arrangment of (motionless) atoms, creating a periodic potential. There is a natural basis for the Hilbert space of quantum particles (electrons) feeling such a potential, namely the one formed by Wannier states. Each state is labelled by a site of the lattice, and represents a particle that is localized around the site. With a few additional assumptions, we obtain a lattice model.

Another class of models consists in spin systems. Here, a spin is attached at each site of the lattice; the phase space is a tensorial product of local phase spaces, these being Hilbert spaces for one spin. The standard spin model is the Heisenberg model, with Hamiltonian involving nearest-neighbour interactions. When the Hamiltonian and all interesting observables are diagonal operators, the model can be reformulated in the context of Classical Statistical Mechanics.

2. Classical lattice models

More than modelization of a given physical system, classical lattice models are illustrations of different phenomena. The most famous and simplest one is the Ising model, "describing" a system of spin $\frac{1}{2}$ on a lattice. A configuration of spins is an assignment of a value ± 1 to each site. The interaction between the spins is nearest-neighbour; more precisely, each pair of neighbouring spins in opposite states [i.e. $(+,-)$ or $(-,+)$] contributes for an amount of energy of J, while pairs with identical spins have energy $-J$. At high temperature, there is a unique phase, that has all the symmetries of the Hamiltonian — in particular, it is invariant under the spin flips. The magnetization is zero. At low temperature, however, there are two phases, one with positive magnetization, the other with negative magnetization. These phases are not invariant under spin flips: there is *symmetry breaking*. Qualitatively, the Ising model describes the behaviour of a magnet.

The proof of these properties was done by Peierls [Pei 1936] (see also [Dob 1965, Gri 1964]) and is called now the "Peierls argument". He introduced geometric concepts, namely the "contours". Retrospectively, these are natural notions in view of probability theory: at high temperature, the spins are essentially independent random variables, and a central limit theorem holds. At low temperature, the spins are strongly dependent, but contours play the role of essentially independent random variables. For boundary conditions "+", respectively "−", contours have low probability of occurrence and most of the sites are in the state "+", respectively "−".

It is interesting to consider now the Ising model with an external magnetic field. When it is positive, there is only one phase with positive magnetization; decreasing the magnetic field, we obtain the "+" phase. The same can be done with a negative magnetic field, so as to obtain the "−" phase. This describes a *first-order* (or *discontinuous*) *phase transition*. The magnetization is a first derivative of the free energy of the system; we see here that it has a discontinuity as a function of the magnetic field, when it is zero.

There exists a beautiful and general theory for first-order phase transitions in lattice models, that is due to Pirogov and Sinai [PS 1975]. It relies on the Peierls argument, but involves new ideas to treat the case where phases are not related by symmetry. It provides a good description of the low temperature phases and of the low temperature

phase diagrams for a large class of models. Important notions are that of phase coexistence and metastable free energy — both have physical as well as mathematical meaning.

3. Quantum lattice models

There is a curious conservation law between the classical and quantum cases, in Statistical Physics. Namely, the modelization process leading to a classical model has no physical justification; for instance, why should Ising spins be only in the z-direction; and why should they interact in their ferromagnetic way? However, given the model, the definition of thermodynamic quantities finds a deep justification in probability theory. On the other hand, basic quantum models are more natural — the Hubbard model, for instance, consists in kinetic energy and Coulomb interaction. But the motivation behind the definition of Gibbs states is not clear.

The study of quantum models is much harder than classical ones, and there is comparatively less results, for less models. The questions we are interested in are roughly the same as for classical systems — namely, to understand which symmetries are broken at low temperatures. An important — negative — result is the Mermin-Wagner theorem, which states that continuous symmetries *cannot* be broken at one or two dimensions.

There are two rather general methods to prove the existence of phases with magnetization or long-range order. One is the "reflection positivity" [DLS 1978, FL 1978], the other is the Peierls argument applied to quantum models [Gin 1969, Rob 1969]. An important advantage of the first one is the possibility to study breakings of continuous symmetries. The second one is more robust to perturbations of the model; it also allows to define pure states.

Beside of the results which enter these two classes, there are numerous contributions where special properties of models are used, together with the imagination of their authors.

4. About this work

There are two aspects. The first one consists in the extension of the Pirogov-Sinai theory to quantum models. In a collaboration with Christian Borgs and Roman Kotecký [BKU 1996, BKU 1997], we showed that "nice" classical models possess low temperature phases that are stable with respect to a quantum perturbation.[1] This amounts to say that classical models may be correct approximations of the quantum reality. The proof consists in an expansion with Duhamel formula (Dyson serie) mapping the quantum model onto a classical model in one more (continuous) dimension. Then it is possible to introduce contours and to use the ideas of Pirogov-Sinai theory. Notice that the quantum model is mathematically very close to a classical one, but the concepts (in particular that of metastability) are physically not so meaningful.

The second aspect is to focus on the "quantum fluctuations", and to show that they bring a new (classical) effective interaction between the particles. This allows to study models where the classical part has degeneracies that are removed by the quantum perturbation.[2] This work was done with Christian Gruber and Roman Kotecký [KU 1998, GKU 1998]. It is possible to compute e.g. the nearest-neighbour antiferromagnetic interaction in the Hubbard model. Conditions are given in order that the low temperature phases are decided by this effective potential. Notice that the Hubbard model

[1] Similar results were obtained at the same time by a group in Zürich consisting in Nilanjana Datta, Roberto Fernández and Jürg Fröhlich [DFF 1996].

[2] Related results were *previously* obtained by the Zürich group, the same persons and Luc Rey-Bellet [DFFR 1996, FR 1996].

does not satisfy one of the assumptions (there is "quantum instability"; it is related to the rotational invariance of the spins). With this effective interaction, we make a small step towards justifying classical models.

A natural question is about true quantum phenomena such as superfluidity and superconductivity. Our results bring some information, but these are negative results: in the domain of applicability of our method, no off-diagonal long-range order may be present (remark that in most of the situations, we have no mathematical statement to support this affirmation). This knowledge is nevertheless useful, because, as noted in [DFF 1996]: "it allows people hunting for quantum effects to rule out large regions of the phase diagram, saving efforts and misunderstandings".

Let us end this introduction by a description of the contents of this thesis.

After a brief heuristical discussion on the definition of macroscopic states in classical systems, Chapter 2 introduces the necessary mathematical definitions.

The results proved in this thesis are written in Chapter 3. The first theorem claims the analyticity of the free energy at high temperature — this result is not new, but is a nice example of the use of cluster expansions. The second theorem is also about analyticity, for all temperature, provided only local interactions are not small. The next section is devoted to the stability of the properties of classical models with respect to the quantum fluctuations (quantum Pirogov-Sinai theory). In the last section the effective potential is introduced, and after a few assumptions, the stability of phases selected by the effective interaction is stated.

The title of Chapter 4 is "Applications to Hubbard models". Notice the plural of "models". It of course suggests that the standard Hubbard model is *not* included in those we consider. Actually, we introduce first the "asymmetric" Hubbard model where electrons of different spins do not have the same hopping. Low temperature phases present chessboard structures; we observe however that when adding longer-range hopping, the phases may be drastically different. Second we study the Bose-Hubbard model describing bosons on a lattice.

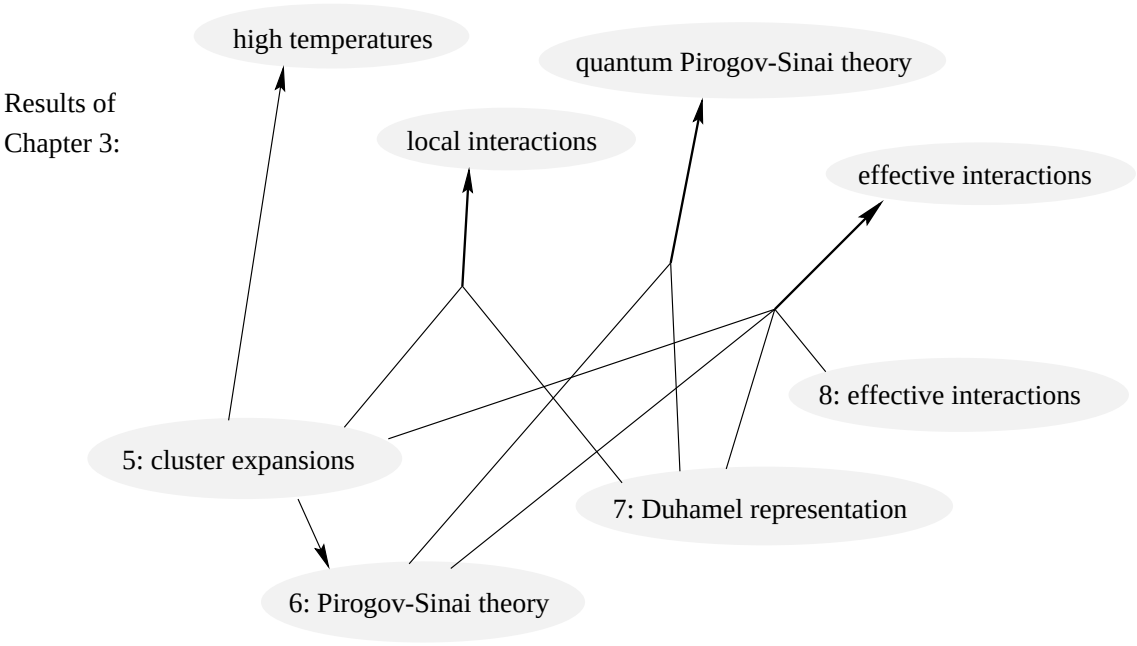
The basic mathematical tool is cluster expansion, that we present in Chapter 5. At the end of the chapter, we illustrate its usefulness with high temperature expansions.

Ideas and results of the Pirogov-Sinai theory are explained in Chapter 6. Ising and Blume-Capel models are discussed, because they allow to introduce both the geometric notions ("contours") and the concept of metastable free energy. The results of this theory are then stated in the framework of an abstract contour model, that will be directly used in quantum systems.

Chapter 7 starts with a description of the Duhamel formula. It is then applied to quantum models of Statistical Physics, in order to obtain a contour model where contours have small activities.

The last Chapter 8 is devoted to the effective potential. The ideas are first presented in the special case of the asymmetric Hubbard model, in a heuristical manner. Next the general situation is considered, and efforts are paid in order to define suitable contours, and finally to prove that their activities are sufficiently small in order to meet the requirements of the Pirogov-Sinai theory.

Let us summarize the structure of this thesis with a diagram. If A and B are two subjects, the notation A$\rightarrow$B means that the proof of the result of B necessitates the tools developped in A.



The diagram shows that the demonstration of the high temperature phase only requires cluster expansions; the absence of phase transitions in systems with local interactions follows from cluster expansions and Duhamel reprentation; the Pirogov-Sinai theory, together with the Duhamel representation of quantum models, lead to the statements of the quantum Pirogov-Sinai theory; finally, the effective interactions due to quantum fluctuations are consequences of all four chapters.

CHAPTER 2

Mathematical modelization

1. Heuristical discussion (classical systems)

Statistical Physics describes systems consisting of a huge number of particles. Having the microscopical description, how can we obtain the thermodynamics of the system? A mathematical answer to this question is the canonical formalism, that we introduce in Section 3. We can take it as a postulate, but it is a very crude one. So let us start with a discussion of physical ideas concerning systems at equilibrium.

Since the number of the particles in the system is enormous, two obvious and fundamental remarks have to be done:

- the microscopic state is impossible to know,
- relevant quantities are *macroscopic observables*, i.e. those involving a huge number of particles.

On the other hand, it is known from Thermodynamics that only a few numbers are necessary to characterize a physical system. For instance, the thermodynamic state of a gas of N particles in a volume V is now specified by its temperature, even though the number of degrees of freedom is about 10^{23}. "To be specified by its temperature" means that if we measure the same physical quantity in two different systems with identical temperature (and identical volume and number of particles), we find the same value, although they are in two different microscopic states. Thermodynamics would be no Science without this property of reproducibility of its experiments. Remark that the state of the system can be thermodynamically specified by choosing other parameters, as for instance the energy.

Let us be more precise — although we keep vague in mathematical notions. Let $\boldsymbol{\Omega} = \Omega^N$ be the phase space for a system of N particles. We suppose that there exists a function $\boldsymbol{E} : \boldsymbol{\Omega} \to \mathbb{R}$ (the energy observable). Let us denote by $\mathcal{M}$ the set of macroscopic observables. For given energy E, let $\boldsymbol{\Omega}(E) \subset \boldsymbol{\Omega}$ be the set of microscopic states ω such that $\boldsymbol{E}(\omega) = E$.

Postulate 1 (Reduction of variables). *There exists $\boldsymbol{\Omega}_{\rm typ}(E) \subset \boldsymbol{\Omega}(E)$ (the set of typical states) on which any macroscopic observable $M \in \mathcal{M}$ is constant; moreover, the system is in a state of $\boldsymbol{\Omega}_{\rm typ}(E)$, any time it is observed.*

The last statement means that $\boldsymbol{\Omega}(E) \setminus \boldsymbol{\Omega}_{\rm typ}(E)$ is a small set, and that its events are so rare that they never really happen (and if they do, people would say there is an error, and the repetition of the experiment would confirm their belief).

We need to introduce the temperature, since we want to discuss the canonical ensemble. Any large system at equilibrium has a temperature, therefore there must exist a function $\boldsymbol{\beta} : \cup_E \boldsymbol{\Omega}_{\rm typ}(E) \to \mathbb{R}$ such that $\boldsymbol{\beta}(\omega)$ is the inverse temperature of the system[1]; in the case of a gas, $\boldsymbol{\beta}$ would be associated to the distribution of the kinetic energy of the particles. $\boldsymbol{\beta}$

[1]Note that the inverse temperature function is not defined on the whole of $\boldsymbol{\Omega}$, and is therefore not an observable.

is also constant on $\mathbf{\Omega}_{\rm typ}(E)$; this means that the temperature is a function of the energy. Assuming it is invertible, it allows to define the set of typical states at inverse temperature β, namely $\mathbf{\Omega}_{\rm typ}(\beta) = \mathbf{\Omega}_{\rm typ}(E(\beta))$.

Since we want to derive the macroscopic behaviour from the microscopic description, we should now consider an element of $\mathbf{\Omega}_{\rm typ}(\beta)$ and compute the values of the observables. This is impossible in practice, already because the set $\mathbf{\Omega}_{\rm typ}(\beta)$ is hard to specify! But since any $M \in \mathcal{M}$ is constant on $\mathbf{\Omega}_{\rm typ}(\beta)$, we have

$$M(\omega) = \int \mathrm{d}\mu(\omega') M(\omega')$$

for any $\omega \in \mathbf{\Omega}_{\rm typ}(\beta)$ and any probability measure μ on $\mathbf{\Omega}$ such that $\mu(\mathbf{\Omega}_{\rm typ}(\beta)) = 1$. We call such a measure a β-equilibrium measure; it describes the equilibrium phases at inverse temperature β.

Postulate 2 (Canonical ensemble). *Let λ be the uniform measure on $\mathbf{\Omega}$. Then*

$$\mathrm{d}\mu(\omega) = \mathrm{e}^{-\beta H(\omega)}\, \mathrm{d}\lambda(\omega) \Big/ \int \mathrm{d}\lambda(\omega')\, \mathrm{e}^{-\beta H(\omega')}$$

is a β-equilibrium measure.

These two postulates are plausible for systems with a lot of particles, since the law of large numbers plays a crucial role — we see here the intrinsic probabilistic nature of statistical physics systems.

Similar ideas are discussed by Lebowitz [Leb 1993]. As for mathematical results to support this discussion, there are considerations on the "triviality of Gibbs measures with respect to the field of global observables" [LR 1969, Lan 1973], and equivalence of microcanonical and canonical ensembles, see e.g. [LPS 1994]. All this holds for classical systems; I prudently choose not to enter deep questions about quantum ones.

2. Mathematical definitions

This section contains all the necessary definitions and notations used throughout this thesis. They are introduced without further justification. We restrict ourselves to lattice systems; the phase space associated to each site will always be countable for classical systems, and is a Hilbert space with a countable basis in the case of quantum systems. A description of the formalism of Classical Statistical Physics may be found in [EFS 1993, Geo 1988, Sim 1993, Sin 1982, Vel 1997]. Concerning Quantum Statistical Mechanics, the mathematical framework for systems with a variable number of particles — the second quantization — is very well explained in [MR 1990]; for lattice models, standard references are [BR 1981, Sim 1993].

We denote by $\Lambda \subset \mathbb{Z}^\nu$ the **lattice**, ν is the **dimension** of the system. The **distance** between $x, y \in \Lambda$ is $|x-y| \equiv \mathrm{dist}(x,y) = \|x-y\|_\infty$. The r**-boundary** of Λ is $\partial_r \Lambda = \{x \in \Lambda : \mathrm{dist}(x, \Lambda^{\rm c}) \leqslant r\}$ and its diameter is $\mathrm{diam}\,\Lambda = \max_{x,y\in\Lambda} |x-y|$. Let $f_\Lambda \in \mathbb{C}$, $\Lambda \subset \mathbb{Z}^\nu$; a *thermodynamic limit* of f_Λ is the limit of a sequence $(f_{\Lambda_n})_n$, such that $\Lambda_m \subset \Lambda_n$ if $m < n$, and $\lim_{n\to\infty} |\partial_r \Lambda_n|/|\Lambda_n| = 0$ for all $r < \infty$. We say that the **thermodynamic limit** of f_Λ exists, and worths f, if any such sequence converges to f; we write $f = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} f_\Lambda$. A set A is **connected** if for any $x, y \in A$, there exists a sequence $(x_0, x_1, \ldots, x_n)$ such that $x_0 = x$, $x_n = y$, $x_j \in A$ and $|x_j - x_{j-1}| = 1$ for all j, $1 \leqslant j \leqslant n$. It is useful to define the symbol $\Cap$ ("intersection"): for $A, B \subset \mathbb{Z}^\nu$,

$$A \Cap B \iff A \cup B \text{ is a connected set.}$$

We shall need a bound for the number of connected sets of given size, that contain a given site. So let[2] $\beth = (2\nu)^2$; then we have the property

$$\#(A \subset \mathbb{Z}^\nu : A \ni x \text{ and } |A| = \ell) \leqslant \beth^\ell. \tag{2.1}$$

2.1. Phase spaces. Our intention is to describe quantum systems that are perturbations of classical ones; this is the reason why we introduce first the classical configurations, which then allow to construct the Hilbert spaces of quantum models.

Three are basically three types of models: spin, fermions and bosons ones.[3] The **single site phase space** Ω is

$$\Omega = \begin{cases} \Omega = \{-S, -S+1, \dots, S-1, S\} & \text{for spin-}S \text{ systems} \\ \{0,1\}^\Sigma & \text{for fermion systems} \\ \mathbb{N}^\Sigma & \text{for boson systems.} \end{cases}$$

Here, Σ is a finite set that represents internal degrees of freedom of particles, such as spins (for the Hubbard model, $\Sigma = \{\uparrow, \downarrow\}$).

The phase space of the classical model is the **configuration space** $\mathbf{\Omega} = \Omega^{\mathbb{Z}^\nu}$, and $n \in \mathbf{\Omega}$ is a **configuration** on the infinite lattice. $n_x \in \Omega$ represents the configuration at site $x \in \mathbb{Z}^\nu$ and n_A is the restriction of n to $A \subset \mathbb{Z}^\nu$. For particle systems, we define $n_{x\sigma}$, $(x, \sigma) \in \mathbb{Z}^\nu \times \Sigma$, in obvious manner ($n_{x\sigma} \in \{0,1\}$ for fermions, $n_{x\sigma} \in \mathbb{N}$ for bosons). The total number of particles in $A \subset \mathbb{Z}^\nu$ is

$$|n_A| = \sum_{x \in A, \sigma \in \Sigma} n_{x\sigma}. \tag{2.2}$$

Finally, we introduce the notation $n_A n'_{\Lambda \setminus A}$ for a configuration of Ω^Λ, whose restriction on A, resp. $\Lambda \setminus A$, is n_A, resp. $n'_{\Lambda \setminus A}$.

The Hilbert space representing the phase space of a quantum system has different structure, in the case of spins, bosons or fermions:

- spin systems: tensorial product of copies of the Hilbert space for one spin attached to a given site of the lattice;
- boson systems: Fock space of symmetric wave functions on Λ;
- fermion systems: Fock space of antisymmetric wave functions on Λ.

In the case of particle systems, a convenient basis of the Fock space is that of occupation numbers of the position operators. The distinction between spins, bosons or fermions is contained in the choice of the single site phase space, and on the action of creation and annihilation operators on the elements of the basis of occupation numbers, that we define below.

Let $\mathcal{H}_\Lambda$ the Hilbert space of the system in a finite volume $\Lambda \subset \mathbb{Z}^\nu$; it is spanned by the classical configurations of Ω^Λ, i.e. $\mathcal{H}_\Lambda$ contains all $|v\rangle$,

$$|v\rangle = \sum_{n_\Lambda \in \Omega_\Lambda} a_{n_\Lambda} |n_\Lambda\rangle, \qquad a_{n_\Lambda} \in \mathbb{C}, \tag{2.3}$$

[2] "$\beth$" is the Hebrew letter "beth".

[3] For sake of simplicity, but regretfully, I assume here that the considered systems are fully fermionic or fully bosonic. However, there are interesting models with mixed particles, as for instance the Helium model that is discussed in the concluding remarks, Chapter 9. The Hilbert space for systems of mixed particles are tensorial products of Hilbert spaces for each species.

and the scalar product is

$$\langle v|v'\rangle = \sum_{n_\Lambda \in \Omega^\Lambda} a^*_{n_\Lambda} a'_{n_\Lambda}. \tag{2.4}$$

2.2. Classical interactions. An **interaction** is a collection of mappings $\Phi = (\Phi_A)_A$, $A \subset \mathbb{Z}^\nu$ connected, $\Phi_A : \Omega^A \to \mathbb{R} \cup \{+\infty\}$. Let $\mathfrak{t}_x$ denote a translation of $x \in \mathbb{Z}^\nu$; its action on the configurations is defined by $(\mathfrak{t}_x n)_y = n_{y-x}$; on the interactions, it is $\mathfrak{t}_x \Phi_A = \Phi_{\mathfrak{t}_x A} = \Phi_{A+x}$. The interaction Φ is **periodic** with period $\ell_0 \in \mathbb{N}$ if $\Phi_A(n_A) = \mathfrak{t}_x \Phi_A((\mathfrak{t}_x n)_{A+x})$ for any $x \in \ell_0 \mathbb{Z}^\nu$, $A \subset \mathbb{Z}^\nu$ and $n_A \in \Omega^A$. It is **translation invariant** if it is periodic with period $\ell_0 = 1$. The set of periodic configurations is denoted $\mathbf{\Omega}^{\mathrm{per}}$.

An interaction Φ is an ***m*-potential** if there exists a set of configurations $G \subset \mathbf{\Omega}$ such that for all $A \subset \Lambda$ for which $\Phi_A \neq 0$,

- $\Phi_A(g_A) = \Phi_A(g'_A)$ for all $g, g' \in G$,
- $\Phi_A(n_A) - \Phi_A(g_A) > 0$ for all $g \in G$ and $n \in \mathbf{\Omega}$, such that $n_A \neq g'_A$ for all $g' \in G$.

G is then the set of ground states of Φ.

There is exponential decay if there is a constant $c > 0$ such that for $r < \infty$

$$\sum_{A \ni x, |A| \geqslant r} |\Phi_A(n_A)|\, \mathrm{e}^{c|A|} < \infty \tag{2.5}$$

for any $n \in \mathbf{\Omega}$ with $\sup_{x \in \mathbb{Z}^\nu} |n_x| < \infty$. (This definition allows the potential to have a hard-core.) The interaction is **stable** if for all x, n,

$$\sum_{A \ni x} \frac{1}{|A|} \Phi_A(n_A) \;\geqslant\; b|n_x| - a \tag{2.6}$$

for some constants $a < \infty$, $b > 0$. The space of all stable interactions is a vector space, if we define $\Phi + \Psi$ by $(\Phi + \Psi)_A(n_A) = \Phi_A(n_A) + \Psi_A(n_A)$; we note $\mathcal{O}$ the zero of this vector space.

The **Hamiltonian** H^Φ_Λ (with free boundary conditions) is the sum of the interactions in the system, defined by

$$H^\Phi_\Lambda(n_\Lambda) = \sum_{A \subset \Lambda} \Phi_A(n_A). \tag{2.7}$$

The **energy** (or mean energy) of a periodic configuration $n \in \mathbf{\Omega}^{\mathrm{per}}$ is

$$e^\Phi(n) = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{1}{|\Lambda|} H^\Phi_\Lambda(n_\Lambda). \tag{2.8}$$

The minimum energy of an interaction Φ is the **ground energy** e^Φ_0,

$$e^\Phi_0 \;\doteq\; \inf_{n \in \mathbf{\Omega}^{\mathrm{per}}} e^\Phi(n). \tag{2.9}$$

The set of the periodic **ground states** of an interaction Φ is

$$G^\Phi = \{g \in \mathbf{\Omega}^{\mathrm{per}} : e^\Phi(g) = e^\Phi_0\}.$$

This set may be empty. There exist systems with finite single site phase space, and finite-range, translation invariant interaction, which do not possess any periodic ground states, see [Mię 1993].

Two interactions Φ and Ψ are **physically equivalent** if for any $\Lambda \subset \mathbb{Z}^\nu$, the difference

$$\sum_{A \cap \Lambda \neq \varnothing} \Big(\Phi_A(n_A) - \Psi_A(n_A) \Big)$$

does not depend on n_Λ. Two physically equivalent interactions have the same set of Gibbs states [Geo 1988], see also [EFS 1993] for useful comments.

Example: Zero-potentials [GJL 1992, Ken 1994].

A *zero-potential* ϕ is an interaction that is physically equivalent to $\mathcal{O}$. Then $\Phi + \phi$ and Φ are physically equivalent.

Zero potentials are useful when studying certain frustrated interactions, since they may allow to replace this interaction by an m-potential. For instance, take a lattice gas model with interaction on sets $B = (x, y, z)$ (where x and z are two opposite neighbours of y):

$$\begin{cases} \Phi_B(\bullet\circ\circ) = \Phi_B(\circ\circ\bullet) = 0 \\ \Phi_B(\circ\bullet\circ) = \frac{4}{3} \\ \Phi_B(\circ\circ\circ) = \Phi_B(\circ\bullet\bullet) = \Phi_B(\bullet\bullet\circ) = \Phi_B(\bullet\circ\bullet) = \Phi_B(\bullet\bullet\bullet) = 1 \end{cases} \tag{2.10}$$

where empty circle means no particle, and filled circle means one particle. If we define $\phi_B(n_x n_y n_z) = n_x - 2n_y + n_z$, then $(\Phi + \frac{4}{9}\phi)$ is a physically equivalent interaction that is an m-potential, the ground configurations being those that contain only patterns $\circ\bullet\circ$, $\circ\circ\bullet$ and $\bullet\circ\circ$ (there are six ground configurations in two dimensions).

An important class of (stable) interactions that we shall often consider is the ones that act only on blocks, and that satisfy a *Peierls condition*. Let $R_0 \in \frac{1}{2}\mathbb{N}$; we define the *$R_0$-neighbourhood* $U(x)$ of $x \in \mathbb{Z}^\nu$ as

$$U(x) = \begin{cases} \{y \in \mathbb{Z}^\nu : |y - x| \leqslant R_0\} & \text{if } R_0 \in \mathbb{N} \\ \{y \in \mathbb{Z}^\nu : |y - (x_1 + \frac{1}{2}, \dots, x_\nu + \frac{1}{2})| \leqslant R_0\} & \text{otherwise.} \end{cases} \tag{2.11}$$

A periodic interaction Φ belongs to the class $\mathcal{C}(R_0, G, \Delta_0, a, b)$, $R_0 \in \frac{1}{2}\mathbb{N}$, $G \subset \mathbf{\Omega}$ is a finite set of periodic configurations, $\Delta_0 > 0$, $a \in \mathbb{R}$, $b > 0$, if it satifies the following properties :

- $\Phi_A = 0$ if $A \neq U(x)$ for all $x \in \mathbb{Z}^\nu$.
- For all $g \in G$, $\Phi_{U(x)}(g_{U(x)})$ is independent of $x \in \mathbb{Z}^\nu$; we write $e(g) = \Phi_{U(x)}(g_{U(x)})$, and define $e_0^\Phi = \min_{g \in G} e(g)$.
- (Peierls condition) If $n_{U(x)} \neq g_{U(x)}$ for all $g \in G$,

$$\Phi_{U(x)}(n_{U(x)}) \geqslant e_0^\Phi + \Delta_0. \tag{2.12}$$

- Finally, the potential is stable

$$\Phi_{U(x)}(n_{U(x)}) \geqslant e_0^\Phi + b|n_x| - a. \tag{2.13}$$

The classes are such that

$$\mathcal{C}(R_0, G, \Delta_0, a, b) \subset \mathcal{C}(R_0, G, \Delta_0', a', b')$$

if $\Delta_0 \geqslant \Delta_0'$, $a \leqslant a'$ and $b \geqslant b'$. Furthermore, if $\Phi \in \mathcal{C}(R_0, G, \Delta_0, a, b)$, and $R_0' \geqslant R_0$, then the interaction Φ'

$$\Phi'_A(n_A) = \begin{cases} \Phi_{U(x)}(n_{U(x)}) & \text{if } A \text{ is the } R_0'\text{-neighbourhood of some } x \in \mathbb{Z}^\nu \\ 0 & \text{otherwise} \end{cases}$$

belongs to $\mathcal{C}(R_0', G, \Delta_0, a, b)$ and is physically equivalent to Φ. In the sequel, we shall often write Φ_x instead of $\Phi_{U(x)}$, for an interaction belonging to such a class.

If the single site phase space is finite, condition (2.13) is no longer useful, and we denote by $\mathcal{C}(R_0, G, \Delta_0)$ the space of interactions that satisfy all the conditions, except (2.13).

2.3. Quantum interactions. We first have to embed classical systems in a quantum framework. The Hilbert space is constructed from quantum configurations, and the **quantum equivalent** $V = (V_A)$ of a classical interaction $\Phi = (\Phi_A)$ is a collection of operators

$$\begin{aligned} V_A : \quad & \mathcal{D}(V_A) \subset \mathcal{H}_A \to \mathcal{H}_A \\ & V_A \,|n_A\rangle = \Phi_A(n_A)\,|n_A\rangle. \end{aligned}$$

Quantum equivalents of classical interactions are diagonal operators in the basis of classical configurations. The domain of V_A is not necessarily the whole of $\mathcal{H}_A$, V_A may even not be densely defined — we want to accept models with hard-cores. It is however useful to notice that (Φ_A) is bounded below, see (2.13), and therefore the operators $\mathrm{e}^{-\beta V_A}$, with $\beta > 0$, are defined everywhere in $\mathcal{H}_A$.

Next we define creation and annihilation operators on the basis of occupation numbers of $\mathcal{H}_\Lambda$.

- Bosons:

$$\begin{aligned} c^\dagger_{x\sigma}\,|n_\Lambda\rangle &= \sqrt{n_{x\sigma}+1}\,|n'_\Lambda\rangle \qquad && \text{with } n'_{y\sigma'} = n_{y\sigma'} + \delta_{xy}\delta_{\sigma\sigma'} \\ c_{x\sigma}\,|n_\Lambda\rangle &= \sqrt{n_{x\sigma}}\,|n'_\Lambda\rangle \qquad && \text{with } n'_{y\sigma'} = n_{y\sigma'} - \delta_{xy}\delta_{\sigma\sigma'}. \end{aligned} \tag{2.14}$$

  Creation and annihilation operators satisfy the commutation relations

$$[c^\dagger_{x,\sigma}, c^\dagger_{y,\sigma'}] = 0, \qquad [c_{x,\sigma}, c_{y,\sigma'}] = 0, \qquad [c_{x,\sigma}, c^\dagger_{y,\sigma'}] = \delta_{x,y}\delta_{\sigma,\sigma'}.$$

- Fermions: we first have to choose an order on Λ and Σ; this induces an order on $\Lambda \times \Sigma$ by

$$(y,\sigma') < (x,\sigma) \iff y < x, \text{ or } y = x \text{ and } \sigma' < \sigma.$$

  Then

$$\begin{aligned} c^\dagger_{x\sigma}\,|n_\Lambda\rangle &= (1-n_{x\sigma})(-1)^{\sum_{(y,\sigma')<(x,\sigma)} n_{y\sigma'}}\,|n'_\Lambda\rangle \qquad && \text{with } n'_{y\sigma'} = n_{y\sigma'} + \delta_{xy}\delta_{\sigma\sigma'} \\ c_{x\sigma}\,|n_\Lambda\rangle &= n_{x\sigma}(-1)^{\sum_{(y,\sigma')<(x,\sigma)} n_{y\sigma'}}\,|n'_\Lambda\rangle \qquad && \text{with } n'_{y\sigma'} = n_{y\sigma'} - \delta_{xy}\delta_{\sigma\sigma'}. \end{aligned} \tag{2.15}$$

  We have the anticommutation relations

$$\{c^\dagger_{x,\sigma}, c^\dagger_{y,\sigma'}\} = 0, \qquad \{c_{x,\sigma}, c_{y,\sigma'}\} = 0, \qquad \{c_{x,\sigma}, c^\dagger_{y,\sigma'}\} = \delta_{x,y}\delta_{\sigma,\sigma'}.$$

In order to have correlation functions or order parameters, we need a notion of **local operator**. K is a local operator with connected support $\operatorname{Supp} K \subset \mathbb{Z}^\nu$, if $|\operatorname{Supp} K| < \infty$ and it satisfies the following conditions, for fermions or bosons, respectively:

- (Fermions) K is a finite sum of *even* monomials in creation and annihilation operators of fermionic particles at a given site, i.e.

$$K = \sum_{\substack{(x_1,\sigma_1),\dots,(x_\ell,\sigma_\ell) \\ (y_1,\sigma'_1)\dots,(y_m,\sigma'_m)}} k_{\{(x_i,\sigma_j)\}} c^\dagger_{x_1,\sigma_1} \dots c^\dagger_{x_\ell,\sigma_\ell} c_{y_1,\sigma'_1} \dots c_{y_m,\sigma'_m}$$

  with $(x_i,\sigma_j), (y_i,\sigma'_j) \in \operatorname{Supp} K \times \Sigma$; $\ell + m$ must be an even number.
- (Spins or bosons) K is densely defined in $\mathcal{H}_\Lambda$ ($\Lambda \supset \operatorname{Supp} K$), and the matrix element

$$\langle n_\Lambda |\, K \,| n'_\Lambda \rangle$$

  is zero whenever $n_{\Lambda\setminus\operatorname{Supp} K} \neq n'_{\Lambda\setminus\operatorname{Supp} K}$ and otherwise it depends on $n_{\operatorname{Supp} K}$ and $n'_{\operatorname{Supp} K}$ only.

We denote with $\mathcal{L}$ the space of all *bounded* local operators. Notice that in the case of bosonic systems, the creation operators $c_x^\dagger$ do not belong to $\mathcal{L}$, neither do the operators number of particles at a given site. Since we would like to consider their expectation values, we introduce the space $\mathcal{L}(c)$, $c < \infty$, of *moderately off-diagonal* local operators, which satisfy

$$\sum_{n' \in \mathbf{\Omega}} |\langle n'| K |n\rangle| \leqslant C_K \, \mathrm{e}^{c|n_{\mathrm{Supp}\, K}|} \tag{2.16}$$

for all $n \in \mathbf{\Omega}$. Notice that $\mathcal{L}(c=0) = \mathcal{L}$.

A **quantum interaction** is a collection of local operators $(T_{\boldsymbol{A}})$, $\boldsymbol{A} = (A, \sigma)$, with support $A \subset \mathbb{Z}^\nu$ connected, and σ represents additional degrees of freedom, as for instance spins.[4] (By abuse of notation, we consider that for any $\Lambda \supset A$, $T_{\boldsymbol{A}} : \mathcal{H}_\Lambda \to \mathcal{H}_\Lambda$.) We write

$$T_A \doteqdot \sum_\sigma T_{\boldsymbol{A}}. \tag{2.17}$$

In view of the space-time representation for quantum systems, see Chapter 7, we call $\boldsymbol{A}$ a *quantum transition*.

When the single site phase space is finite, a convenient definition for the **norm** $\|T\|$ of a quantum interaction $(T_{\boldsymbol{A}})$ is[5]

$$\|T\| = \sup_{A \subset \mathbb{Z}^\nu} \Big[\max_{n_A, n'_A \in \Omega^A} \big| \langle n'_A| T_A |n_A\rangle \big| \Big]^{1/|A|} \tag{2.18}$$

This is a norm, provided the multiplication of an interaction T by a scalar λ is defined to be $(\lambda T)_{\boldsymbol{A}} = \lambda^{|A|} T_{\boldsymbol{A}}$. In this case the space of quantum interactions is no vector space, but it does not matter. Let $\mathcal{Q}$ the space of interactions with finite norm.

In the case of boson systems, this definition is inconvenient, already because hopping terms $T_{\boldsymbol{A}} = c_x^\dagger c_y$ do not belong to $\mathcal{Q}$. Therefore we define the following norm

$$\|T\| = \sup_{A \subset \mathbb{Z}^\nu} \Big(\sup_{n_A \in \Omega^A} \Big\{ \sum_{n'_A \in \Omega^A} \frac{|\langle n_A| T_A |n'_A\rangle|}{|n_A|+1}, \sum_{n'_A \in \Omega^A} \frac{|\langle n_A| T_A |n'_A\rangle|}{|n'_A|+1} \Big\} \Big)^{1/|A|} \tag{2.19}$$

and we denote by $\mathcal{Q}_{\mathrm{b}}$ the space of interactions for which this norm is finite. A hopping term of the form $(t_{xy} c_x^\dagger c_y)_{x,y \in \mathbb{Z}^\nu}$ with $|t_{xy}| \leqslant \mathrm{e}^{-\gamma|x-y|}$ belongs to $\mathcal{Q}_{\mathrm{b}}$.[6]

Notice the inequalities

$$\sum_{\boldsymbol{A}: A=B} \sum_{n'_B \in \Omega^B} \frac{1}{|n_B|+1} |\langle n_B| T_{\boldsymbol{A}} |n'_B\rangle| \leqslant \|T\|^{|B|} \tag{2.20}$$

$$\sum_{\boldsymbol{A}: A=B} \sum_{n'_B \in \Omega^B} \frac{1}{|n'_B|+1} |\langle n_B| T_{\boldsymbol{A}} |n'_B\rangle| \leqslant \|T\|^{|B|} \tag{2.21}$$

for any $B \subset \mathbb{Z}^\nu$ and $n_B \in \Omega^B$. If $\|T\| < \infty$, each operator $T_{\boldsymbol{A}}$ is densely defined in $\mathcal{H}_A$ (and hence in $\mathcal{H}_\Lambda$, $\Lambda \supset A$); we denote by $\mathcal{Q}$ the space of quantum interactions with finite norm.

[4] These degrees of freedom may coincide with the set Σ.

[5] In the sequel, we should not mix up the norm $\|T\|$ of an interaction T, with the operator norm $\|T_{\boldsymbol{A}}\|$ of the local operator $T_{\boldsymbol{A}}$.

[6] *Stricto sensu* it does not, because supports are not necessarily connected. However, it is clear that one can rewrite it into another interaction with connected supports.

2.4. Phase diagrams. So far we have considered only one thermodynamic parameter, namely the inverse temperature β. But other quantities such as the external magnetic field or the chemical potential have to be taken into account. Notice that a non zero magnetic field modifies the Hamiltonian; the chemical potential is present whenever we are considering the grand-canonical ensemble, and a common trick consists in redefining a new Hamiltonian by substracting to the ancient one the number of particles times the chemical potential, and to go to the canonical ensemble. The Hamiltonian is then a function of these two thermodynamic parameters:

$$\begin{aligned} H_\Lambda(n_\Lambda) &= \sum_{A\subset\Lambda} \Phi_A(n_A) - h\sum_{x\in\Lambda} S_x(n_x) - \mu\sum_{x\in\Lambda} N_x(n_x) \\ &\equiv \sum_{A\subset\Lambda} \Phi_A^{h,\mu}(n_A). \end{aligned}$$

Consequently let $\boldsymbol{\mu} = (\mu_1, \dots, \mu_{p-1}) \in \mathcal{U}$ be a family of **external fields** where $\mathcal{U}$ is an open subset of $\mathbb{R}^{p-1}$. The interaction Φ is now supposed to depend on $\boldsymbol{\mu}$.

Let us write $G^{\boldsymbol{\mu}} = G^{\Phi(\boldsymbol{\mu})}$ the set of periodic ground states of $\Phi^{\boldsymbol{\mu}}$ and $G^{\mathcal{U}} = \cup_{\boldsymbol{\mu}\in\mathcal{U}} G^{\boldsymbol{\mu}}$. We suppose that $|G^{\mathcal{U}}| = p$, with $1 \leqslant p < \infty$; we note $G^{\mathcal{U}} = \{g^{(1)}, \dots, g^{(p)}\}$. The **zero-temperature phase diagram** of $\Phi(\boldsymbol{\mu})$ is the decomposition of $\mathcal{U}$:

$$\mathcal{U} = \bigcup_{Q\subset G^{\mathcal{U}}} \mathfrak{M}(Q)$$

with $\mathfrak{M}(Q)$ the set of $\boldsymbol{\mu}$ where the set of ground states is Q, i.e.

$$\mathfrak{M}(Q) = \{\boldsymbol{\mu} \in \mathcal{U} : G^{\boldsymbol{\mu}} = Q\}.$$

Remark that $\mathfrak{M}(\varnothing) = \varnothing$ and $\mathfrak{M}(Q) \cap \mathfrak{M}(Q') = \varnothing$ if $Q \neq Q'$.

An alternative description of the zero-temperature phase diagram, which admits a generalization to low temperatures in the framework of the Pirogov-Sinai theory, is to define, for each $g \in G^{\mathcal{U}}$:

$$\mathfrak{M}(g) = \{\boldsymbol{\mu} \in \mathcal{U} : e^{\boldsymbol{\mu}}(g) = \min_{g'\in G^{\mathcal{U}}} e^{\boldsymbol{\mu}}(g')\}. \tag{2.22}$$

Then[7] $\mathfrak{M}(Q)$ is the subset of $\mathcal{U}$ where all $g \in Q$ are ground states, and all $g \notin Q$ have strictly bigger energy; that is,

$$\mathfrak{M}(Q) = \bigcap_{g\in Q} \mathfrak{M}(g) \setminus \bigcup_{g\notin Q} \mathfrak{M}(g). \tag{2.23}$$

This phase diagram is said to be **regular**, or alternatively to satisfy the **Gibbs phase rule**, if the function

$$\mathcal{U} \to \text{ boundary of the positive octant of } \mathbb{R}^p \tag{2.24}$$

$$\boldsymbol{\mu} \mapsto \left(e^{\boldsymbol{\mu}}(g^{(1)}) - e_0^{\boldsymbol{\mu}}, \dots, e^{\boldsymbol{\mu}}(g^{(p)}) - e_0^{\boldsymbol{\mu}}\right) \tag{2.25}$$

is a homeomorphism whose image contains a neighbourhood of the origin of $\mathbb{R}^p$. In other words, the zero-temperature phase diagram has the following structure: there exist $\boldsymbol{\mu}_0 \in \mathcal{U}$ where all the energies are equal, p different lines where $(p-1)$ configurations are ground states, $\frac{1}{2}p(p-1)$ 2-dimensional surfaces with $(p-2)$ ground states, ... , p $(p-1)$-dimensional manifolds where only one state has minimum energy. We have the following relations for the closures of the manifolds: $\overline{\mathfrak{M}}(Q) \cap \overline{\mathfrak{M}}(Q') = \overline{\mathfrak{M}}(Q \cup Q')$.

[7] One should not mix $\mathfrak{M}(g)$ with $\mathfrak{M}(\{g\})$; actually, $\mathfrak{M}(\{g\}) \subset \mathfrak{M}(g)$ is the set of external fields $\boldsymbol{\mu}$ where g is unique ground state.

Actually we shall need a stronger condition than regularity of the phase diagram, namely that the μ_i removes the degeneracy at $\boldsymbol{\mu}_0$ linearly: we suppose that there exists $\boldsymbol{\mu}_0 \in \mathcal{U}$ where $e^{\boldsymbol{\mu}_0}(g) = e_0^{\boldsymbol{\mu}_0}$ for any $g \in G^{\mathcal{U}}$, and that the matrix of derivatives

$$\left(\frac{\partial}{\partial \mu_i} \left[e^{\boldsymbol{\mu}}(g^{(j)}) - e^{\boldsymbol{\mu}}(g^{(p)}) \right] \right)_{1 \leqslant i,j \leqslant p-1} \tag{2.26}$$

exists and has non zero determinant for all $\boldsymbol{\mu} \in \mathcal{U}$. If an interaction $\Phi^{\boldsymbol{\mu}}$ satisfies this condition, we say that its zero-temperature phase diagram is **linearly regular**.

Our main goal is to show the stability of such phase diagrams when the temperature is small but non zero, as well as when a quantum perturbation is added to the interaction. The p ground states have to be replaced by p *phases*, or *thermodynamic states*, that represent small deformations of these ground states, in a sense that will be given more precise meaning later.

3. Thermodynamic states

We define thermodynamic states starting from finite systems, and then taking the thermodynamic limit.

Let us start with free boundary conditions. The **canonical partition function** at temperature β is

$$Z_\Lambda = \mathrm{Tr}_{\mathcal{H}_\Lambda} \exp\Big(-\beta \sum_{A \subset \Lambda} (T_A + V_A) \Big). \tag{2.27}$$

This allows to define the **free energy** of the system, namely

$$f = - \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{1}{\beta |\Lambda|} \log Z_\Lambda \tag{2.28}$$

(if the limit exists).

3.1. Periodic boundary conditions. Let $L \in \mathbb{N}$; we define $\Lambda^{\,\mathrm{per}}(L) = \mathbb{Z}^\nu / (L\mathbb{Z})^\nu$. The Hamiltonian with periodic boundary conditions is

$$H^\Phi_{\Lambda^{\,\mathrm{per}}}(n_\Lambda) = \sum_{A \subset \Lambda^{\,\mathrm{per}}} \Phi_A(n_A). \tag{2.29}$$

The notion of physical equivalence is simpler in the case of periodic systems. Indeed, two finite-range interactions Φ and Ψ (with range smaller than the size of lattice) are physically equivalent if

$$\sum_{A \subset \Lambda^{\,\mathrm{per}}} \Big(\Phi_A(n_A) - \Psi_A(n_A) \Big) = |\Lambda^{\,\mathrm{per}}| \mathrm{const} \tag{2.30}$$

for any n.

3.2. Boundary conditions with boundary operators. In the classical case, given an interaction Φ, a usual way to introduce boundary conditions is to take a fixed configuration $g \in \boldsymbol{\Omega}$, and for any finite $\Lambda \in \mathbb{Z}^\nu$ to define the Hamiltonian

$$H^{(0)g}_\Lambda(n_\Lambda) = \sum_{A \subset \Lambda} \Phi_A(n_A) + \sum_{A \not\subset \Lambda, A \cap \Lambda \neq \varnothing} \Phi_A(n_{A \cap \Lambda} g_{A \setminus \Lambda}).$$

In words, the idea is to freeze the configuration outside of Λ, and to take into account the interactions across the boundary. The same can be described by introducing a *boundary interaction* $\partial^{\Lambda,\Phi,g}$:

$$\partial_A^{\Lambda,\Phi,g}(n_A) = \sum_{A' \not\subset \Lambda, A' \cap \Lambda = A} \Phi_{A'}(n_A g_{A' \setminus \Lambda}); \tag{2.31}$$

then $H_\Lambda^{(0)g}$ is given by the Hamiltonian with free boundary conditions, plus this boundary interaction, namely

$$H_\Lambda^{(0)g} = H_\Lambda^{(0)} + \sum_{A \subset \Lambda} \partial_A^{\Lambda,\Phi,g}(n_A). \tag{2.32}$$

If Φ is of finite range, only terms close to the boundary contribute in the second sum. Such a generalization of boundary conditions was considered in [BLP 1979].

In a sense the boundary interaction modelizes much better the boundary of a physical system than interactions with configurations outside of Λ, which do not exist in reality. However, it should be clear that boundary conditions are only a mathematical tool useful for the description of phase coexistence, and their physical interpretation should not be overstressed.

A natural generalization of these classical boundary conditions is quantum ones. Here we would replace the classical boundary interaction by quantum operators. Good examples should be, for bosons,

$$\partial^\Lambda = \sum_{x \in \partial_1 \Lambda} (c_x^\dagger + c_x), \tag{2.33}$$

and for fermions,

$$\partial^\Lambda = \sum_{\substack{x,y \in \partial_1 \Lambda \\ |x-y| \leqslant r}} (c_x^\dagger c_y^\dagger + c_x c_y). \tag{2.34}$$

As in the classical situation, these operators break some symmetries of the system, although the symmetries are now different. The total number of particles is no more a constant, which means that the system is not necessarily gauge invariant. In this case, the system displays features of superfluidity or superconductivity. Their order parameters are[8] $\langle c_0^\dagger \rangle$ (superfluidity for bosonic systems), see Penrose and Onsager [PO 1956], or $\langle c_{0\uparrow}^\dagger c_{0\downarrow}^\dagger \rangle$ (superconductivity in some fermionic systems) [Yang 1962]. With free, periodic or classical boundary conditions, these order parameters are obviously zero if the Hamiltonian conserves the total number of particles. However, they may differ from zero with quantum boundary conditions. If they are non zero (in the thermodynamic limit), the heuristical meaning is that a particle created at site 0 travels and eventually disappears at the far boundary. It is therefore reasonable to expect special transport and conductivity properties in systems with such equilibrium states.

3.3. States. A thermodynamic state, or state, or phase, in Quantum Statistical Physics is a linear, normalized, positive functional on the space of local operators. Let H

[8] The operator $c_0^\dagger$ is unbounded, and this may create technical difficulties. An alternative is to consider the order parameter $\langle (n_0)^{-\frac{1}{2}} c_0^\dagger \rangle$.

be a Hamiltonian. If for all local operators $K \in \mathcal{L}$ the limit

$$\langle K \rangle = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{\mathrm{Tr}_{\mathcal{H}_\Lambda} K \, \mathrm{e}^{-\beta H_\Lambda}}{\mathrm{Tr}_{\mathcal{H}_\Lambda} \, \mathrm{e}^{-\beta H_\Lambda}} \tag{2.35}$$

exists, we call $\langle \cdot \rangle$ a **Gibbs state** at inverse temperature β and with free boundary conditions. Similarly, a Gibbs state with periodic boundary conditions is a limit

$$\langle K \rangle^{\mathrm{per}} = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{\mathrm{Tr}_{\mathcal{H}_\Lambda} K \, \mathrm{e}^{-\beta H_{\Lambda \, \mathrm{per}}}}{\mathrm{Tr}_{\mathcal{H}_\Lambda} \, \mathrm{e}^{-\beta H_{\Lambda \, \mathrm{per}}}} \tag{2.36}$$

(provided it exists for all $K \in \mathcal{L}$).

Finally, we define Gibbs states with boundary interactions. For instance, $\langle \cdot \rangle^g$ is constructed by considering finite volumes Hamiltonians[9] $H_\Lambda + \partial^{\Lambda,\Phi,g}$ where $\partial^{\Lambda,\Phi,g}$ is given by (2.31).

Phase coexistence and first-order phase transitions are present when the thermodynamic states are sensitive to boundary conditions. Actually, since the system jumps from one phase to another when varying the corresponding thermodynamic parameter, it is also sensitive to external perturbations; for instance, by slightly modifying this parameter. We are lead to the notion of thermodynamic stability.

A state $\langle \cdot \rangle^H$, constructed with a Hamiltonian H, is **thermodynamically stable** if for any $P \in \mathcal{Q}$,

$$\langle K \rangle^H = \lim_{\alpha \to 0} \langle K \rangle^{H + \alpha P} \tag{2.37}$$

for all $K \in \mathcal{L}$.

The link between boundary and thermodynamic stability should be the following.

Conjecture.

A state is thermodynamically stable iff it is insensitive to boundary conditions (i.e. to the effect of a boundary operator).

Another important notion is that of clustering. Namely, a thermodynamic state is **exponentially clustering** if for any two local observables $K, K' \in \mathcal{L}$,

$$|\langle K \, \mathrm{t}_x(K') \rangle - \langle K \rangle \langle \mathrm{t}_x(K') \rangle| \leqslant C(K, K') \, \mathrm{e}^{-|x|/\xi} \tag{2.38}$$

with constants $\xi < \infty$ that depends on the state only, and $C(K, K') < \infty$ that depends on the operators only. In other words, a state is exponentially clustering whenever all correlations decay exponentially quickly.

Conjecture.

A thermodynamically stable state is exponentially clustering.

The converse of this conjecture is wrong. For instance, the " + " phase of the Ising model below the critical temperature and with zero external magnetic field is exponentially clustering, but unstable with respect to a small negative magnetic field.

External perturbations can break symmetries of the Hamiltonian, as may do boundary conditions. The gauge invariance of a quantum model can be broken by the field $\sum_{x \in \Lambda} (c_x^\dagger + c_x)$ [Gin 1968]. The corresponding physical properties of the system should be that of a superfluid.

Extremal states of Classical Statistical Physics can be constructed as thermodynamic limits of finite systems with suitable boundary conditions. In the sequel we shall consider

[9] More precisely, we consider the quantum equivalent of $\partial^{\Lambda,\Phi,g}$.

such an approach with quantum models. However, when discussing the effect of quantum fluctuations, we shall be into technical troubles, and it simplifies the task to consider external fields and periodic boundary conditions. Pure states at a coexistence point will be constructed by taking limits of thermodynamically stable states. This motivates the following definition of pureness: a linear, normalized, positive functional $\langle\cdot\rangle$ is a **pure state** if there exists $P \in Q$ such that

- for all $\alpha \in (0, \alpha_0]$, $\langle\cdot\rangle^{H+\alpha P}$ is a thermodynamically stable Gibbs state;
- $\langle\cdot\rangle = \lim_{\alpha\to 0}\langle\cdot\rangle^{H+\alpha P}$.

Notice that any thermodynamically stable state is pure. We call **phase coexistence** the situation where two or more pure states exist for a given Hamiltonian, or a given external field.

Let us end this chapter by mentionning the following standard convention on sums and products, that is used throughout this thesis: $\sum_{n\in\varnothing} a_n \doteq 0$, $\prod_{n\in\varnothing} a_n \doteq 1$ (this convention makes partition functions of contour models simple and elegant).

CHAPTER 3

Low temperature phases and stability of phase diagrams

This chapter summarizes the results for quantum lattice models proven throughout this thesis. Their common point is that all of them are obtained using the Duhamel representation of a quantum system (see Section 1, Chapter 7) and the cluster expansion (Chapter 5). Some of them also rely on the Pirogov-Sinai theory (Chapter 6).

1. High temperature phases

It may seem bizarre to discuss high temperature phases in this chapter devoted to the low temperatures, but high temperature expansions constitute a simple and nice illustration of the use of cluster expansion, hence we introduce them in Chapter 5.

Interactions between the particles are unimportant at high temperature, and thus we are left with a nearly ideal gas, whose physical state shows all the symmetries of the system. All this is known for more than 30 years, see e.g. [Dob 1968, Kunz 1978], ... Concerning quantum systems, boson lattice systems were considered in [PY 1995].

THEOREM 3.1. **Analyticity at high temperature.**

Let $\mathcal{H}$ be the Hilbert space constructed from the single site phase space Ω with $|\Omega| = S < \infty$. $T^{\boldsymbol{\mu}} = (T^{\boldsymbol{\mu}}_{\boldsymbol{A}})$ is a translation invariant quantum interaction that depends on a parameter $\boldsymbol{\mu} \in \mathcal{U} \subset \mathbb{R}^s$, such that

- $[T^{\boldsymbol{\mu}}_{\boldsymbol{A}}, T^{\boldsymbol{\mu}}_{\boldsymbol{A}'}] = 0$ *when* $A \cap A' = \varnothing$;
- $\langle n_A | \, T^{\boldsymbol{\mu}}_{\boldsymbol{A}} \, | n'_A \rangle$ *is analytic in* $\boldsymbol{\mu}$, *for any* $\boldsymbol{A}$, n, n';
- $\sum_{A \ni x} \| T^{\boldsymbol{\mu}}_A \| \, \mathrm{e}^{c|A|} < \infty$ *for a constant* $c > 2\nu + 1 + \log 2$.

Then the free energy

$$f(\beta, \boldsymbol{\mu}) = -\frac{1}{\beta} \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{1}{|\Lambda|} \log \mathrm{Tr} \; \mathrm{e}^{-\beta \sum_{A \subset \Lambda} T^{\boldsymbol{\mu}}_A}$$

exists and is analytic in β and $\boldsymbol{\mu}$ in the domain

$$\Big\{ (\boldsymbol{\mu}, \beta) \in \mathcal{U} \times \mathbb{R}_+ : \beta \sum_{A \ni x} \| T^{\boldsymbol{\mu}}_A \| \, \mathrm{e}^{c|A|} < 1 \Big\}.$$

The corresponding Gibbs state exists in the thermodynamic limit, is thermodynamically stable, pure and exponentially clustering.

This result is obtained in Section 3 of Chapter 5.

2. Quantum models with local interactions

When the (classical) interaction is only on-site, i.e.

$$V^{\boldsymbol{\mu}}_A = \begin{cases} V^{\boldsymbol{\mu}}_x & \text{if } A = \{x\} \\ 0 & \text{otherwise,} \end{cases} \tag{3.1}$$

with $V_x^{\boldsymbol{\mu}} : \mathcal{H}_{\{x\}} \to \mathcal{H}_{\{x\}}$, then the free energy is analytic in a domain where β and $T^{\boldsymbol{\mu}}$ are small enough, independently of $V^{\boldsymbol{\mu}}$. Actually, the statement shows similarities with the high temperature case. Here, each site is almost isolated, and the free energy is close to that of a system with only one site; no phase transition occurs, for the same reason that there are none in zero-dimensional systems.

THEOREM 3.2. **Analyticity with local interactions.**

We consider a model with single site state space Ω, $|\Omega| = S < \infty$, and Hamiltonian $H^{\boldsymbol{\mu}} = V^{\boldsymbol{\mu}} + T^{\boldsymbol{\mu}}$ where $V^{\boldsymbol{\mu}}$ is an on-site interaction, and $T^{\boldsymbol{\mu}}$ is translation invariant. We assume that

- $[T_{\boldsymbol{A}}^{\boldsymbol{\mu}}, T_{\boldsymbol{A}'}^{\boldsymbol{\mu}}] = 0$ *when* $A \cap A' = \varnothing$;
- $\langle n_A | \, T_{\boldsymbol{A}}^{\boldsymbol{\mu}} \, | n'_A \rangle$ *is analytic in* $\boldsymbol{\mu}$, *for any* $\boldsymbol{A}$, n, n';
- $\sum_{A \ni x} \|T_A^{\boldsymbol{\mu}}\| \, \mathrm{e}^{c|A|} < \infty$ *for a constant* $c > 2\nu + 1 + \log 2\beth + \log S$.

Then the thermodynamic limit of the free energy exists and is analytic in β and $\boldsymbol{\mu}$ in the domain

$$\Big\{ (\boldsymbol{\mu}, \beta) \in \mathcal{U} \times \mathbb{R}_+ : \beta \sum_{A \ni x} \|T_A^{\boldsymbol{\mu}}\| \, \mathrm{e}^{c|A|} < 1 \Big\},$$

and the corresponding Gibbs state exists in the thermodynamic limit, is thermodynamically stable, pure and exponentially clustering.

The proof combines Duhamel representation and cluster expansion, see Section 2, Chapter 7. The Hubbard model is an example of a Hamiltonian with on-site interaction; Theorem 3.2 establishes the existence of a paramagnetic phase in a domain $\beta|t| < \text{const}$ (at half filling, one can improve this result by showing analyticity in a domain $\beta t^2/U < \text{const}$ [Uel 1998]); see Chapter 4 for more discussion. Another example is the Falicov-Kimball model, for which this statement was proved in [KL 1986] (as well as in the domain $\beta t^2/U < \text{const}$).

3. Results of the quantum Pirogov-Sinai theory

We consider in this section quantum models that consist in a classical interaction which has well-understood low temperature phase diagram, and a quantum perturbation. We show that the latter does not destroy the classical picture, i.e. that quantum fluctuations do not play an important role. This amounts to say that the classical model is a good approximation for the description of the quantum system.

Results in this direction start with Ginibre [Gin 1969] and Robinson [Rob 1969], who proved long-range order in some spin systems. An important model is the Heisenberg one; if the coupling between neighbouring spins is anisotropic, i.e. if the coupling between the spins in the z-direction, say, is stronger than the coupling in the directions x and y, Kennedy proved that there is long-range order at low enough temperature [Ken 1985]. When the anisotropy is high, this result is a special case of our theorem below, but it does not cover the situation with weak anisotropy.

A fermion model with nearest-neigbour couplings was studied in [LM 1993]; here the "classical term" is the antiferromagnetic Ising model, and the phases of the quantum systems are shown to display chessboard features. All these results rely on the Peierls argument, so that it is necessary that the phases are related by some symmetry. In the context of Classical Physics, the generalization of the Peierls argument to situations without such symmetry was achieved by Pirogov and Sinai [PS 1975, Sin 1982] and bears now the name of its authors. Its application to quantum spin systems was suggested

in [Pir 1978], but was realized only twenty years later [BKU 1996, DFF 1996]. Fermion systems present an additional technical difficulty; in the contour representation of the quantum system, one has to deal with a sign arising from the anticommutation relations, and it is necessary to show its factorization with respect to the contours. This factorization was proved in [DFF 1996], so that their results also apply to fermion systems.

Here we present a theorem valid for spin, fermion, and boson systems, that is summarizing — and slightly extending — results of [BKU 1996, DFF 1996, BKU 1997]. It follows from Chapters 6 and 7.

THEOREM 3.3. **Stability of the phase diagram against quantum fluctuations.**

Let ν, the dimension of the system, be bigger or equal to 2.[1] *We consider a Hamiltonian $H^{\boldsymbol{\mu}} = T^{\boldsymbol{\mu}} + V^{\boldsymbol{\mu}}$, depending on a parameter $\boldsymbol{\mu} \in \mathcal{U} \subset \mathbb{R}^{p-1}$, where $V^{\boldsymbol{\mu}}$ is the quantum equivalent of a classical interaction $\Phi^{\boldsymbol{\mu}} \in \mathcal{C}(R_0, G^{\boldsymbol{\mu}}, \Delta_0, a, b)$, with $|\cup_{\boldsymbol{\mu}\in\mathcal{U}} G^{\boldsymbol{\mu}}| = |G^{\mathcal{U}}| = p < \infty$, and with linearly regular zero-temperature phase diagram. $T^{\boldsymbol{\mu}} \in \mathcal{Q}_{\rm b}$ is a differentiable quantum perturbation. Then for any $\delta > 0$, there exist $\beta_0 < \infty$ and $\varepsilon_0 > 0$ such that if $\beta \geqslant \beta_0$ and $\|T^{\boldsymbol{\mu}}\| + \sum_{i=1}^{p-1} \|\frac{\partial}{\partial\mu_i} T^{\boldsymbol{\mu}}\| \leqslant \varepsilon_0$ for all $\boldsymbol{\mu}$, there exist p functions $f^{\boldsymbol{\mu}}(g)$, $g \in G^{\mathcal{U}}$, such that*

- *if $\operatorname{Re} f^{\boldsymbol{\mu}}(g_0) = \min_{g\in G^{\mathcal{U}}} \operatorname{Re} f^{\boldsymbol{\mu}}(g)$, $f^{\boldsymbol{\mu}}(g_0)$ is the (infinite volume) free energy of the system.*
- *The matrix of derivatives*

$$\Big(\frac{\partial}{\partial\mu_i}\big[\operatorname{Re} f^{\boldsymbol{\mu}}(g^{(j)}) - \operatorname{Re} f^{\boldsymbol{\mu}}(g^{(p)})\big]\Big)_{1\leqslant i,j\leqslant p-1}$$

  exists and has an inverse matrix that is uniformly bounded in $\boldsymbol{\mu}$.
- *For all local operators $K \in \mathcal{L}(0)$, and if $\operatorname{Re} f^{\boldsymbol{\mu}}(g_0) = \min_{g\in G^{\mathcal{U}}} \operatorname{Re} f^{\boldsymbol{\mu}}(g)$, the expectation value (with classical boundary conditions g_0)*

$$\langle K\rangle_{g_0}^{\beta,\boldsymbol{\mu}} = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{\operatorname{Tr} K\, \mathrm{e}^{-\beta H^{\boldsymbol{\mu}}_{\Lambda,g_0}}}{\operatorname{Tr}\, \mathrm{e}^{-\beta H^{\boldsymbol{\mu}}_{\Lambda,g_0}}}$$

  exists, and is close to the value of K in the ground state g_0: there exists $C_K < \infty$ such that

$$\big|\langle K\rangle_{g_0}^{\beta,\boldsymbol{\mu}} - \langle g_0|\, K\, |g_0\rangle\big| \leqslant C_K\delta.$$

  This describes a pure state with exponential decay of correlations, i.e. there exists ξ such that for all $K, K' \in \mathcal{L}(0)$,

$$\big|\langle K\,\mathfrak{t}_x K'\rangle_{g_0}^{\beta,\boldsymbol{\mu}} - \langle K\rangle_{g_0}^{\beta,\boldsymbol{\mu}}\langle \mathfrak{t}_x K'\rangle_{g_0}^{\beta,\boldsymbol{\mu}}\big| \leqslant C_{K,K'}\, \mathrm{e}^{-|x|/\xi}\,,$$

  with $C_{K,K'} < \infty$.
- *If g_0 is the unique minimum of $\{\operatorname{Re} f^{\boldsymbol{\mu}}(g)\}$, the state $\langle\cdot\rangle_{g_0}^{\beta,\boldsymbol{\mu}}$ is thermodynamically stable.*

In the case of boson systems, we would like to have statements concerning the expectation value of local operators such as the operator number of particles in a subset A, or the operator creation of a particle at site x. But $N_A, c_x^\dagger \notin \mathcal{L}(0)$, since they are not bounded. To obtain a statement for local operators of $\mathcal{L}(c)$, we need a further assumption, namely that the quantum interaction conserves the number of particles.

[1] One-dimensional models could be included, but only at $\beta \to \infty$. The reason why this does not hold at finite temperature is that the system may create arbitrarily large excitations having fixed energy cost.

THEOREM 3.4. **Bosonic states.**

Under the same assumption as in Theorem 3.3, and supposing moreover that T satisfies $[T_{\boldsymbol{A}}, N_A] = 0$ for any $\boldsymbol{A}$, then if $\operatorname{Re} f^{\boldsymbol{\mu}}(g_0) = \min_{g\in G^{\mathcal{U}}} \operatorname{Re} f^{\boldsymbol{\mu}}(g)$, the expectation value of $K \in \mathcal{L}(c)$

$$\langle K\rangle_{g_0}^{\beta,\boldsymbol{\mu}} = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{\operatorname{Tr} K\, \mathrm{e}^{-\beta H^{\boldsymbol{\mu}}_{\Lambda,g_0}}}{\operatorname{Tr}\, \mathrm{e}^{-\beta H^{\boldsymbol{\mu}}_{\Lambda,g_0}}}$$

exists, and is close to the value of K in the ground state g_0. The state $\langle\cdot\rangle_{g_0}^{\beta,\boldsymbol{\mu}}$ describes a pure state with exponential decay of correlations.

This result is true for all c, but not uniformly: constants β_0 and ε_0 depend on c.

4. Effective interactions due to quantum fluctuations

When the classical interaction has an infinite number of ground states, the quantum perturbation may stabilize some of them. Examples of quantum lattice models with degenerate classical ground states are Hubbard and Falicov-Kimball models.[2] The first one is certainly the most interesting, but the latter allows rigorous studies. Kennedy and Lieb succeeded in applying the Peierls argument to exhibit a region of low temperatures where the quantum fluctuations are more important than the thermal ones [KL 1986]. The method was generalized in [LM1 1994, LM2 1994]. In the latter the degrees of freedom can be continuous.

A general method to study the low temperature behaviour of these systems was recently proposed by Datta, Fernández, Fröhlich and Rey-Bellet [DFFR 1996]. The idea is to replace the original Hamiltonian by a unitary equivalent one, that is diagonal up to negligible terms, and that has only a finite number of ground states. These are stable by virtue of Pirogov-Sinai theory.

The approach of [KU 1998], that we consider here, is different, although it leads to comparable results. We show that "quantum fluctuations" act as a classical effective potential. One has then to study the ground states of both the original interaction and the effective potential, and whenever this new classical model satisfies a suitable Peierls condition, and that there is "no quantum instability" (see below), its ground states are stable with respect to thermal, and other quantum, fluctuations.

4.1. The model. Different assumptions are needed. First, we restrict ourselves to systems with finite single site phase space, i.e. $|\Omega| = S < \infty$. The extension to lattice boson systems should be straightforward, but it is nevertheless a hard task that is not done so far. Second, since we are unable to include boundary conditions, we consider a periodic lattice $\Lambda^{\,\mathrm{per}}$. As before, the dimension ν of the system is bigger or equal to 2.

The Hamiltonian of the system is, as before, given by a classical interaction Φ and a quantum perturbation $T \in \mathcal{Q}$.

We suppose that a fixed collection of reference configurations $G \subset \boldsymbol{\Omega}$ is given[3] and we let $\bar{A} = \cup_{x\in A} U(x)$ (recall that $U(x)$ is the R_0-neighbourhood of x) and $G_A = \{g_A : g \in G\}$, $A \subset \mathbb{Z}^\nu$. G may be an infinite set.

[2] Reviews on these models include [Lieb 1993] for the Hubbard model, and [GM 1996] for the Falicov-Kimball model.

[3] In some situations G is simply the set of all ground configurations of Φ. When discussing the full phase diagram, however, we will typically extend the interaction Φ to a class of interactions by adding certain "external fields". The set G then will actually play the role of ground states of the interaction with particular values of external fields (the point of maximal coexistence of the ground state phase diagram).

We assume that the local energy gap of excitations is uniformly bounded from below, while the spread of local energies of reference states is not too big:

ASSUMPTION 1. **Classical interaction.**
Φ is a block interaction with finite range $R_0 \in \frac{1}{2}\mathbb{N}$ and is periodic with period $\ell_0 < \infty$. There exists a set $G \subset \mathbf{\Omega}$, possibly infinite, such that for all $n_{U(x)} \notin G_{U(x)}$,

$$\Phi_x(n_{U(x)}) - \max_{g \in G} \Phi_x(g_{U(x)}) \;\geqslant\; \Delta_0 \tag{3.2}$$

with $\Delta_0 > 0$, and

$$\max_{g,g' \in G} \bigl|\Phi_x(g_{U(x)}) - \Phi_x(g'_{U(x)})\bigr| \;\leqslant\; \delta_0, \tag{3.3}$$

$\delta_0 < \infty$. Furthermore, we assume the following extension property on the set of reference states G: if, for a connected $A \subset \mathbb{Z}^\nu$, a configuration n is such that $n_{U(x)} \in G_{U(x)}$ for any $x \in A$, then $n_{\bar{A}} \in G_{\bar{A}}$.

In view of the definition of the effective potential, it is useful to note the following property.

PROPERTY. *Let Φ satisfy Assumption 1, R be such that $R^\nu \;\leqslant\; \Delta_0/\delta_0$, and $A \subset \mathbb{Z}^\nu$ with $\operatorname{diam} A \;\leqslant\; R$. Then any pair of configurations $g_{\bar{A}} \in G_{\bar{A}}$ and $n_{\bar{A}} \notin G_{\bar{A}}$, with $n_{\bar{A}\setminus A} = g_{\bar{A}\setminus A}$, satisfies the lower bound*

$$\sum_{x \in A} \Bigl[\Phi_x(n_{U(x)}) - \Phi_x(g_{U(x)})\Bigr] \;\geqslant\; R^{-\nu}\Delta_0. \tag{3.4}$$

PROOF. Since $n_{\bar{A}} \notin G_{\bar{A}}$, there exists at least one site $x \in A$ such that $n_{U(x)} \notin G_{U(x)}$. From the assumption, this implies that

$$\sum_{x \in A} \Bigl[\Phi_x(n_{U(x)}) - \Phi_x(g_{U(x)})\Bigr] \;\geqslant\; \Delta_0 - \sum_{y \in A, y \neq x} \delta_0.$$

Using $|A| \;\leqslant\; R^\nu$, we obtain the property. □

4.2. The effective potential. It is actually a cumbersome task to write down a compact formula for the effective potential in the general case. A lot of notation has to be introduced, and one pays for the generality by the fact that the resulting formulæ look rather obscure; nevertheless, the logic behind the following definitions and equations appears rather naturally along the steps in Chapter 8. In the next subsection we shall discuss a special case where the effective interaction is due to at most four transitions resulting in much simpler and straightforward formulæ. We would like to stress that for typical concrete models this is entirely sufficient. The reader might thus skip the present subsection on the first reading and consider only the simplified situation of the next subsection.

The real meaning of the next definitions [in particular (3.7)] will appear more clearly only in Chapter 8, but, in the general case, we cannot leave it aside. First of all, we assume that a list $\mathcal{S}$ of sequences of quantum transitions $\boldsymbol{A}$ is given to represent the leading quantum fluctuations. The particular choice of $\mathcal{S}$ depends on properties of the considered model. Often the obvious choice like "any sequence of transitions not surpassing a given order" is sufficient. In the general case, certain conditions (specified later in Assumption

3) involving $\mathcal{S}$ are to be met. For any $g_A \in G_A$, the effective potential Ψ is defined to equal

$$\Psi_A(g_A) = -\sum_{n \geqslant 1} \frac{1}{n!} \sum_{k_1,\dots,k_n \geqslant 2} \sum_{\substack{(\boldsymbol{A}_1^1,\dots,\boldsymbol{A}_{k_1}^1,\boldsymbol{A}_1^2,\dots,\boldsymbol{A}_{k_n}^n)\in\mathcal{S} \\ \cup_{i,j}\bar{A}_j^i = A}}$$

$$\prod_{i=1}^{n}\Big\{ \sum_{n_A^{i,1},\dots,n_A^{i,k_i-1}\notin G_A} \mathcal{I}(A_1^i,\dots,A_{k_i}^i; n_A^{i,1}g_{\Lambda\setminus A},\dots,n_A^{i,k_i-1}g_{\Lambda\setminus A}) \Big[\prod_{j=1}^{k_i} \langle n_A^{i,j-1}|\, T_{\boldsymbol{A}_j^i}\, |n_A^{i,j}\rangle\Big]$$

$$\int_{-\infty<\tau_1^i<\dots<\tau_{k_i}^i<\infty} \mathrm{d}\tau_1^i\dots\mathrm{d}\tau_{k_i}^i \Big[\prod_{j=1}^{k_i-1} \mathrm{e}^{-(\tau_{j+1}^i-\tau_j^i)\sum_{x\in A^i}[\Phi_x(n_{U(x)}^{i,j})-\Phi_x(g_{U(x)})]}\Big]\Big\}$$

$$\frac{\mathbb{I}\left[\min_{i,j}\tau_j^i < 0 \text{ and } \max_{i,j}\tau_j^i > 0\right]}{\max_{i,j}\tau_j^i - \min_{i,j}\tau_j^i} \varphi^{\mathrm{T}}(B_1,\dots B_n). \quad (3.5)$$

To begin to decode this formula, notice first that the second sum is over all sequences $(\boldsymbol{A}_1^1,\dots,\boldsymbol{A}_{k_1}^1,\boldsymbol{A}_1^2,\dots,\boldsymbol{A}_{k_n}^n)$ of transitions that are in the list $\mathcal{S}$ and are just covering the set A, $\cup_{i,j}\bar{A}_j^i = A$. The sum in the braces (for a given $i = 1,\dots,n$) is taken over collections of configurations $n_A^{i,1},\dots,n_A^{i,k_i-1} \notin G_A$ with $n_A^{i,0} \equiv n_A^{i,k_i} \equiv g_A$, while the integral is taken over "times" attributed to transitions, with the energy term in the exponent taken over the set $A^i = \cup_{j=1}^{k_i} A_j^i$, $\bar{A} = \cup_{x\in A}U(x)$.

Finally, there are some restrictions on the sums and integrals encoded in functions $\frac{\mathbb{I}\left[\min_{i,j}\tau_j^i<0 \text{ and } \max_{i,j}\tau_j^i>0\right]}{\max_{i,j}\tau_j^i-\min_{i,j}\tau_j^i}$, $\varphi^{\mathrm{T}}(B_1,\dots B_n)$, and $\mathcal{I}(A_1^i,\dots,A_{k_i}^i; n_A^{i,1}g_{\Lambda\setminus A},\dots,n_A^{i,k_i-1}g_{\Lambda\setminus A})$. The easiest is the first one. One just assumes that the interval between the first and the last of concerned "times" contains the origin and the integrand is divided by the length of this interval. The function $\varphi^{\mathrm{T}}(B_1,\dots B_n)$ in terms of the sets $B_i = A^i \times [\tau_1^i,\tau_{k_i}^i] \subset \mathbb{Z}^\nu \times [-\infty,\infty]$, $i = 1,\dots,n$, is the standard factor from the theory of cluster expansions defined as

$$\varphi^{\mathrm{T}}(B_1,\dots,B_n) = \begin{cases} 1 & \text{if } n = 1 \\ \sum_{\mathcal{G}} \prod_{e(i,j)\in\mathcal{G}} \big(-\mathbb{I}\left[B_i \cup B_j \text{ is connected }\right]\big) & \text{if } n \geqslant 2 \end{cases}$$

with the sum over all connected graphs $\mathcal{G}$ of n vertices. Connectedness of a set $B \subset \mathbb{Z}^\nu \times [-\infty,\infty]$ is defined by combining connection in continuous direction with connection in slices $\{x|(x,\tau) \in B\} \subset \mathbb{Z}^\nu$ through pairs of sites of distance one. The most difficult to define is the restriction given by the function $\mathcal{I}$ that characterizes whether the collection of transitions is connected, in some generalized sense, through the intertwining configurations. A consolation might be that in lowest orders it is always true. Namely, whenever $k \leqslant 5$ and $\prod_{j=1}^{k}\langle n_A^{j-1}|\, T_{\boldsymbol{A}_j}\, |n_A^j\rangle \neq 0$,

$$\mathcal{I}(A_1,\dots,A_k; n_A^1 g_{\Lambda\setminus A},\dots,n_A^{k-1}g_{\Lambda\setminus A}) = \begin{cases} 1 & \text{if } \cup_j \bar{A}_j \text{ is connected} \\ 0 & \text{if } \cup_j \bar{A}_j \text{ is not connected.} \end{cases} \quad (3.6)$$

(When $\prod_{j=1}^{k}\langle n_A^{j-1}|\, T_{\boldsymbol{A}_j}\, |n_A^j\rangle = 0$, the value of $\mathcal{I}(\cdot)$ is not relevant.) To define it in a general case, consider $A_1,\dots,A_k \subset \mathbb{Z}^\nu$ and $n^1,\dots,n^{k-1} \in \Omega^{\mathbb{Z}^\nu}$. Taking $\bar{A} = \cup_{x\in A}U(x)$

and $E(n) = \{x \in \Lambda : n_{U(x)} \neq g_{U(x)} \text{ for any } g \in G\}$, we consider the set $\hat{B}^{(0)} \subset \mathbb{Z}^{\nu+1}$,

$$\hat{B}^{(0)} = \bigcup_{j=1}^{k} \Big[\bar{A}_j \times \{2j-2\}\Big] \cup \bigcup_{j=1}^{k-1} \Big[E(n^j) \times \{2j-1\}\Big].$$

Think of layers, one on top of another — configurations on odd levels interspersed with transitions on even levels. The set $\hat{B}^{(0)}$ decomposes into connected components, $\hat{B}^{(0)} = \cup_{\ell \geqslant 1} \hat{B}^{(0)}_\ell$. To any $\hat{B}^{(0)}_\ell$, define the box $\tilde{B}^{(0)}_\ell \subset \mathbb{Z}^{\nu+1}$ as the smallest rectangle containing $\hat{B}^{(0)}_\ell$. Then let $\hat{B}^{(1)} = \cup_{\ell \geqslant 1} \tilde{B}^{(0)}_\ell$; decompose into connected components $\hat{B}^{(1)} = \cup_{\ell \geqslant 1} \hat{B}^{(1)}_\ell$, and repeat the procedure until no change occurs any more, i.e. until $\hat{B}^{(m)} = \cup_{\ell \geqslant 1} \tilde{B}^{(m)}_\ell$. The function $\mathcal{I}$ characterizes whether this final set, the result of the above construction, is connected or not,

$$\mathcal{I}(A_1, \dots, A_k; n^1, \dots, n^{k-1}) = \begin{cases} 1 & \text{if } \hat{B}^{(m)} \text{ is connected} \\ 0 & \text{otherwise.} \end{cases} \tag{3.7}$$

4.3. Quantum fluctuations with less than four transitions. The equation (3.5) for the effective potential is hard to handle in general case. However, in many situations it is enough to consider only small sequences of less than four quantum transitions to define it. We rewrite in this section the explicit formulæ for the effective potential in such a case.

We assume thus that a list $\mathcal{S}$ of sequences of quantum transitions $\boldsymbol{A}$, containing at most 4 transitions, is given to represent the most important quantum fluctuations. Let us decompose $\mathcal{S} = \mathcal{S}^{(2)} \cup \mathcal{S}^{(3)} \cup \mathcal{S}^{(4)}$, with $\mathcal{S}^{(k)}$ denoting the list of sequences with exactly k transitions, and write

$$\Psi = \Psi^{(2)} + \Psi^{(3)} + \Psi^{(4)}. \tag{3.8}$$

Here $\Psi^{(k)}$ is the contribution to the effective potential due to the fluctuations from $\mathcal{S}^{(k)}$.

Let

$$\phi_A(n_A; g_A) = \sum_{x, U(x) \subset A} \Big[\Phi_x(n_{U(x)}) - \Phi_x(g_{U(x)})\Big].$$

Then, for any connected $A \subset \mathbb{Z}^\nu$ and $g_A \in G_A$, we define

$$\Psi^{(2)}_A(g_A) = - \sum_{\substack{(\boldsymbol{A}_1, \boldsymbol{A}_2) \in \mathcal{S}^{(2)} \\ \bar{A}_1 \cup \bar{A}_2 = A}} \sum_{n_A \notin G_A} \frac{\langle g_A | T_{\boldsymbol{A}_1} | n_A \rangle \langle n_A | T_{\boldsymbol{A}_2} | g_A \rangle}{\phi_A(n_A; g_A)}, \tag{3.9}$$

$$\Psi^{(3)}_A(g_A) = - \sum_{\substack{(\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{A}_3) \in \mathcal{S}^{(3)} \\ \bar{A}_1 \cup \bar{A}_2 \cup \bar{A}_3 = A}} \sum_{n_A, n'_A \notin G_A} \frac{\langle g_A | T_{\boldsymbol{A}_1} | n_A \rangle \langle n_A | T_{\boldsymbol{A}_2} | n'_A \rangle \langle n'_A | T_{\boldsymbol{A}_3} | g_A \rangle}{\phi_A(n_A; g_A) \phi_A(n'_A; g_A)}. \tag{3.10}$$

The expression for $\Psi^{(4)}$ becomes more complicated (we shall see in Chapter 8 that clusters of excitations are actually occurring here),

$$\Psi^{(4)}_A(g_A) = - \sum_{\substack{(\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{A}_3, \boldsymbol{A}_4) \in \mathcal{S}^{(4)} \\ \bar{A}_1 \cup \bar{A}_2 \cup \bar{A}_3 \cup \bar{A}_4 = A}} \Bigg[\sum_{n_A, n'_A, n''_A \notin G_A} \frac{\langle g_A | T_{\boldsymbol{A}_1} | n_A \rangle \langle n_A | T_{\boldsymbol{A}_2} | n'_A \rangle \langle n'_A | T_{\boldsymbol{A}_3} | n''_A \rangle \langle n''_A | T_{\boldsymbol{A}_4} | g_A \rangle}{\phi_A(n_A; g_A) \phi_A(n'_A; g_A) \phi_A(n''_A; g_A)}$$

$$- \frac{1}{2} \sum_{n_A, n'_A \notin G_A} \frac{\langle g_A | T_{\boldsymbol{A}_1} | n_A \rangle \langle n_A | T_{\boldsymbol{A}_2} | g_A \rangle \langle g_A | T_{\boldsymbol{A}_3} | n'_A \rangle \langle n'_A | T_{\boldsymbol{A}_4} | g_A \rangle}{\phi_{A^1}(n_A; g_A) + \phi_{A^2}(n'_A; g_A)} \Big\{ \frac{1}{\phi_{A^1}(n_A; g_A)} + \frac{1}{\phi_{A^2}(n'_A; g_A)} \Big\}^2 \Bigg]. \tag{3.11}$$

Above we denoted $A^1 = \bar{A}_1 \cup \bar{A}_2$ and $A^2 = \bar{A}_3 \cup \bar{A}_4$. All the denominators are strictly positive.

These equations simplify further if $T_{\boldsymbol{A}}$ is a monomial in creation and annihilation operators; indeed in the sums over intermediate configurations only one element has to be taken into account.

Notice, finally, that the diagonal terms in T are not playing any role in the previous definitions; we consider that they are small, since otherwise we would have included them into the diagonal potential.

4.4. Stability of the dominant states. The aim of rewriting a class of quantum transitions in terms of the effective potential was to get a control over stable low temperature phases. To this end, the three conditions, expressed first only vaguely and then in precise terms in the following Assumptions 2, 3, and 4, must be met. Namely, we suppose that

- the Hamiltonian corresponding to the sum $\Phi + \Psi$ of the classical (diagonal) and effective interactions has a finite number of ground configurations, and its excitations have strictly positive energy;[4]
- the list $\mathcal{S}$ contains all the lowest quantum fluctuations;
- there is no "quantum instability"; the transition probability from a "ground state" g to another "ground state" g' is small compared to the energy cost of the excitations.

Each component of the effective interaction Ψ_A is a mapping $G_A \to \mathbb{R}$; let us first extend it to $\Omega^A \to \mathbb{R}$ by putting $\Psi_A(n_A) = 0$ if $n_A \notin G_A$. To give a precise meaning to the first condition, we suppose that a finite number of periodic reference configurations $D \subset G$ is given such that the interaction $\Phi + \Psi$ satisfies the Peierls condition with respect to D. We choose a formulation in which it is very easy to verify the condition and, in addition, it takes into account the fact that the configurations from D are not necessarily translation invariant. Namely, we will formulate the condition in terms of a potential Υ that is equivalent to $\Phi + \Psi$ and is chosen in a suitable way. Of course, in many particular cases this is not necessary and the condition as stated below is valid directly for $\Phi + \Psi$. However, in several important cases treated in Chapter 4, the interaction $\Phi + \Psi$ turns out not to be so called m-potential and the use of the equivalent m-potential Υ not only simplifies the formulation of the Peierls condition, but also makes the task of its verification much easier.

ASSUMPTION 2. **Peierls condition.**

There exist a finite set of periodic configurations $D \subset G$ with the smallest common period L_0, a constant Δ such that $\Delta > \|T\|^k$ for some finite constant k, and a periodic interaction Υ (with period ℓ_0) that is physically equivalent to $\Phi + \Psi$ such that the following conditions are satisfied. The interaction Υ is a block interaction that belongs to $\mathcal{C}(R, D, \Delta)$, where the range R is finite[5] *and is such that*

$$R^\nu \leqslant \Delta_0/\delta_0, \tag{3.12}$$

with the constants δ_0 and Δ_0 determined by the interaction Φ in Assumption 1. Excitations with respect to G and D are separated by gaps $\frac{1}{2}\Delta_0$ and Δ respectively:

[4] Again, when exploring a region of phase diagram at once, we have a fixed finite set of reference configurations that, strictly speaking, turn out to be ground configurations of the corresponding Hamiltonian for a particular value of "external fields". See below for a more detailed formulation.

[5] We will suppose, taking larger R if necessary, that it is larger or equal to the range R_0 of Φ, as well as to the range of the effective interaction Ψ and to L_0.

- *for any* $x \in \Lambda$ *and any* n *with* $n_{U(x)} \notin G_{U(x)}$, *we have*
$$\Upsilon_x(n_{U'(x)}) - \max_{g\in G} \Upsilon_x(g_{U'(x)}) \geqslant \tfrac{1}{2}\Delta_0;$$
- *for any* $x \in \Lambda$ *and any* n *with* $n_{U'(x)} \notin D_{U'(x)}$, *we have*
$$\Upsilon_x(n_{U'(x)}) - \min_{d\in D} \Upsilon_x(d_{U'(x)}) \geqslant \Delta.$$

The following assumption is a condition demanding that the list $\mathcal{S}$ should contain all transitions that are relevant for the effective potential. We define

$$\boldsymbol{m}(T_{\boldsymbol{A}_1}, \dots, T_{\boldsymbol{A}_k}) = \max_{g\in G} \max_{n^1,\dots,n^{k-1}\notin G} |\langle g| T_{\boldsymbol{A}_1} |n^1\rangle\langle n^1| T_{\boldsymbol{A}_2} |n^2\rangle \dots \langle n^{k-1}| T_{\boldsymbol{A}_k} |g\rangle|. \quad (3.13)$$

Assumption 3. **Completeness of the set of quantum transitions.**
There exists a function $b_1(\cdot)$ *with* $\lim_{\lambda\to 0} b_1(\lambda) = 0$ *such that for any sequence* $(\boldsymbol{A}_1, \dots, \boldsymbol{A}_m) \notin \mathcal{S}$ *with connected* $\cup_{i=1}^m \bar{A}_i$ *one has*

$$\boldsymbol{m}(T_{\boldsymbol{A}_1}, \dots, T_{\boldsymbol{A}_{k_1}})\boldsymbol{m}(T_{\boldsymbol{A}_{k_1+1}}, \dots, T_{\boldsymbol{A}_{k_2}}) \dots \boldsymbol{m}(T_{\boldsymbol{A}_{k_{n-1}+1}}, \dots, T_{\boldsymbol{A}_m}) \leqslant b_1(\|T\|)\Delta.$$

Finally, we have a condition assuring that there is *no quantum instability.*

Assumption 4. **Absence of quantum instability.**
There exists a function $b_2(\cdot)$ *with* $\lim_{\lambda\to 0} b_2(\lambda) = 0$ *such that for any sequence* $(\boldsymbol{A}_1, \dots, \boldsymbol{A}_m)$, *and any* $g, g' \in G$, $g \neq g'$, *one has*

$$\left|\langle g| T_{\boldsymbol{A}_1} \dots T_{\boldsymbol{A}_m} |g'\rangle\right| \leqslant b_2(\|T\|)\Delta.$$

Our first result concerns the existence of the thermodynamic limit for the state under periodic boundary conditions. Taking L_0 to be the smallest common period of periodic configurations from D, we always consider in the following the limit over tori $\Lambda \nearrow \mathbb{Z}^\nu$ whose sides are multiples of L_0 and ℓ_0.

Theorem 3.5. **Thermodynamic limit.**
Suppose that the Hamiltonian is $H = T + V$, $T \in \mathcal{Q}$, *and satisfies the Assumptions 1–4. Then there exist constants* $\varepsilon_0 > 0$ *and* $\beta_0 = \beta_0(\Delta)$ *(depending on* ν, S, R, ℓ_0*) such that the limit*

$$\langle K\rangle_\beta^{\mathrm{per}} = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{\operatorname{Tr} K\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}}{\operatorname{Tr}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}} \quad (3.14)$$

exists whenever $\|T\| \leqslant \varepsilon_0$, $\beta \geqslant \beta_0$, *and* K *is a local observable.*

Notice the logic of constants in the theorem above (as well as in the remaining two theorems stated below). We first choose ε_0. Then, for any $\|T\| \leqslant \varepsilon_0$ one can choose β_0 (depending on Δ that is determined in terms of T through the effective potential Ψ) such that the claim is valid for the given T and any $\beta \geqslant \beta_0(\Delta)$. With $\|T\| \to 0$ we may have to go to lower temperatures (higher β) to keep the control. Of course, if Δ does not vanish with vanishing $\|T\|$ (i.e. Assumption 2 is valid for Φ alone) as was the case in Theorem 3.3, one can choose the constant β_0 uniformly in $\|T\|$.

If there are coexisting phases for a given temperature and Hamiltonian, the state $\langle\cdot\rangle_\beta^{\mathrm{per}}$ will actually turn out to be a linear combination of several pure states. A standard way how to select such a pure state is to consider a thermodynamic limit with a suitably chosen fixed boundary condition. In many situations to which the present theory should apply, this approach is not easy to implement. The classical part of the Hamiltonian might actually consist only of on-site terms and to make the system "feel" the boundary, the

truly quantum terms must be used. One possibility is, of course, to couple the system with the boundary with the help of the effective potential. The problem here is, however, that since we are interested in a genuine quantum model, we would have to introduce the effective potential directly in the finite volume quantum state. Expanding this state, in a similar manner as it will be done in Chapters 7–8, we would actually obtain a new, boundary dependent effective potential. One can imagine that it would be possible to cancel the respective terms by assuming that the boundary potential satisfies certain "renormalizing self-consistency conditions". However, the details of such an approach remain to be clarified.

Hence we prefer to consider only periodic boundary conditions, and to talk about thermodynamically stable states.

THEOREM 3.6. **Pure low temperature phases.**

If the Hamiltonian is $H = T+V$, with $T \in \mathcal{Q}$, and if the Assumptions 1–4 are satisfied, then for any $\eta > 0$, there exist $\varepsilon_0 > 0$ and $\beta_0 = \beta_0(\Delta)$ (depending on ν, S, R, ℓ_0) such that if $\|T\| \leqslant \varepsilon_0$ and $\beta \geqslant \beta_0$, there exists for every $d \in D$ a function $f^\beta(d)$ such that the set $Q = \{d \in D;\, \mathrm{Re}\, f^\beta(d) = \min_{d' \in D} \mathrm{Re}\, f^\beta(d')\}$ characterizes the set of pure phases. Namely, for any $d \in Q$:

a) *The function $f^\beta(d)$ is equal to the free energy of the system, i.e.*

$$f^\beta(d) = -\frac{1}{\beta} \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{1}{|\Lambda|} \log \mathrm{Tr}\ \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}.$$

b) *There exists a pure state $\langle\cdot\rangle_\beta^d$. Moreover, it is close to the state $|d_\Lambda\rangle$ in the sense that for any bounded local observable K and any sufficiently large Λ, one has*

$$\left| \langle K \rangle_\beta^d - \langle d_\Lambda |\, K\, | d_\Lambda \rangle \right| \leqslant \eta |\,\mathrm{Supp}\, K\,| \|K\|.$$

c) *There is an exponential decay of correlations in the state $\langle\cdot\rangle_\beta^d$, i.e. there exists a constant $\xi^d > 0$ such that*

$$\left| \langle K K' \rangle_\beta^d - \langle K \rangle_\beta^d \langle K' \rangle_\beta^d \right| \leqslant |\,\mathrm{Supp}\, K\,|\,|\,\mathrm{Supp}\, K'\,| \|K\| \|K'\|\, \mathrm{e}^{-\,\mathrm{dist}(\mathrm{Supp}\, K, \mathrm{Supp}\, K')/\xi^d}$$

for any bounded local observables K and K'.

d) *The state $\langle\cdot\rangle_\beta^{\mathrm{per}}$ is a linear combination of the states $\langle\cdot\rangle_\beta^d$, $d \in Q$, with equal weights,*

$$\langle K \rangle_\beta^{\mathrm{per}} = \frac{1}{|Q|} \sum_{d \in Q} \langle K \rangle_\beta^d$$

for each local observable K.

e) *If $Q = \{d\}$, the states $\langle\cdot\rangle_\beta^d$ and $\langle\cdot\rangle_\beta^{\mathrm{per}}$ are identical, and they are thermodynamically stable.*

4.5. Phase diagram. We now turn to the phase diagram at low temperatures. Let p be the number of dominant states, i.e. $p = |D|$. To be able to investigate the phase diagram, we suppose that $p-1$ suitable "external fields" are added to the Hamiltonian H_Λ^{per}. Or, in other words, we suppose that classical potential Φ and quantum interaction T depend on a vector parameter $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_{p-1}) \in \mathcal{U}$, where $\mathcal{U}$ is an open set of $\mathbb{R}^{p-1}$, and that the zero-temperature phase diagram of $\Phi + \Psi$ is linearly regular.

ASSUMPTION 5. **Phase diagram of the effective potential.**

Φ and T are differentiable with respect to $\boldsymbol{\mu}$ and there exists a constant $M < \infty$ such that

$$\max_{n_{U(x)} \in \Omega^{U(x)}} \Big| \frac{\partial}{\partial \mu_i} \Phi_x(n_{U(x)}) \Big| \;\leqslant\; M$$

for all $x \in \mathbb{Z}^\nu$, and

$$\|T\| + \sum_{i=1}^{p-1} \Big\| \frac{\partial T}{\partial \mu_i} \Big\| \;\leqslant\; M$$

for all $\boldsymbol{\mu} \in \mathcal{U}$.

Further, there exists a point $\boldsymbol{\mu}_0 \in \mathcal{U}$ such that

$$e^{\boldsymbol{\mu}_0}(d) = e^{\boldsymbol{\mu}_0}(d') \text{ for all } d, d' \in D,$$

and the inverse of the matrix of derivatives

$$\left(\frac{\partial}{\partial \mu_i} \big[e^{\boldsymbol{\mu}}(d_j) - e^{\boldsymbol{\mu}}(d_p) \big] \right)_{1 \leqslant i,j \leqslant p-1}$$

has a uniform bound for all $\boldsymbol{\mu} \in \mathcal{U}$.

Let $\mathcal{P}^*$ be the corresponding phase diagram, i.e. the decomposition of $\mathcal{U}$ into manifolds with configurations of minimum energy. The statement of the following theorem is that the collection $\mathcal{P} = \{\mathfrak{M}(Q)\}_{Q \subset D}$ of manifolds where the configurations of Q yield pure phases of the full model is also a regular phase diagram and differs only slightly from $\mathcal{P}^*$. To measure the distance of two manifolds $\mathfrak{M}$ and $\mathfrak{M}'$, we introduce the Hausdorff distance

$$\mathrm{dist}_{\mathrm{H}}(\mathfrak{M}, \mathfrak{M}') = \max\big(\sup_{\boldsymbol{\mu} \in \mathfrak{M}} \mathrm{dist}(\boldsymbol{\mu}, \mathfrak{M}'),\; \sup_{\boldsymbol{\mu} \in \mathfrak{M}'} \mathrm{dist}(\boldsymbol{\mu}, \mathfrak{M}) \big).$$

THEOREM 3.7. **Low temperature phase diagram.**

$H = T + V$, $T \in \mathcal{Q}$. Under the Assumptions 1–5 there exist $\varepsilon_0 > 0$ and $\beta_0 = \beta_0(\Delta)$ such that if $\|T\| + \sum_{i=1}^{r-1} \|\frac{\partial}{\partial \mu_i} T\| \;\leqslant\; \varepsilon_0$ and $\beta \;\geqslant\; \beta_0$, there exists a collection of manifolds $\mathcal{P}^\beta = \{\mathfrak{M}^\beta(Q)\}_{Q \subset D}$ such that

(a) *The collection $\mathcal{P}^\beta$ determines a regular phase diagram;*

(b) *If $\boldsymbol{\mu} \in \mathfrak{M}^\beta(Q)$, the corresponding pure state $\langle \cdot \rangle_\beta^d$ exists for every $d \in Q$ and satisfies the properties b), c), d) and e), from Theorem 3.6;*

(c) *The Hausdorff distance* $\mathrm{dist}_{\mathrm{H}}$ *between the manifolds of $\mathcal{P}^\beta$ and their correspondent in $\mathcal{P}^*$ is bounded,*

$$\mathrm{dist}_{\mathrm{H}}(\mathfrak{M}^\beta(Q), \mathfrak{M}^*(Q)) \;\leqslant\; O(\,\mathrm{e}^{-\beta} + \|T\| + \sum_{i=1}^{r-1} \Big\| \frac{\partial T}{\partial \mu_i} \Big\|),$$

for all $Q \subset D$.

The proofs of these theorems are given in Chapter 8.

CHAPTER 4

Applications to Hubbard models

As illustrations we consider two systems, with fermions and bosons respectively. The first one is a modified Hubbard model in which the hopping of the particles depends on their spin — this modification being introduced for mathematical rather than physical reasons. The second one is the Bose-Hubbard model, which described hopping bosons on a lattice, with on-site and/or longer-range interactions.

1. The asymmetric Hubbard model

The physical system consists of quantum particles with spin on a lattice $\Lambda \subset \mathbb{Z}^\nu$ ($\nu \geqslant 2$). The phase space could be constructed as the Fock space for fermions in Λ; however, it is simpler to proceed as in Chapter 2, i.e. to choose a single site phase space and to construct the Hilbert space spanned by the classical configurations. Hence we take $\Omega = \{0, \uparrow, \downarrow, 2\}$; a basis of $\mathcal{H}_\Lambda$ is $\{\, |n_\Lambda\rangle : n_\Lambda \in \Omega^\Lambda\}$. The Hamiltonian has kinetic and potential parts; the potential part depends on a chemical potential μ and an external magnetic field h:

$$H^{\mu,h} = T + V^{\mu,h}. \tag{4.1}$$

$T = (T_{\boldsymbol{A}})$, $\boldsymbol{A} = (< x, y >, \sigma)$, where $< x, y >$ is an ordered pair of nearest neighbours ($\|x - y\|_1 = 1$) and $\sigma \in \{\uparrow, \downarrow\}$ is the spin; in this case

$$T_{\boldsymbol{A}} = t_\sigma c^\dagger_{x\sigma} c_{y\sigma}, \tag{4.2}$$

with $t_\sigma \in \mathbb{R}$ being the hopping coefficient, that depends on σ. In other words [see (2.17)],

$$T_A = \begin{cases} t_\uparrow (c^\dagger_{x\uparrow} c_{y\uparrow} + c^\dagger_{y\uparrow} c_{x\uparrow}) + t_\downarrow (c^\dagger_{x\downarrow} c_{y\downarrow} + c^\dagger_{y\downarrow} c_{x\downarrow}) & \text{if } A = \{x, y\} \text{ with } \|x - y\|_1 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

If $t_\uparrow = t_\downarrow$ we have the usual Hubbard model. However in the sequel we shall restrict our attention to the range of parameters

$$U \gg |t_\uparrow| \gg |t_\downarrow|,$$

when discussing the antiferromagnetic phase. Hopping coefficients are related to the mass of particles, and there is no physical justification why the mass of spin up particles should be much smaller than the one for spin down electrons. However, this model can have different meaning, e.g. describing electrons interacting with ions; the latter are heavier and thus their hopping constant is smaller. This model is a generalization of the Falicov-Kimball one. One has to remark that the physics of the model is significantly modified by setting $t_\uparrow \neq t_\downarrow$; this artificially breaks a continuous symmetry of the Hubbard model, namely the rotation invariance of the magnetization.

The potential $V^{\mu,h}$ is the quantum equivalent of a classical on-site interaction $\Phi^{\mu,h}$,

$$\Phi^{\mu,h}_x(n_x) = U n_{x\uparrow} n_{x\downarrow} - \mu(n_{x\uparrow} + n_{x\downarrow}) - h(n_{x\uparrow} - n_{x\downarrow}). \tag{4.3}$$

We can solve this model exactly, at least in the "atomic limit" $t_\uparrow, t_\downarrow \to 0$. The free energy per site is

$$f(\beta,\mu,h) = \frac{U}{2} - \mu - \frac{1}{\beta}\log\Big[2\cosh\big(\beta\frac{U}{2} - \beta\mu\big) + 2\,\mathrm{e}^{\beta U/2}\,\cosh(\beta h)\Big] \tag{4.4}$$

(it does not depend on the dimension). $f(\beta,\mu,h)$ is analytic in β,μ,h and therefore no phase transition may occur. The magnetization is

$$-\frac{\partial f}{\partial h}(\beta,\mu,h) = \frac{\sinh(\beta h)}{\mathrm{e}^{-\beta U/2}\,\cosh\big(\beta\frac{U}{2} - \beta\mu\big) + \cosh(\beta h)}. \tag{4.5}$$

It is an increasing function of h, which is zero at $h = 0$; this describes a paramagnetic phase.

Since the potential is only on-site, there is a domain of thermodynamic parameters with analyticity of the free energy, extending to low temperatures:

THEOREM 4.1. **Paramagnetic phase.**
There exists $c_1, c_2 > 0$ such that the free energy is analytic in the union of the two domains

$$\beta(|t_\uparrow| + |t_\downarrow|) < c_1$$
$$\frac{\beta(t_\uparrow^2 + t_\downarrow^2)}{\min(\mu, U-\mu) - |h|} < c_2 \qquad \textit{(provided } \min(\mu, U-\mu) - |h| > 0\textit{)}$$

and the corresponding Gibbs state exists in the thermodynamic limit, is thermodynamically stable and exponentially clustering.

Analyticity in the first domain results from Theorem 3.2; the second domain is proved in [Uel 1998] (and in the case $t_\downarrow = 0$, i.e. for the Falicov-Kimball model, this was done in [KL 1986]).

To study the effects of quantum fluctuations, let us rewrite the potential as

$$\Phi_x^{\mu,h}(n_x) = \frac{U}{2}\Big(n_{x\uparrow} + n_{x\downarrow} - \frac{\mu}{U} - \frac{1}{2}\Big)^2 - h(n_{x\uparrow} - n_{x\downarrow}) - C \tag{4.6}$$

with $C = \frac{\mu^2}{2U} + \frac{\mu}{2} + \frac{U}{8}$. We take for G the set of all configurations with exactly one particle per site. G is an infinite set (for all finite Λ, we have $|G_\Lambda| = 2^{|\Lambda|}$). Constants Δ_0 and δ_0 of Assumption 1 (page 27) can be chosen as

$$\Delta_0 = \frac{1}{2^\nu}\big[\min(\mu, U-\mu) - |h|\big]$$
$$\delta_0 = 2|h|.$$

Actually, (3.2) holds with the lower bound $\min(\mu, U-\mu) - |h|$; but Δ_0 also appears in Assumption 2, and it will turn out that the factor $1/2^\nu$ is necessary). The list $\mathcal{S}$ of transitions that we consider for the effective potential is

$$\mathcal{S} = \{(\boldsymbol{A}, \boldsymbol{A}') : \boldsymbol{A} = (<x,y>,\uparrow) \text{ and } \boldsymbol{A}' = (<y,x>,\uparrow) \text{ for some } x,y \in \mathbb{Z}^\nu, \|x-y\|_2 = 1\}.$$

The effective potential is given by (3.9). We have $\phi_{\{x,y\}}(n_{\{x,y\}}; g_{\{x,y\}}) = U$ if $n_{\{x,y\}} \in \{(0,2),(2,0)\}$ and $g_{\{x,y\}} \in G_{\{x,y\}}$; furthermore

$$\langle g_{\{x,y\}}|\, c_{x\uparrow}^\dagger c_{y\uparrow} c_{y\uparrow}^\dagger c_{x\uparrow}\, |g_{\{x,y\}}\rangle + \langle g_{\{x,y\}}|\, c_{y\uparrow}^\dagger c_{x\uparrow} c_{x\uparrow}^\dagger c_{y\uparrow}\, |g_{\{x,y\}}\rangle = \begin{cases} 1 & \text{if } g_{\{x,y\}} \in \{(\uparrow,\downarrow),(\downarrow,\uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \tag{4.7}$$

The effective potential is then

$$\Psi_{\{x,y\}}(g_{\{x,y\}}) = \begin{cases} -t_\uparrow^2/U & \text{if } g_{\{x,y\}} \in \{(\uparrow,\downarrow),(\downarrow,\uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \tag{4.8}$$

This interaction is nearest-neighbour and can be inscribed in blocks $2 \times \cdots \times 2$. We take $R = \frac{1}{2}$ and choose for the physically equivalent interaction Υ

$$\Upsilon_x(n_{U'(x)}) = \frac{1}{2^\nu} \sum_{y \in U'(x)} \Phi_y^{\mu,h}(n_y) + \frac{1}{2^{\nu-1}} \sum_{\substack{\{y,z\} \subset U'(x) \\ \|y-x\|_2 = 1}} \Psi_{\{x,y\}}(n_{\{x,y\}}). \tag{4.9}$$

The set D of dominant states has two elements, namely the two chessboard configurations $d^{(1)}$ and $d^{(2)}$; if $(-1)^x \doteq \prod_{i=1}^\nu (-1)^{x_i}$,

$$d_x^{(1)} = \begin{cases} \uparrow & \text{if } (-1)^x = 1 \\ \downarrow & \text{if } (-1)^x = -1 \end{cases} \qquad d_x^{(2)} = \begin{cases} \uparrow & \text{if } (-1)^x = -1 \\ \downarrow & \text{if } (-1)^x = 1. \end{cases}$$

To find the Peierls constant Δ of Assumption 2, page 30, let us make the following observation. Consider a cube $2 \times \cdots \times 2$ in $\mathbb{Z}^\nu$, that we denote C, and a configuration n_C on it. First, only configurations with one particle per site need to be taken into account, the others having an increase of energy of the order U. If $n_C \in G_C$, then all edges of the cubes are either ferromagnetic, or antiferromagnetic. If a spin at a site is flipped, then exactly ν edges are changing of state. Since any configuration can be created by starting from the chessboard one, and flipping the spins at some sites, we see that the minimum number of ferromagnetic edges, for configurations that are not chessboard, is ν. This leads to $\Delta = \frac{\nu}{2^{\nu-1}} \frac{t_\uparrow^2}{U} - |h|$. Let us introduce $\epsilon = 1 - \frac{2^{\nu-1}}{\nu} \frac{U}{t_\uparrow^2} |h|$, so that $\Delta = \frac{\nu}{2^{\nu-1}} \frac{t_\uparrow^2}{U} \epsilon$.

The maximum of the expression in Assumption 3 is equal to $\max(t_\downarrow^2, t_\uparrow^4)$. If there exists $\varepsilon > 0$ such that $|t_\downarrow| \leqslant |t_\uparrow|^{1+\varepsilon}$, the bound of Assumption 3 can be chosen to be $b_1 = \frac{2^{\nu-1}U}{\nu\epsilon} |t_\uparrow|^{2\varepsilon}$. For Assumption 4 the expression has maximum equals to $|t_\downarrow t_\uparrow|$ and we can take $b_2 = \frac{2^{\nu-1}U}{\nu\epsilon} |t_\uparrow|^\varepsilon$ (this Assumption is not true in the symmetric Hubbard model; the effective potential is not strong enough in order to forbid the model to jump from one g to another g').

As a consequence of Theorem 3.6, the chessboard states are stable at low temperatures.

THEOREM 4.2. **Chessboard phases in asymmetric Hubbard model.**

We assume $\nu \geqslant 2$, $0 < \mu < U$, $h < \frac{2^{\nu-1}}{\nu} \frac{t_\uparrow^2}{U}$, and $|t_\downarrow| \leqslant |t_\uparrow|^{1+\varepsilon}$ with $\varepsilon > 0$. Then for any $\delta > 0$, there exist $t_0 > 0$ and $\beta_0(t_\uparrow, h) < \infty$ ($\lim_{t_\uparrow \to 0} \beta_0(t_\uparrow, 0) = \infty$) such that if $|t_\uparrow| \leqslant t_0$ and $\beta \geqslant \beta_0$,

- *The free energy exists in the thermodynamic limit, as well as expectation values of observables.*
- *There are two pure periodic phases, $\langle\cdot\rangle^{(1)}$ and $\langle\cdot\rangle^{(2)}$, with exponential decay of correlations.*
- *$\langle\cdot\rangle^{(1)}$ represents a pure phase that is a small deformation of the first chessboard configuration:*

$$\langle n_{x\uparrow}\rangle^{(1)} \begin{cases} \geqslant 1-\delta & \text{if } (-1)^x = 1 \\ \leqslant \delta & \text{if } (-1)^x = -1 \end{cases} \qquad \langle n_{x\downarrow}\rangle^{(1)} \begin{cases} \leqslant \delta & \text{if } (-1)^x = 1 \\ \geqslant 1-\delta & \text{if } (-1)^x = -1, \end{cases}$$

and $\langle\cdot\rangle^{(2)}$ *represents a pure phase that is a small deformation of the second chessboard.*

To construct the two pure phases, one way is to add to the Hamiltonian a staggered magnetic field

$$\tilde{h}\tilde{V}_x \doteq -(-1)^x\tilde{h}(n_{x\uparrow}-n_{x\downarrow}).$$

Then

$$\langle\cdot\rangle^{(1)} = \lim_{\tilde{h}\to 0+}\langle\cdot\rangle^{\mathrm{per}}(\tilde{h})$$

and

$$\langle\cdot\rangle^{(2)} = \lim_{\tilde{h}\to 0-}\langle\cdot\rangle^{\mathrm{per}}(\tilde{h}),$$

where $\langle\cdot\rangle^{\mathrm{per}}(\tilde{h})$ is the thermodynamic limit of the state with periodic boundary conditions, and Hamiltonian $H^{\mu,h,\tilde{h}} = V^{\mu,h} + T + \tilde{h}\tilde{V}$. $\tilde{V}$ is no physical object. However, the notion of thermodynamic stability *is* physical, and any possible instability has to be considered, including staggered magnetization.

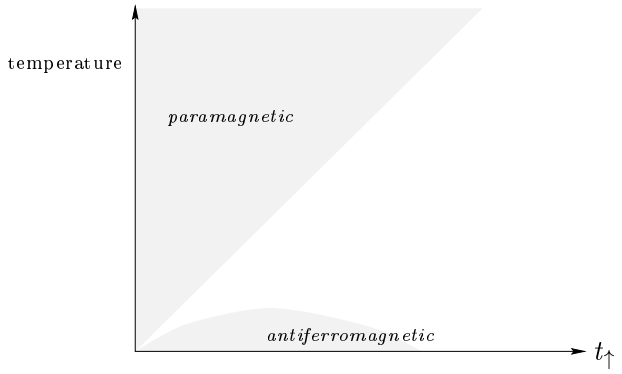


FIGURE 4.1. Phase diagram of the asymmetric Hubbard model.

Notice that the Hamiltonian conserves the number of particles, and the magnetization in both directions. Following [BKU 1997], one expects to have bounds on compressibility coefficient and on susceptibility; namely, if $t_\uparrow \neq 0$,

$$\left|\frac{\partial}{\partial\mu}\langle(n_{x\uparrow}+n_{x\downarrow})\rangle^{\mu,h,\beta}\right| \leqslant C\,\mathrm{e}^{-c\beta} \tag{4.10}$$

$$\left|\frac{\partial}{\partial h}\langle(n_{x\uparrow}-n_{x\downarrow})\rangle^{\mu,h,\beta}\right| \leqslant C'\,\mathrm{e}^{-c'\beta}\,. \tag{4.11}$$

In particular, these quantities vanish in the ground state (see the concluding remarks, Chapter 9, for additional discussion).

Hubbard model with longer-range hopping. A natural question is whether the approximation of considering hopping only betweeen nearest-neighbours is correct. In other words, what happens if the particles have the posibility to hop onto next-nearest-neighbours? The answer depends on the value of the longer-range hoppings; if they are strong enough, other phases occur, namely planar and lamellar ones [GKU 1998].

We consider the case of dimension $\nu = 3$; the hopping matrix is $T = (T_{\boldsymbol{A}})$, where

$$T_{\boldsymbol{A}} = \begin{cases} t_\sigma^{(j)} c_{x\sigma}^\dagger c_{y\sigma} & \text{if } \boldsymbol{A} = ((x,y),\sigma) \text{ with } \|x-y\|_2 = \sqrt{j},\ j = 1,2,3 \\ 0 & \text{otherwise.} \end{cases} \tag{4.12}$$

Actually, the quantum matrix is not a quantum interaction with connected supports, and so does not fulfill our assumptions. This could be corrected by defining a new equivalent interaction with connected supports. For simplicity, we only refer to [GKU 1998] where the effective interaction is explicitely written in the case of lattice systems of hopping particles.

The potential is as before given by an on-site Coulomb repulsion; to simplify, we set $U = 1$.

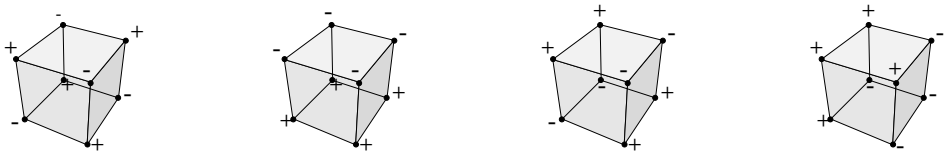
The list of transitions leading to the effective potential is

$$\mathcal{S} = \{(\boldsymbol{A}, \boldsymbol{A}') : \boldsymbol{A} = (<x, y>, \uparrow) \text{ and } \boldsymbol{A}' = (<y, x>, \uparrow), x, y \in \mathbb{Z}^\nu \text{ with } \|x-y\|_2 = 1, \sqrt{2}, \sqrt{3}\}.$$

From (3.9) we obtain

$$\Psi_{\{x,y\}}(g_{\{x,y\}}) = \begin{cases} -(t_\uparrow^{(j)})^2 & \text{if } g_{\{x,y\}} \in \{(\uparrow,\downarrow),(\downarrow,\uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \tag{4.13}$$

The physically equivalent potential Υ may be chosen as to act on cubes of size 1 (i.e. with 8 sites). Candidates for minimizing Υ are



chessboard planar lamellar enigmatic

(here "+" stands for "↑" and "−" stands for "↓"). The corresponding energies are

$$\begin{aligned}
\Upsilon_x(n_C^{\mathrm{cb}}) &= -3(t_\uparrow^{(1)})^2 - 4(t_\uparrow^{(3)})^2 \\
\Upsilon_x(n_C^{\mathrm{pl}}) &= -(t_\uparrow^{(1)})^2 - 4(t_\uparrow^{(2)})^2 - 4(t_\uparrow^{(3)})^2 \\
\Upsilon_x(n_C^{\mathrm{lam}}) &= -2(t_\uparrow^{(1)})^2 - 4(t_\uparrow^{(3)})^2 \\
\Upsilon_x(n_C^{\mathrm{en}}) &= -\tfrac{3}{2}(t_\uparrow^{(1)})^2 - 3(t_\uparrow^{(2)})^2 - 4(t_\uparrow^{(3)})^2.
\end{aligned}$$

It is not hard to check that for any $t_\uparrow^{(1)}$, $t_\uparrow^{(2)}$, $t_\uparrow^{(3)}$, the ground configurations are among these four (and all obtained by rotations and reflections). Domains where they are ground states are shown in Fig. 4.2; enigmatic configuration is present on the coexistence line between chessboard and planar.

The zero-temperature phase diagram of the effective potential is *not* regular. However, it is possible to prove stability of chessboard, planar and lamellar phases, but the transitions from one phase to another are not understood. Between the chessboard and the planar phases, either there is first-order phase transitions, or there are two transitions, one from chessboard to enigmatic, and one from enigmatic to planar. Transitions from chessboard to lamellar, or planar to lamellar, are a mystery; it is even not clear if there are phase transitions. An open question is whether enigmatic phase is present?

2. The Bose-Hubbard model

2.1. Introduction. Lattice models of interacting bosons have been considered for different reasons. On the one hand they were used as models capturing important features of such systems as, for instance, ^{4}He absorbed in porous media, or superconductors where Cooper pairs are approximately bosonic quasiparticles. But more importantly, it was

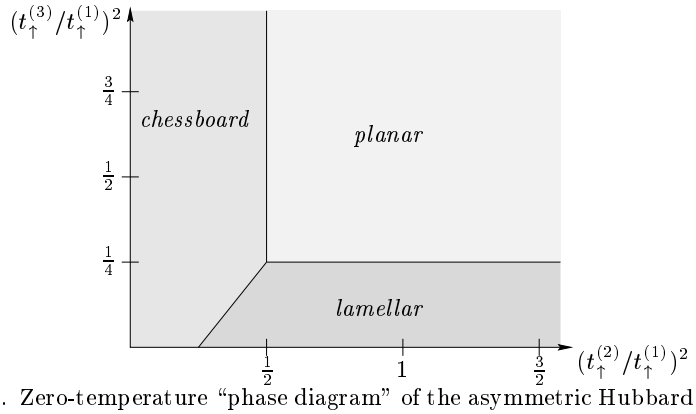


FIGURE 4.2. Zero-temperature "phase diagram" of the asymmetric Hubbard model with extended hopping. Enigmatic configuration appears in-between chessboard and planar ones.

suggested that these systems could play an important role in the study of Bose-Einstein condensation[1] and superfluidity in interacting systems.

Widely used is the *Bose-Hubbard model* [FWGF 1989] which describes bosonic particles hopping on a lattice. The basic ingredients are a hopping term for the kinetic energy of the bosons, and an on-site interaction proportional to the number of pairs of bosons at the same site,

$$H_\Lambda = -t \sum_{<x,y>\subset\Lambda} (c_x^\dagger c_y + c_y^\dagger c_x) + U_0 \sum_{x\in\Lambda} \big(n_x^2 - n_x\big) - \mu \sum_{x\in\Lambda} n_x. \tag{4.14}$$

Here the sum of hopping terms runs over nearest neighbours, and the on-site repulsive potential per pair is $2U_0$; μ is the chemical potential.

The zero temperature phase diagram was studied by Fisher *et al.* [FWGF 1989] (with and without an additional random potential); their discussion suggested the phase diagram according to Fig. 4.3. It consists of domains of incompressible phases with integer densities near the $t = 0$ axis, and a domain of the superfluid phase. The nature of the transition between incompressible and superfluid phases is still not understood.

A natural way to extend the Bose-Hubbard model is to introduce longer-range interactions between bosons. Let us consider the Hamiltonian defined on a d-dimensional lattice $\Lambda \subset \mathbb{Z}^\nu$ ($\nu \geqslant 2$) by

$$H_\Lambda = -t \sum_{<x,y>\subset\Lambda} (c_x^\dagger c_y + c_y^\dagger c_x) + U_0 \sum_{x\in\Lambda} \big(n_x^2 - n_x\big) + \sum_{k=1}^{\nu} U_k \sum_{\substack{\|x-y\|_2=\sqrt{k} \\ |x-y|\leqslant 1}} n_x n_y - \mu \sum_{x\in\Lambda} n_x. \tag{4.15}$$

The ground states are not difficult to find in two extremal cases, $t = 0$ and $t = \infty$ (i.e. setting all the couplings U_k to 0). The first case reduces to a problem of finding the ground states of a classical system. In the latter case, the bosons are independent and a Fourier transform diagonalizes the one-body Hamiltonian associated with the kinetic part; at zero temperature the particles exhibit a Bose-Einstein condensation.

In the case of large enough U_0 and $U_1 > 2U_2 > 0$, the zero-temperature phase diagram of the two-dimensional version of (4.15) is depicted in Fig. 4.4. The translation invariant

[1] The Indian name "Bose" has to be pronounced "Bosh"; we thank Nilanjana Datta for this crucial information. Please pay attention in the sequel to boshons and boshonic systems.

phases $\rho = n$ were also present for the on-site Bose-Hubbard model. Nearest neighbour interactions are responsible for the occurrence of chessboard phases (with $\rho = n + \frac{1}{2}$). These phases are not translation invariant — the system exhibits symmetry breaking. Finally, phases with quarter integer densities with alternating rows of density n and $n + \frac{1}{2}$ are present because of next nearest neighbour interactions.

It is interesting to discuss the degeneracy of the classical ($t = 0$) ground states of (4.15). While the integer and half integer phases have finite degeneracies, the quarter integer phases do not. Taking, e.g., the phase $\rho = 1/4$, there is alternatively an empty row without any boson and a row of staggered (antiferromagnetic) occupation pattern with 0 or 1 boson at each site. The degeneracy is roughly proportional to the exponential of $|\Lambda|^{\frac{1}{2}}$. Theorem 3.3 applies in the darker domains, where the number of classical ground states is finite. For quarter-integer densities, we can use Theorem 3.6, provided some hard-core is added to the model, in such a way to have finite single site phase space.

In three dimensions the model exhibits even more interesting degenerated phases. With well chosen parameters, the classical part of (4.15) has infinitely many ground states such that their restriction to any cube is a configuration of the following form (up to rotations and reflections)
Here all ground configurations have density 1/8. To evaluate their number, we can look at all the possibilities of putting blocks $3 \times 3 \times 3$ with one particle at the middle, in a given volume. There must be no intersection, and no empty space between the blocks. It is not clear how much possibilities there are; however, we can observe that given boundary conditions (i.e. with fixed boundaries of the volume), there is at most one way to make a covering without intersection nor empty space. This means that their total number does not grow faster than the exponential of the boundary of the volume. In other words, there is no residual entropy in this system.

For a different choice of parameters, the base cube is as follows,
The density is locked to 1/4 and the degeneracy is roughly proportional to the exponential of $|\Lambda|^{\frac{1}{3}}$.

At non-zero temperature we expect the degeneracy to be removed since a finite number of particular configurations of alternated staggered rows have lower excitation energy; this

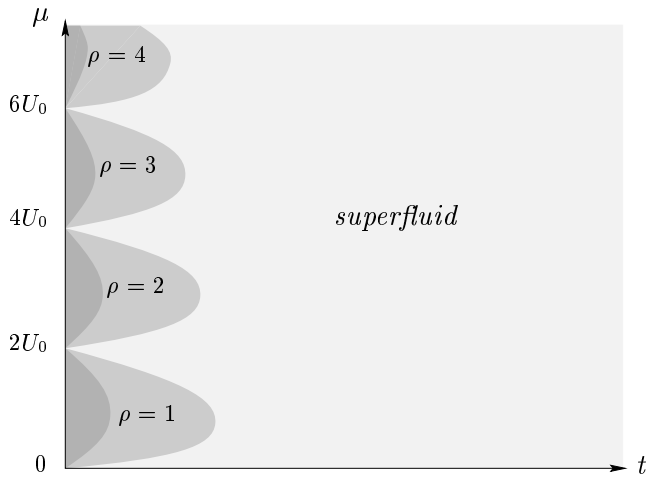


FIGURE 4.3. Zero temperature phase diagram for the Bose-Hubbard model in two dimensions. Lobes are incompressible phases with integer densities. Our results hold in darker regions near the $t = 0$ axis (and also for low temperatures).

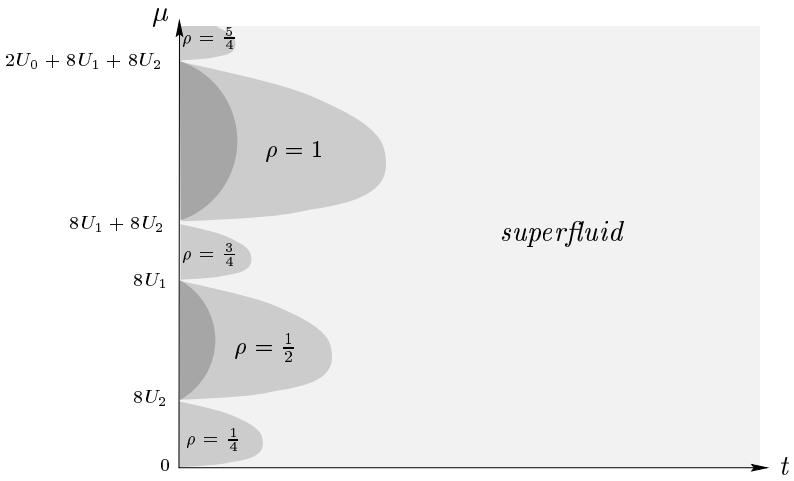
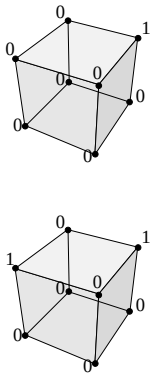


FIGURE 4.4. Zero temperature phase diagram for the Bose-Hubbard model in two dimensions with nearest and next nearest neighbour interactions. Incompressible (insulating) phases of given density are expected to exist in grey regions. In the darker regions the existence of such phases can be rigorously established.



theory of "dominating ground states" preferred by low energy fluctuations was presented in [BS 1989]. It seems here that selected phases have alternating empty planes, and chessboard of a given type. One should expect that they are stable against perturbations with a small hopping term. On the other hand, the effective potential from quantum fluctuations selects phases with alternating empty planes, and chessboard of alternating types.

If a coexistence surface separates the domain in the t, β plane where thermal fluctuations dominate from that where quantum fluctuations dominate, an interesting transition occurs, driven by the competition between two different kinds of fluctuations. Another possibility is that the transition goes through many other phases, maybe with a devil's staircase structure.

2.2. Results. We consider the two-dimensional case and make the following assumptions on the coupling constants.

$$U_0 > 4U_1 + 4U_2, \qquad U_1 > 2U_2 \geqslant 0 \tag{4.16}$$

For each $k \in \mathbb{N}$ consider the disjoint intervals

$$\begin{aligned} I_k &= \{\mu : (2U_0 + 8U_1 + 8U_2)k - 2U_0 < \mu < (2U_0 + 8U_1 + 8U_2)k\}, \\ H_k &= \{\mu : (2U_0 + 8U_1 + 8U_2)k + 8U_2 < \mu < (2U_0 + 8U_1 + 8U_2)k + 8U_1\}, \\ Q_k^{(1)} &= \{\mu : (2U_0 + 8U_1 + 8U_2)k < \mu < (2U_0 + 8U_1 + 8U_2)k + 8U_2\}, \\ Q_k^{(2)} &= \{\mu : (2U_0 + 8U_1 + 8U_2)k + 8U_1 < \mu < (2U_0 + 8U_1 + 8U_2)k + 8U_1 + 8U_2\}. \end{aligned}$$

The relevance of this decomposition is clear when comparing with the vertical axis of Fig. 4.4.

Hereafter we give two theorems. The first one for the existence of phases in the thermodynamic limit; we shall prove it in the sequel, using Theorem 3.4. The second theorem is about the incompressibility of the quantum ground states; it was proved in [BKU 1997]. These results do not cover the case of quarter densities, because of the degeneracies of the classical ground states; we shall study this situation in the next section. At high temperatures there is a unique translation invariant phase; the proof of this statement is in [PY 1995].

THEOREM 4.3. **Two-dimensional Bose-Hubbard model.**
Assume that the coupling constant satisfy the conditions (4.16). *Then for each* $\mu \in I_k$, *or* $\mu \in H_k$, *there exists* $t_0(\mu)$ *and* $\beta_0(\mu)$ *such that for* $\beta \geqslant \beta_0(\mu)$, $t \leqslant t_0(\mu)$,

- *if* $\mu \in I_k$, *there is a unique state that is close to the classical ground state* $|n\rangle^{(k)}$, *with* $n_x^{(k)} = k$ *for all* $x \in \mathbb{Z}^\nu$,
- *if* $\mu \in H_k$, *there are two states, each one being close to a chessboard configuration with* k *particles on each site of one sublattice, and* $k+1$ *particles on each site of the other sublattice.*

THEOREM 4.4. **Incompressibility of ground state.**
Assume that the coupling constant satisfy the conditions (4.16). *Then for each* $\mu \in I_k$, *or* $\mu \in H_k$, *there exists* $t_0(\mu)$ *and* $\beta_0(\mu)$ *such that for* $\beta \geqslant \beta_0(\mu)$, $t \leqslant t_0(\mu)$,

- *if* $\mu \in I_k$, *then*
$$\left|\langle n_x\rangle^{\beta,\mu} - k\right| \leqslant C\,\mathrm{e}^{-c\beta},$$
and
$$\left|\frac{\partial}{\partial\mu}\langle n_x\rangle^{\beta,\mu}\right| \leqslant C'\,\mathrm{e}^{-c'\beta}.$$
- *if* $\mu \in H_k$, *then for nearest neighbours* x, y,
$$\left|\langle \tfrac{1}{2}(n_x + n_y)\rangle^{\beta,\mu} - (k + \tfrac{1}{2})\right| \leqslant C\,\mathrm{e}^{-c\beta},$$
and
$$\left|\frac{\partial}{\partial\mu}\langle \tfrac{1}{2}(n_x + n_y)\rangle^{\beta,\mu}\right| \leqslant C'\,\mathrm{e}^{-c'\beta}.$$

The physical significance of the theorem may be more clear when considering the relation between density and pressure. Recall that $\frac{\partial\rho}{\partial\mu} = \rho\frac{\partial\rho}{\partial p}$ (fixed variables are the temperature and the volume). Then we can derive the existence of plateaux in the graph of Fig. 4.5.

This incompressibility theorem should not be mixed up with the uniform density theorem of [LLM 1993], although there is some overlap. The latter uses special symmetries of the system and shows uniformity of the density with respect to coupling constant *and temperature*, for a class of models of the Hubbard type (the "classical ground states" may

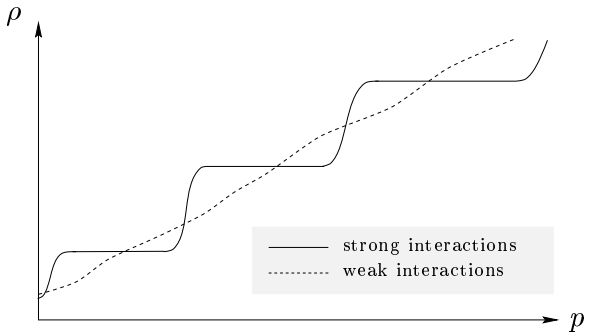


FIGURE 4.5. Graph of the density as a function of the pressure, at zero temperature (and in the case of the Bose-Hubbard model with only on-site interactions).

be infinitely degenerate). However, it is not uniform with respect to the chemical potential, because only for special values of the latter the system has the necessary symmetries; the compressibility coefficient does not vanish in general.

In the case of small hopping, there is one (or two) pure state with exponential decay of correlations. These states are thermodynamically stable against an external field $\sum_{x\in\Lambda}(c_x^\dagger + c_x)$, and therefore these phases are not superfluid. On the contrary, a system of free bosons without interactions features Bose-Einstein condensation. The situation here is analogous to Mott insulator transition in fermionic systems, where an insulating phase may appear because of the interactions between fermions — in contrast to the situation in band theory, where the insulating phase is due to an external periodic potential. So it is generally said that the Bose-Hubbard system forms a Mott insulator in the incompressible phase.[2]

PROOF OF THEOREM 4.3. Let us first establish the Peierls condition (2.12). The classical part of the (two-dimensional) Bose-Hubbard Hamiltonian (4.15) — with chemical potential — may be written as a block interaction over plaquettes of 4 sites,

$$\Phi_P(n_P) = \sum_{x\in P} \tfrac{1}{4}(U_0 n_x^2 - U_0 n_x - \mu n_x) + \tfrac{1}{2}U_1 \sum_{\substack{x,y\in P\\ |x-y|=1}} n_x n_y + U_2 \sum_{\substack{x,y\in P\\ |x-y|=\sqrt{2}}} n_x n_y. \qquad (4.17)$$

With k an integer we introduce new variables, $n_x = k + m_x$, and with $\Phi_P(k, m_P) = \Phi_P(n_P)$, a straightforward calculation leads to

$$\Phi_P(k, m_P) = C_k + \sum_{x\in P} \tfrac{1}{4}(U_0 m_x^2 - U_0 m_x - \mu_k m_x) + \tfrac{1}{2}U_1 \sum_{\substack{x,y\in P\\ |x-y|=1}} m_x m_y + U_2 \sum_{\substack{x,y\in P\\ |x-y|=\sqrt{2}}} m_x m_y, \qquad (4.18)$$

where we defined $C_k = \frac{1}{4}U_0(k^2 - k) - \frac{1}{4}\mu k + 4k^2(U_1 + U_2)$, and

$$\mu_k = \mu - (2U_0 + 8U_1 + 8U_2)k. \qquad (4.19)$$

In the following, we show that, for a given k,

a) if $\mu_k \in [-2U_0, 0]$, $m_P = \left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ minimizes $\Phi_P(k, m_P)$,

b) if $\mu_k \in [0, 8U_2]$, $m_P = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ (and the three obtained by rotation) minimizes $\Phi_P(k, m_P)$,

[2]We intentionally avoid the term "Mott insulating phase" because *stricto sensu* it is not a phase: the fact that a system can be considered to have Mott insulator behaviour depends actually on the chosen microscopic description.

c) if $\mu_k \in [8U_2, 8U_1]$, $m_P = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ (and the other obtained by rotation) minimizes $\Phi_P(k, m_P)$,

d) if $\mu_k \in [8U_1, 8U_1 + 8U_2]$, $m_P = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ (and the three obtained by rotation) minimizes $\Phi_P(k, m_P)$.

Clearly, from this and (4.19) we obtain the classical ground states for all $\mu \geqslant 0$ [and in the case $\mu < 0$, we see immediately in (4.17) that $n_x = 0$, for any x, minimizes $\Phi_P(k_P)$].

For the point a), let us introduce a such that $\mu_k = -2U_0(a + \frac{1}{2})$; it is easy to check that

$$\Phi_P(k, m_P) = C'_k + (\tfrac{1}{4}U_0 - U_1 - U_2) \sum_{x \in P} (m_x + a)^2 + \tfrac{1}{4}U_1 \sum_{\substack{x,y \in P \\ |x-y|=1}} (m_x + m_y + a)^2 + \tfrac{1}{2}U_2 \sum_{\substack{x,y \in P \\ |x-y|=\sqrt{2}}} (m_x + m_y + a)^2, \quad (4.20)$$

and this is minimum for $m_x = 0$, for any $x \in P$, when $a \in [-\frac{1}{2}, \frac{1}{2}]$, i.e. $\mu_k \in [-2U_0, 0]$.

Moreover, we obtain a Peierls condition if $\mu_k \neq -2U_0, 0$.

Point c) is similar; we define a such that $\frac{1}{4}\mu_k = U_1 + U_2 - 2a(U_1 - U_2)$; in this case

$$\Phi_P(k, m_P) = C''_k + (\tfrac{1}{4}U_0 - U_1 + U_2) \sum_{x \in P} (m_x - \tfrac{1}{2})^2 + (\tfrac{1}{4}U_1 - \tfrac{1}{2}U_2) \sum_{\substack{x,y \in P \\ |x-y|=1}} (m_x + m_y - 1 + a)^2 + U_2 \big(\sum_{x \in P} m_x - 2 + a \big)^2. \quad (4.21)$$

$\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ is ground state when $a \in [-\frac{1}{2}, \frac{1}{2}]$, i.e. $\mu_k \in [8U_2, 8U_1]$ (recall that $U_1 > 2U_2$). The Peierls condition is also straightforward.

Finally, we show that $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ is ground state for $\mu_k \in [0, 8U_2]$ and $\left(\begin{smallmatrix} -1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ for $\mu_k \in [-2U_0 - 8U_2, -2U_0]$. With $\varepsilon = +1$ in the first case and $\varepsilon = -1$ in the second case, we have

$$\Phi_P(k, m_P) = C^{\varepsilon}_k + (\tfrac{1}{4}U_0 - U_1 + U_2) \sum_{x \in P} (m_x - \tfrac{1}{2}\varepsilon)^2 + (\tfrac{1}{4}U_1 - \tfrac{1}{2}U_2) \sum_{\substack{x,y \in P \\ |x-y|=1}} (m_x + m_y - \tfrac{1}{2}\varepsilon)^2 + U_2 \big(\sum_{x \in P} m_x - \varepsilon + a \big)^2 \quad (4.22)$$

where $a = \frac{1}{2} - \mu_k/8U_2$ in the first case, and $a = -\frac{1}{2} - (\mu_k + 2U_0)/8U_2$ in the second case; the condition $a \in [-\frac{1}{2}, \frac{1}{2}]$ yields the intervals for μ_k.

Theorem 4.3 is then a consequence of Theorem 3.4.

□

2.3. Quarter integer densities and effective potential. We need a finite single site phase space when studying the quantum fluctuations. This is the reason why we choose $U_0 \to \infty$ in (4.15). This amounts to consider a new model with $\Omega = \{0, 1\}$ and with an interaction on plaquettes

$$\Phi_P(n_P) = \tfrac{1}{2}U_1 \sum_{\substack{x,y \in P \\ \|x-y\|_2=1}} n_x n_y + U_2 \sum_{\substack{x,y \in P \\ \|x-y\|_2=\sqrt{2}}} n_x n_y - \tfrac{1}{4}\mu \sum_{x \in P} n_x, \quad (4.23)$$

and $\Phi_A = 0$ if A is not a plaquette. When $0 < \mu < 8U_2$, we have from (4.22) that $\Phi_P(n_P)$ is minimum if $n_P = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$, or any configuration obtained from $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ by rotation. Hence we define

$$G = \left\{ n \in \{0,1\}^{\mathbb{Z}^2} : n_P \in \left\{ \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right), \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right), \left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right), \left(\begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix}\right) \right\} \text{ for any plaquette } P \right\}$$

(G is here the set of ground states of the interaction Φ). Since $\Phi_P(n_P) - \Phi_P(g_P) \geqslant \frac{1}{4}\min(\mu, 8U_2 - \mu)$, for any $n_P \notin G_P$, $g_P \in G_P$, Assumption 1 holds with $\Delta_0 = \frac{1}{36}\min(\mu, 8U_2 - \mu)$ and $\delta_0 = 0$ (the factor $\frac{1}{36}$, rather than $\frac{1}{4}$, has been chosen in view of Assumption 2, see below).

We take as sequence of transitions for the smallest quantum fluctuations

$$\mathcal{S} = \{(\boldsymbol{A}, \boldsymbol{A}') : \boldsymbol{A} = <x, y> \text{ and } \boldsymbol{A}' = <y, x> \text{ for some } x, y \in \mathbb{Z}^2, \|x - y\|_2 = 1\}.$$

The effective potential follows from (3.9). Let $\mathcal{P}_{xy} = \cup_{P \cap \{x,y\} \neq \varnothing} P$ and more generally we denote by $\mathcal{P}$ any 3×4 or 4×3 rectangle. Up to rotations and reflections, we have to take into account five configurations, namely

$$\begin{array}{ccccc} \begin{smallmatrix} 0&1&0 \\ 0&0&0 \\ 0&1&0 \\ 0&0&0 \end{smallmatrix} & \begin{smallmatrix} 0&1&0 \\ 0&0&0 \\ 1&0&1 \\ 0&0&0 \end{smallmatrix} & \begin{smallmatrix} 1&0&1 \\ 0&0&0 \\ 0&1&0 \\ 0&0&0 \end{smallmatrix} & \begin{smallmatrix} 1&0&1 \\ 0&0&0 \\ 1&0&1 \\ 0&0&0 \end{smallmatrix} & \begin{smallmatrix} 1&0&0 \\ 0&0&1 \\ 1&0&0 \\ 0&0&1 \end{smallmatrix} \\ g_{\mathcal{P}}^{(A)} & g_{\mathcal{P}}^{(B)} & g_{\mathcal{P}}^{(C)} & g_{\mathcal{P}}^{(D)} & g_{\mathcal{P}}^{(E)} \end{array}$$

We find $\Psi_{\mathcal{P}}(g_{\mathcal{P}}^{(A)}) = -t^2/2U_1$, $\Psi_{\mathcal{P}}(g_{\mathcal{P}}^{(C)}) = -t^2/4U_2$, and $\Psi_{\mathcal{P}}(g_{\mathcal{P}}^{(B)}) = \Psi_{\mathcal{P}}(g_{\mathcal{P}}^{(D)}) = \Psi_{\mathcal{P}}(g_{\mathcal{P}}^{(E)}) = 0$.

We can choose $R = \frac{3}{2}$; $U'(x)$ is a block 4×4 centered on $(x_1 + \frac{1}{2}, x_2 + \frac{1}{2})$. The configuration $g_{U'(x)} \in G_{U'(x)}$ are (up to rotations and reflections)

$$\begin{array}{cc} \begin{smallmatrix} 1&0&1&0 \\ 0&0&0&0 \\ 1&0&1&0 \\ 0&0&0&0 \end{smallmatrix} & \begin{smallmatrix} 1&0&1&0 \\ 0&0&0&0 \\ 0&1&0&1 \\ 0&0&0&0 \end{smallmatrix} \\ g_{U'(x)}^{(a)} & g_{U'(x)}^{(b)} \end{array}$$

We choose for Υ

$$\Upsilon_x(n_{U'(x)}) = \frac{1}{9} \sum_{P \subset U'(x)} \tilde{\Phi}_P(n_P) + \frac{1}{2} \sum_{\mathcal{P} \subset U'(x)} \Psi_{\mathcal{P}}(n_{\mathcal{P}}), \tag{4.24}$$

with $\tilde{\Phi}_P(n_P) = \Phi_P(n_P) - \min_{g \in G} \Phi_P(g_P)$. Which configurations, among the ones generated by $g^{(a)}$ and the ones generated by $g^{(b)}$, allows for more quantum fluctuations? The effective potential yields

$$\Upsilon_x(g_{U'(x)}^{(a)}) = -\frac{t^2}{2U_1}$$
$$\Upsilon_x(g_{U'(x)}^{(b)}) = -\frac{t^2}{4U_1} - \frac{t^2}{8U_2}.$$

We see that the set of dominant states D is formed by all the configurations generated by $g^{(b)}$ ($|D| = 8$). Heuristically, there is more freedom for the bosons to move in $g^{(b)}$, since they can go to a nearest-neighbour site and feel a small repulsion of strength U_2; as for bosons of the configuration $g^{(a)}$, any nearest-neighbour move brings them at distance 1 of another boson, and they feel a bigger repulsion U_1.

As a result we can choose $\Delta = t^2(\frac{1}{8U_2} - \frac{1}{4U_1})$ in Assumption 2. The maximum of the expression in Assumption 3 is $b_1 = t^2(\frac{1}{8U_2} - \frac{1}{4U_1})^{-1}$. In Assumption 4 $b_2 = 0$, because $g \neq g'$ means that g and g' must differ on a whole row, and the matrix element is zero for any finite m.

These eight dominant states bring eight pure periodic phases, $\langle\cdot\rangle^{(1)}, \ldots, \langle\cdot\rangle^{(8)}$; each one can be constructed by adding a suitable field in the Hamiltonian (e.g. the projector onto the dominant state).

THEOREM 4.5. **Hard-core Bose-Hubbard model.**
Consider the hard-core Bose-Hubbard model on the lattice $\mathbb{Z}^2$, and suppose $U_1 > 2U_2$ and $0 < \mu < 8U_2$. There exist $t_0 > 0$ and $\beta_0(t) < \infty$ ($\lim_{t\to 0} \beta_0(t) = \infty$) such that if $t \leqslant t_0$ and $\beta \geqslant \beta_0$,

- *the free energy exists in the thermodynamic limit with periodic boundary conditions, as well as expectation values of observables,*
- *there are 8 pure periodic phases with exponential decay of correlations.*

Each of these eight phases is a perturbation of a dominant state d, and the expectation value of any operator is close to its value in the state d, see Theorem 3.6 for more precise statement.

CHAPTER 5

Cluster expansions

Cluster expansions (or swarm expansions[1]) appeared in Statistical Physics in the 30's (see Chapter 3 of [Pfi 1991] and references therein) — we met the works of Mayer and collaborators in the prolog. Its use in classical lattice systems began with the study of polymer models [Kunz 1971]. A proof of the convergence of the cluster expansion was given by Gruber and Kunz [GK 1971]. We present two approaches. The first one is inspired by Kotecký and Preiss [KP 1986]; a nice feature consists in its independence with respect to detailed properties of the bees. The proof of Proposition 5.1 that we give here is due to Dobrushin [Dob 1994]. The second approach follows Pfister [Pfi 1991], himself following Brydges' lectures [Bry 1986]. It allows for a continuous set of bees.

The bees sting, but also produce honey; similarly the swarm expansion is rather painful, but brings very nice results in Statistical Physics. We shall see later in this chapter that in all reasonable lattice models, a unique thermodynamic phase exists at high temperature.[2] All the perturbative approach to the theory of first order phase transitions (the Pirogov-Sinai theory) is actually based on cluster expansions — even though we shall see in Chapter 6 that it is certainly more than just an application.

1. The hive or the abstract polymer model

Let $\mathbb{B}$ be the *hive*, i.e. the set of bees, that we suppose to be finite. A reflexive and symmetric relation ι is given on $\mathbb{B}$; we say that $b, b' \in \mathbb{B}$ are *incompatible* if $b \iota b'$, otherwise they are *compatible*. A set of bees $B \subset \mathbb{B}$ is called *admissible* if its elements are mutually compatible. The partition function of a hive $\mathbb{B}$ is

$$Z(\mathbb{B}) = \sum_{\substack{B \subset \mathbb{B} \\ B \text{ admissible}}} \prod_{b \in B} w(b) \tag{5.1}$$

where $w : \mathbb{B} \to \mathbb{C}$ is called the *weight* of the bee b. If $\mathbb{B} = \varnothing$, we set $Z(\varnothing) = 1$.

Let $C = (b_1, \dots, b_n)$, $b_j \in \mathbb{B}$, and consider the graph $\mathcal{G}(C)$ with n vertices and with an edge between different vertices i and j whenever $b_i \iota b_j$. C is a *swarm*, or a *cluster*, if $\mathcal{G}(C)$ is connected. Then if the weights $w(b)$ are small enough, we have the following expansion.

[1] The name "swarm expansion" is the English translation of "développement en essaims", the French expression for "cluster expansion". Hence bees and hives. As for Dobrushin, he chose to expand animals and herds of animals, and he obtained gangs of animals [Dob 1994].

[2] Typical results of cluster expansions are the analyticity of free energies; but they also find a use in probability theory, to prove e.g. central limit theorems. Assumptions can be weakened in this situation [FFG 1998].

PROPOSITION 5.1. **Swarm expansion.**
Let $w_0, v : \mathbb{B} \to \mathbb{R}_+$ two positive functions on bees, with $w_0(b) > 0$ for all $b \in \mathbb{B}$, and assume the following inequality:

$$1 - w_0(b) \exp\Big\{ \sum_{\substack{b' \in \mathbb{B} \\ b' \iota b, b' \neq b}} w_0(b') v(b') \Big\} \;\geqslant\; \mathrm{e}^{-w_0(b) v(b)} \tag{5.2}$$

for any $b \in \mathbb{B}$; then if $|w(b)| \leqslant w_0(b)$ for all $b \in \mathbb{B}$, we have

$$\log Z(\mathbb{B}) = \sum_{C=(b_1,\dots,b_n),\, b_j \in \mathbb{B}} \Phi^{\mathrm{T}}(C), \tag{5.3}$$

and $\Phi^{\mathrm{T}}(C)$ satisfies the bound

$$|\Phi^{\mathrm{T}}(C)| \;\leqslant\; \sum_{j=1}^{n} w_0(b_j) v(b_j) \prod_{j=1}^{n} \frac{|w(b_j)|}{w_0(b_j)}. \tag{5.4}$$

Before proving Proposition 5.1, we establish a useful lemma.[3]

LEMMA 5.2.
If the inequality (5.2) is valid, then

$$\Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B}')} \Big| \;\leqslant\; \sum_{b \in \mathbb{B} \setminus \mathbb{B}'} w_0(b) v(b) \tag{5.5}$$

for any finite $\mathbb{B}, \mathbb{B}'$ with $\mathbb{B}' \subset \mathbb{B}$.

PROOF. By induction on the number of elements in $\mathbb{B}$. The lemma clearly holds if $\mathbb{B} = \varnothing$ or if $\mathbb{B}' = \mathbb{B}$. Otherwise there exists at least one bee $b_0 \in \mathbb{B} \setminus \mathbb{B}'$.

$$\Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B}')} \Big| = \Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B} \setminus \{b_0\})} \frac{Z(\mathbb{B} \setminus \{b_0\})}{Z(\mathbb{B}')} \Big| \;\leqslant\; \Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B} \setminus \{b_0\})} \Big| + \Big| \log \frac{Z(\mathbb{B} \setminus \{b_0\})}{Z(\mathbb{B}')} \Big|. \tag{5.6}$$

From the induction assumption,

$$\Big| \log \frac{Z(\mathbb{B} \setminus \{b_0\})}{Z(\mathbb{B}')} \Big| \;\leqslant\; \sum_{\substack{b \in \mathbb{B} \setminus \mathbb{B}' \\ b \neq b_0}} w_0(b) v(b); \tag{5.7}$$

the lemma is proved if we can show that

$$\Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B} \setminus \{b_0\})} \Big| \;\leqslant\; w_0(b_0) v(b_0). \tag{5.8}$$

From the definition (5.1) of the partition function, we have

$$Z(\mathbb{B}) = Z(\mathbb{B} \setminus \{b_0\}) + w(b_0) Z(\mathbb{B}_0) \tag{5.9}$$

with $\mathbb{B}_0 \subset \mathbb{B} \setminus \{b_0\}$ the set of all bees compatible with b_0. Therefore

$$\Big| \log \frac{Z(\mathbb{B})}{Z(\mathbb{B} \setminus \{b_0\})} \Big| = \Big| \log \Big(1 + w(b_0) \frac{Z(\mathbb{B}_0)}{Z(\mathbb{B} \setminus \{b_0\})} \Big) \Big|. \tag{5.10}$$

[3] The lemma is slightly stronger than the one of [Dob 1994] and *is needed so* in the proof of Proposition 5.1. This was pointed out by Kotecký.

The induction assumption implies

$$\Big|w(b_0)\frac{Z(\mathbb{B}_0)}{Z(\mathbb{B}\setminus\{b_0\})}\Big| \;\leqslant\; w_0(b_0)\exp\Big\{\sum_{\substack{b\in\mathbb{B}\\ b\imath b_0, b\neq b_0}} w_0(b)v(b)\Big\} < 1 \tag{5.11}$$

[the last term is strictly smaller than 1 because of (5.2)]. For any $z, z_0 \in \mathbb{C}$, $|z| \leqslant |z_0| < 1$, it is not hard to check that (for the first inequality, simply expand the logarithm with Taylor series)

$$\big|\log(1+z)\big| \;\leqslant\; -\log(1-|z|) \;\leqslant\; -\log(1-|z_0|).$$

As a consequence

$$\Big|\log\frac{Z(\mathbb{B})}{Z(\mathbb{B}\setminus\{b_0\})}\Big| \;\leqslant\; -\log\Big(1-\,w_0(b_0)\exp\Big\{\sum_{b\imath b_0} w_0(b)v(b)\Big\}\Big) \tag{5.12}$$

and the RHS is smaller than $w_0(b_0)v(b_0)$ because of (5.2). □

Proof of Proposition 5.1. $\log Z(\mathbb{B})$ may be viewed as a function of the numbers $w(b)$, $b \in \mathbb{B}$. More precisely, let $\boldsymbol{w} = (w(b))_{b\in\mathbb{B}}$, and

$$\begin{aligned} F_{\mathbb{B}}(\boldsymbol{w}) : \mathcal{U} = \big\{w(b)\in\mathbb{C} : |w(b)| \;\leqslant\; w_0(b)\big\} &\to \mathbb{C}\\ \boldsymbol{w} &\mapsto F_{\mathbb{B}}(\boldsymbol{w}) = \log \sum_{\substack{B\subset\mathbb{B}\\ B \text{ admissible}}} \prod_{b\in B} w(b). \end{aligned} \tag{5.13}$$

$F_{\mathbb{B}}$ is the logarithm of a polynomial in $\{w(b), b\in\mathbb{B}\}$ which has no zero in $\mathcal{U}$ because of Lemma 5.2. Therefore $F_{\mathbb{B}}$ is holomorphic and we can write its Taylor serie:

$$F_{\mathbb{B}}(\boldsymbol{w}) = \sum_{n\geqslant 1}\sum_{b_1,\dots,b_n\in\mathbb{B}} \frac{1}{n!}\varphi^{\mathrm{T}}(b_1,\dots,b_n)\prod_{j=1}^{n} w(b_j) \tag{5.14}$$

with

$$\varphi^{\mathrm{T}}(b_1,\dots,b_n) = \Big\{\prod_{j=1}^{n}\frac{\partial}{\partial w(b_j)}\Big\}F_{\mathbb{B}}(\boldsymbol{w})\Big|_{\boldsymbol{w}=0}. \tag{5.15}$$

Let us see that $\varphi^{\mathrm{T}}(b_1,\dots,b_n)$ is zero if $(b_1,\dots,b_n)$ is not a cluster. Let $B = \{b_1,\dots,b_n\}$ ($|B| < n$ if $(b_1,\dots,b_n)$ contains many times a same bee) and decompose $B = B_1 \cup B_2$, $B_1, B_2 \neq \varnothing$, in such a way that any element of B_1 is compatible with any element of B_2. Observe that we can substitute $F_{\mathbb{B}}(\boldsymbol{w})$ by $F_B(\boldsymbol{w})$ in (5.15), and that from (5.13),

$$F_B(\boldsymbol{w}) = F_{B_1}(\boldsymbol{w}) + F_{B_2}(\boldsymbol{w}).$$

Since $F_{B_1}(\boldsymbol{w})$ does not depend on $\{w(b) : b\in B_2\}$, its contribution vanishes in (5.15); the same with $F_{B_2}(\boldsymbol{w})$.

Finally, the bound (5.4) can be obtained by the use of Cauchy formula. Let α_b denote the number of occurences of b in $(b_1,\dots,b_n)$; then

$$\varphi^{\mathrm{T}}(b_1,\dots,b_n) = \frac{1}{n!}\Big\{\prod_{b\in B}\frac{\alpha_b!}{2\pi\mathrm{i}}\oint_{|w(b)|=w_0(b)}\frac{\mathrm{d}w(b)}{w(b)^{\alpha_b+1}}\Big\}F_B(\boldsymbol{w}). \tag{5.16}$$

Using Lemma 5.2, we get

$$|F_B(\boldsymbol{w})| \;\leqslant\; \sum_{b\in B} w_0(b)v(b). \tag{5.17}$$

Taking the modulus in the integrals, we find the bound (5.4). □

2. The polymer expansion

The previous approach is beautifully abstract and the proof is very elegant. It has however an important limitation: the set of bees must be finite, while we shall face a continuous one in Chapter 8. So we present an alternate theory of swarm expansion, that we refer to as the *polymer expansion*. It is mostly a simplification of the Chapter 3 of [Pfi 1991]: we restrict to the case where the polymers interact only through a condition of non-intersection (hard-core). Let $\mathbb{X}$ the space of polymers. We note $\xi \in \mathbb{X}$ a polymer, and suppose that a measure has been defined on $\mathbb{X}$; if $f : \mathbb{X} \to \mathbb{C}$ is a measureable function, we write $\int_{\mathbb{X}} \mathrm{d}\xi\, f(\xi)$ the integral of f with this measure. $\mathbb{T} \subset \mathbb{R}^\nu$ is a discrete or continuous subset of $\mathbb{R}^\nu$, with a notion of *connectedness*; if $A, B \subset \mathbb{T}$, we note $A \Cap B$ the property "$A \cup B$ is connected".

The polymers have a *support* $\operatorname{Supp}\xi \subset \mathbb{T}$ and a *length* $|\xi| > 0$ (the bees had not), and a weight $w : \mathbb{X} \to \mathbb{C}$.

As before, we write $C = (\xi_1, \dots, \xi_n)$, $\xi_j \in \mathbb{X}$; $\operatorname{Supp} C = \cup_{\xi \in C} \operatorname{Supp}\xi$ and $|C| = \sum_{\xi \in C} |\xi|$. $\mathcal{G}(C)$ is the graph with n vertices and with an edge between different vertices i and j whenever $\operatorname{Supp}\xi_i \Cap \operatorname{Supp}\xi_j$. C is a cluster whenever $\mathcal{G}(C)$ is connected. We define the truncated function $\Phi^{\mathrm{T}}(C)$ by

$$\Phi^{\mathrm{T}}(C) = \frac{1}{n!} \varphi^{\mathrm{T}}(\mathcal{G}(C)) \prod_{j=1}^{n} w(\xi_j) \tag{5.18}$$

with

$$\varphi^{\mathrm{T}}(\mathcal{G}(C)) = \begin{cases} 1 & \text{if } n = 1 \\ \sum_{\mathcal{G}} \prod_{e(i,j) \in \mathcal{G}} \Big(- \mathbb{I}\left[\operatorname{Supp}\xi_i \Cap \operatorname{Supp}\xi_j \right] \Big) & \text{if } n \geqslant 2, \end{cases} \tag{5.19}$$

where the sum is over all connected graphs $\mathcal{G}$ of n vertices. Notice that $\Phi^{\mathrm{T}}(C) = 0$ whenever C is not a cluster. It is natural to conjecture that $\varphi^{\mathrm{T}}(\mathcal{G}(C)) = \varphi^{\mathrm{T}}(\xi_1, \dots, \xi_n)$ introduced in (5.15).

We start with a proposition that gives the polymer expansion in the simple case where the polymers are connected subsets of $\mathbb{Z}^\nu$. Here $\mathbb{T} = \mathbb{Z}^\nu$, $\operatorname{Supp}\xi = \xi$, and $|\xi| = |\operatorname{Supp}\xi|$.

Proposition 5.3. **Polymer expansion.**
Let $\Lambda \subset \mathbb{Z}^\nu$, $|\Lambda| < \infty$, and $\mathbb{X}(\Lambda) = \{\xi \subset \Lambda : \xi$ connected$\}$. A complex function $w : \mathbb{X}(\Lambda) \to \mathbb{C}$ is given, that satisfies

$$|w(\xi)| \leqslant \mathrm{e}^{-\gamma|\xi|}. \tag{5.20}$$

Then if $\gamma > 2\nu + \log 2$, we have

$$\log \sum_{\substack{\{\xi_1, \dots, \xi_n\} \\ \xi_j \subset \Lambda, \xi_i \not\Cap \xi_j}} \prod_{j=1}^{n} w(\xi_j) = \sum_{\substack{C = (\xi_1, \dots, \xi_n) \\ \xi_j \subset \Lambda}} \Phi^{\mathrm{T}}(C) \tag{5.21}$$

with $\Phi^{\mathrm{T}}(C)$ the truncated function defined in (5.18).

For any $c < \infty$ and $\delta > 0$ there exists $\gamma_0 < \infty$ (depending on ν, c and δ) such that if $\gamma \geqslant \gamma_0$,

$$\sum_{C, \operatorname{Supp} C \ni x} |\Phi^{\mathrm{T}}(C)|\, \mathrm{e}^{c|C|} \leqslant \delta \tag{5.22}$$

for any $x \in \mathbb{Z}^\nu$.

Suppose furthermore that w depends on a parameter $\boldsymbol{\mu} \in \mathcal{U} \subset \mathbb{R}^p$, $w \equiv w^{\boldsymbol{\mu}}$, and that we have a bound on the derivatives

$$\Big|\frac{\partial}{\partial \mu_i} w^{\boldsymbol{\mu}}(\xi)\Big| \;\leqslant\; \mathrm{e}^{-(\gamma-1)|\xi|}, \qquad 1 \;\leqslant\; i \;\leqslant\; p. \tag{5.23}$$

Then for any $c < \infty$ and $\delta > 0$ there exists $\gamma_0 < \infty$ (depending on ν, c and δ) such that if $\gamma \;\geqslant\; \gamma_0$,

$$\sum_{C, \mathrm{Supp}\, C \ni x} \Big|\frac{\partial}{\partial \mu_i} \Phi^{\mathrm{T}}(C)\Big| \, \mathrm{e}^{c|C|} \;\leqslant\; \delta \tag{5.24}$$

for any $x \in \mathbb{Z}^\nu$.

When considering the exponential decay of correlation functions, and in many other situations, one may have to estimate a sum over clusters with length bigger than a number ℓ. From (5.22) we obtain

$$\begin{aligned} \sum_{C, \mathrm{Supp}\, C \ni x, |C| \,\geqslant\, \ell} |\Phi^{\mathrm{T}}(C)| \;&\leqslant\; \mathrm{e}^{-c\ell} \sum_{C, \mathrm{Supp}\, C \ni x} |\Phi^{\mathrm{T}}(C)| \, \mathrm{e}^{c|C|} \\ &\leqslant\; \delta \, \mathrm{e}^{-c\ell}, \end{aligned} \tag{5.25}$$

for any $c < \infty$ and $\delta > 0$, by choosing γ large enough (depending on c and δ, but not on ℓ).

Actually, the motivation to state Proposition 5.3, that is equivalent to Proposition 5.1, is double. First because we shall use it when dealing with contour models, second because its proof follows from the more abstract Proposition 5.4, that we can now better understand.

Proposition 5.4. **Generalized polymer expansion.**
Let $\mathbb{X}$ be a measurable space of polymers, and $w : \mathbb{X} \to \mathbb{C}$ the weight. Assume that the weight is measurable, as well as the indicator function $\mathbb{I}\big[\mathrm{Supp}\, \xi_i \Cap \mathrm{Supp}\, \xi_j\big]$. Define $\Phi^{\mathrm{T}}(C)$ by (5.18) and (5.19), and write $\int \mathrm{d}C \equiv \sum_{n \,\geqslant\, 1} \int_{\mathbb{X}^n} \mathrm{d}\xi_1 \dots \mathrm{d}\xi_n$. Then if

$$\int \mathrm{d}C |\Phi^{\mathrm{T}}(C)| < \infty, \tag{5.26}$$

we have the polymer expansion, that is,

$$\exp\Big(\int \mathrm{d}C \Phi^{\mathrm{T}}(C)\Big) = 1 + \sum_{n \,\geqslant\, 1} \frac{1}{n!} \int_{\mathbb{X}^n} \mathrm{d}\xi_1 \dots \mathrm{d}\xi_n \Big[\prod_{j=1}^n w(\xi_j)\Big] \prod_{i<j} \mathbb{I}\big[\mathrm{Supp}\, \xi_i \not\Cap \mathrm{Supp}\, \xi_j\big]. \tag{5.27}$$

This proposition will be useful in Chapter 8, in a situation with more complicated polymers than just subsets of $\Lambda \subset \mathbb{Z}^\nu$.

Proof. We start with the RHS of (5.27). Since

$$\mathbb{I}\big[\mathrm{Supp}\, \xi_i \not\Cap \mathrm{Supp}\, \xi_j\big] = 1 - \mathbb{I}\big[\mathrm{Supp}\, \xi_i \Cap \mathrm{Supp}\, \xi_j\big],$$

we have

$$\prod_{1 \,\leqslant\, i<j \,\leqslant\, n} \mathbb{I}\big[\mathrm{Supp}\, \xi_i \not\Cap \mathrm{Supp}\, \xi_j\big] = \sum_{\mathcal{G}} \prod_{e(i,j) \in \mathcal{G}} \big(-\mathbb{I}\big[\mathrm{Supp}\, \xi_i \Cap \mathrm{Supp}\, \xi_j\big]\big) \tag{5.28}$$

where the sum is over all graphs of n vertices, not necessarily connected. We can decompose $\mathcal{G}$ into connected components, namely $\mathcal{G} = \{\mathcal{G}_1, \dots, \mathcal{G}_k\}$; $\mathcal{G}_\ell$, $1 \leqslant \ell \leqslant k$, is a connected graph with m_ℓ vertices, and $m_1 + ... + m_\ell = n$.

The RHS of (5.27) can be rewritten

$$... = 1 + \sum_{n \geqslant 1} \frac{1}{n!} \sum_{k=1}^{n} \frac{1}{k!} \sum_{(\mathcal{G}_1,\dots,\mathcal{G}_k)} \prod_{\ell=1}^{k} \int \mathrm{d}\xi_1^\ell \dots \mathrm{d}\xi_{m_\ell}^\ell \Big[\prod_{j=1}^{m_\ell} w(\xi_j^\ell)\Big] \prod_{e(i,j)\in\mathcal{G}_\ell} \big(-\mathbb{I}\left[\operatorname{Supp}\xi_i \Cap \operatorname{Supp}\xi_j\right]\big). \quad (5.29)$$

The sum over seqences $(\mathcal{G}_1, \dots, \mathcal{G}_k)$ can be done by first summing over $m_1, \dots, m_k$ with $m_1 + ... + m_\ell = n$; next by partitionning $\{1, 2, \dots, n\}$ into k sets with $m_1, \dots, m_k$ elements (there are $\frac{n!}{m_1!...m_k!}$ different partitions); then by summing over connected graphs in each set. Therefore

$$\begin{aligned} \dots &= 1 + \sum_{n \geqslant 1} \frac{1}{n!} \sum_{k=1}^{n} \frac{1}{k!} \sum_{\substack{m_1,\dots,m_k \geqslant 1 \\ m_1+\dots+m_k=n}} \frac{n!}{m_1! \dots m_k!} \prod_{\ell=1}^{k} \int \mathrm{d}\xi_1^\ell \dots \mathrm{d}\xi_{m_\ell}^\ell \\ &\qquad \Big[\prod_{j=1}^{m_\ell} w(\xi_j^\ell)\Big] \sum_{\mathcal{G}_\ell} \prod_{e(i,j)\in\mathcal{G}_\ell} \big(-\mathbb{I}\left[\operatorname{Supp}\xi_i \Cap \operatorname{Supp}\xi_j\right]\big) \\ &= 1 + \sum_{k \geqslant 1} \frac{1}{k!} \Big\{ \sum_{m \geqslant 1} \int \mathrm{d}\xi_1 \dots \mathrm{d}\xi_m \Phi^{\mathrm{T}}(\xi_1, \dots, \xi_m) \Big\}^k \end{aligned} \quad (5.30)$$

where we have used the definitions (5.18) and (5.19). We get the LHS of (5.27).

It s clear that all these expressions are convergent: condition (5.26) implies absolute convergence of the series in n of (5.30), and the same with (5.29) and (5.27).

□

In view of the proof of Proposition 5.3, we need a lemma.

LEMMA 5.5.

$$0 \leqslant (-1)^{n-1} \varphi^{\mathrm{T}}(\mathcal{G}(C)) \leqslant \sum_{\mathcal{T}:\text{tree of } n \text{ vertices}} \prod_{e(i,j)\in\mathcal{T}} \mathbb{I}\left[\operatorname{Supp}\xi_i \Cap \operatorname{Supp}\xi_j\right].$$

As a consequence, $|\varphi^{\mathrm{T}}(\mathcal{G}(C))| \leqslant n^{n-2}$, *since* n^{n-2} *is the number of trees with* n *vertices.*

PROOF. In this proof we consider only graphs with n vertices, and the notation $\mathcal{G} \subset \mathcal{G}'$ means that the set of edges of $\mathcal{G}$, is a subset of the set of edges of $\mathcal{G}'$.

The following property is true: to any tree $\mathcal{T}$ we can associate a graph $\mathcal{G}^*(\mathcal{T})$ such that

- $\mathcal{G}^*(\mathcal{T}) \supset \mathcal{T}$;
- the sets $\mathcal{E}(\mathcal{T}) = \{\mathcal{G} : \mathcal{T} \subset \mathcal{G} \subset \mathcal{G}^*(\mathcal{T})\}$ constitute a partition of the set of all connected graphs.

This can be proven by defining a procedure that attributes a tree to each connected graph, by deleting some edges [Pen 1967, Pfi 1991].

The sum over all connected graphs in (5.19) can be done by first summing over trees $\mathcal{T}$, then summing over graphs in $\mathcal{E}(\mathcal{T})$.

$$\begin{aligned}\varphi^{\mathrm{T}}(\mathcal{G}(C)) &= \sum_{\mathcal{T}} \sum_{\mathcal{G}\in\mathcal{E}(\mathcal{T})} \prod_{e(i,j)\in\mathcal{G}} \big(-\mathbb{I}\left[\mathrm{Supp}\,\xi_i \Subset \mathrm{Supp}\,\xi_j\right]\big) \\ &= \sum_{\mathcal{T}} \prod_{e(i,j)\in\mathcal{T}} \big(-\mathbb{I}\left[\mathrm{Supp}\,\xi_i \Subset \mathrm{Supp}\,\xi_j\right]\big) \prod_{e(i,j)\in\mathcal{G}^*(\mathcal{T})\setminus\mathcal{T}} \big(1-\mathbb{I}\left[\mathrm{Supp}\,\xi_i \Subset \mathrm{Supp}\,\xi_j\right]\big).\end{aligned} \tag{5.31}$$

The bound is clear, since the last product is smaller or equal to 1.

□

Proof of Proposition 5.3. It is enough to prove the last two claims, since (5.21) follows from (5.22) with $c = 0$ and Proposition 5.4.

We estimate (5.22) using the Lemma 5.5.

$$\sum_{C,\mathrm{Supp}\,C\ni x} |\Phi^{\mathrm{T}}(C)|\,\mathrm{e}^{c|C|} \;\leqslant\; \sum_{n\geqslant 1} \sum_{\substack{\xi_1,\dots,\xi_n \\ \xi_1\ni x}} \frac{1}{(n-1)!}\Big(\prod_{j=1}^{n} \mathrm{e}^{-(\gamma-c)|\xi_j|}\Big) \sum_{\mathcal{T}} \prod_{e(i,j)\in\mathcal{T}} \mathbb{I}\left[\xi_i \Subset \xi_j\right]. \tag{5.32}$$

Let $i_1, \dots, i_n$ the incidence numbers of a tree with n vertices. We first proceed with the summation over polymers $k \neq 1$ for which $i_k = 1$; in the tree $\mathcal{T}$, k shares an edge with a vertex m, and this means that $\xi_k \Subset \xi_m$, so that we find a bound

$$\sum_{\xi_k:\xi_k\Subset\xi_m} \mathrm{e}^{-(\gamma-c)|\xi_k|} \;\leqslant\; 2\nu|\xi_m| \sum_{\xi_k\ni x} \mathrm{e}^{-(\gamma-c)|\xi_k|}. \tag{5.33}$$

Then

$$\begin{aligned}&\sum_{C,\mathrm{Supp}\,C\ni x} |\Phi^{\mathrm{T}}(C)|\,\mathrm{e}^{c|C|} \;\leqslant \\ &\leqslant \sum_{n\geqslant 1} \frac{1}{(n-1)!} \sum_{\mathcal{T}} \Big(\sum_{\xi_1\ni x} (2\nu|\xi_1|)^{i_1}\,\mathrm{e}^{-(\gamma-c)|\xi_1|}\Big) \prod_{j=2}^{n} \Big(\sum_{\xi_j\ni x} (2\nu|\xi_j|)^{i_j-1}\,\mathrm{e}^{-(\gamma-c)|\xi_j|}\Big).\end{aligned} \tag{5.34}$$

The sum over trees $\mathcal{T}$ can be done by first choosing the incidence numbers, then summing over the trees. There are

$$\frac{(n-2)!}{(i_1-1)!\dots(i_n-1)!} \;\leqslant\; \frac{(n-1)!}{i_1!(i_2-1)!\dots(i_n-1)!}$$

trees with incidence numbers $i_1, \dots\ i_n$. Summing now over the incidence numbers, we get

$$\sum_{C,\mathrm{Supp}\,C\ni x} |\Phi^{\mathrm{T}}(C)|\,\mathrm{e}^{c|C|} \;\leqslant\; \sum_{n\geqslant 1} \Big(\sum_{\xi\ni x} \mathrm{e}^{-(\gamma-c-2\nu)|\xi|}\Big)^n. \tag{5.35}$$

From (2.1), we have

$$\sum_{\xi\ni x} \mathrm{e}^{-(\gamma-c-2\nu)|\xi|} \;\leqslant\; \frac{\mathrm{e}^{-(\gamma-c-2\nu)\,\beth}}{1-\mathrm{e}^{-(\gamma-c-2\nu)\,\beth}} \;\doteqdot\; \varepsilon. \tag{5.36}$$

ε can be put as small as necessary by taking γ large enough; this proves the bound (5.22). To prove (5.21), we take $c = 0$ and $\varepsilon < 1$; this brings the condition $\gamma > 2\nu + \log 2\beth$.

The bound (5.24) may be proven in the same way; since

$$\frac{\partial}{\partial\mu_i}\Phi^{\mathrm{T}}(C) = \frac{1}{n!}\varphi^{\mathrm{T}}(\mathcal{G}(C))\sum_{j=1}^{n}\Big[\prod_{k\neq j} w(\xi_k)\Big]\frac{\partial}{\partial\mu_i}w(\xi_j), \tag{5.37}$$

we have

$$\Big|\frac{\partial}{\partial\mu_i}\Phi^{\mathrm{T}}(C)\Big| \;\leqslant\; \frac{1}{(n-1)!}|\varphi^{\mathrm{T}}(\mathcal{G}(C))|\prod_{j=1}^{n}\mathrm{e}^{-(\gamma-1)|\xi_j|}\,. \tag{5.38}$$

Retracing the steps leading to the first bound, we arrive at

$$\sum_{C,\mathrm{Supp}\,C\ni x}\Big|\frac{\partial}{\partial\mu_i}\Phi^{\mathrm{T}}(C)\Big|\,\mathrm{e}^{c|C|} \;\leqslant\; \sum_{n\,\geqslant\,1} n\Big(\sum_{\xi\ni x}\mathrm{e}^{-(\gamma-c-1-2\nu)|\xi|}\Big)^n \tag{5.39}$$

and since $\sum_{n\,\geqslant\,1} n\varepsilon^n = \varepsilon/(1-\varepsilon)^2$, we obtain the bound if γ is large enough.

□

3. High temperature expansions

We prove Theorem 3.1 by means of high temperature expansions. The idea is to obtain a convergent expansion for the free energy in terms of clusters, with a weight that is analytic in β and $\boldsymbol{\mu}$.

$$Z_\Lambda = \mathrm{Tr}\;\mathrm{e}^{-\beta\sum_{A\subset\Lambda}T_A^{\boldsymbol{\mu}}} = \sum_{m\,\geqslant\,0}\sum_{A_1,\dots,A_m\subset\Lambda}\frac{(-\beta)^m}{m!}\,\mathrm{Tr}_{\mathcal{H}_\Lambda}\,T_{A_1}^{\boldsymbol{\mu}}\dots T_{A_m}^{\boldsymbol{\mu}}. \tag{5.40}$$

To each choice of $A_1,\dots A_m$ corresponds a choice of k connected, disjoint sets $\mathcal{A}_1,\dots,\mathcal{A}_k$. We first sum over sets $\{\mathcal{A}_i\}$, then over compatible $\{A_j\}$; observing that $[T_{A_i},T_{A_j}]=0$ when $A_i\subset\mathcal{A}_k$, $A_j\subset\mathcal{A}_\ell$ and $k\neq\ell$, we find

$$\begin{aligned} Z_\Lambda = \sum_{\substack{\{\mathcal{A}_1,\dots,\mathcal{A}_k\}\\ \mathcal{A}_i\not\sim\mathcal{A}_j}}\;\sum_{m_1\,\geqslant\,1}\;\sum_{\substack{A_1^1,\dots,A_{m_1}^1\\ \cup_i A_i^1=\mathcal{A}_1}}\;\dots\;\sum_{m_k\,\geqslant\,1}\;\sum_{\substack{A_1^k,\dots,A_{m_k}^k\\ \cup_i A_i^k=\mathcal{A}_k}} \\ \frac{(-\beta)^{m_1+\dots+m_k}}{(m_1+\dots+m_k)!}\frac{(m_1+\dots+m_k)!}{m_1!\dots m_k!}\,\mathrm{Tr}_{\mathcal{H}_\Lambda}\,T_{A_1^1}^{\boldsymbol{\mu}}\dots T_{A_{m_1}^1}^{\boldsymbol{\mu}}T_{A_1^2}^{\boldsymbol{\mu}}\dots T_{A_{m_k}^k}^{\boldsymbol{\mu}}\,. \end{aligned} \tag{5.41}$$

We call $\mathcal{A}$ a polymer and define its weight:

$$\rho(\mathcal{A}) = S^{-|\mathcal{A}|}\sum_{m\,\geqslant\,1}\sum_{\substack{A_1,\dots,A_m\\ \cup_i A_i=\mathcal{A}}}\frac{(-\beta)^m}{m!}\,\mathrm{Tr}_{\mathcal{H}_\mathcal{A}}\,T_{A_1}^{\boldsymbol{\mu}}\dots T_{A_m}^{\boldsymbol{\mu}}. \tag{5.42}$$

The partition function takes the form

$$Z_\Lambda = S^{|\Lambda|}\sum_{\{\mathcal{A}_1,\dots\mathcal{A}_k\}}\prod_{i=1}^{k}\rho(\mathcal{A}_i), \tag{5.43}$$

where the sum is restricted to sets of disjoint polymers. In order to apply our swarm expansion, we must check that the weight of the polymers is small.

$$\begin{aligned} |\rho(\mathcal{A})| &\leqslant S^{-|\mathcal{A}|}\,\mathrm{e}^{-c|\mathcal{A}|} \sum_{m\geqslant 1}\frac{\beta^m}{m!} \sum_{A_1,\dots,A_m\subset\mathcal{A}} \sum_{n_{\mathcal{A}}\in\Omega^{\mathcal{A}}} \bigl|\langle n_{\mathcal{A}}|\, T^{\boldsymbol{\mu}}_{A_1}\dots T^{\boldsymbol{\mu}}_{A_m}\,|n_{\mathcal{A}}\rangle\bigr|\,\mathrm{e}^{c\sum_{j=1}^m|A_j|} \\ &\leqslant \mathrm{e}^{-c|\mathcal{A}|}\sum_{m\geqslant 1}\frac{\beta^m}{m!}\Bigl[|\mathcal{A}|\sum_{A\ni x}\|T^{\boldsymbol{\mu}}_A\|\,\mathrm{e}^{c|A|}\Bigr]^m \\ &\leqslant \mathrm{e}^{-(c-1)|\mathcal{A}|}, \end{aligned} \tag{5.44}$$

since $\beta\sum_{A\ni x}\|T^{\boldsymbol{\mu}}_A\|\,\mathrm{e}^{c|A|}\ \leqslant\ 1$.

Analyticity of the free energy follows from Proposition 5.3. Concerning the expectation values of local operators, we define $\mathcal{A}_K$ to be a polymer containing $\operatorname{Supp} K$, and

$$\rho_K(\mathcal{A}_K) = S^{-|\mathcal{A}_K|}\Bigl[\operatorname{Tr}_{\mathcal{H}_{\mathcal{A}_K}} K + \sum_{m\geqslant 1}\sum_{\substack{A_1,\dots,A_m\\ \cup_i A_i\cup\operatorname{Supp} K=\mathcal{A}_K}} \frac{(-\beta)^m}{m!}\operatorname{Tr}_{\mathcal{H}_{\mathcal{A}_K}} K T^{\boldsymbol{\mu}}_{A_1}\dots T^{\boldsymbol{\mu}}_{A_m}\Bigr]. \tag{5.45}$$

Proceeding as before, we find a bound

$$|\rho_K(\mathcal{A}_K)| \ \leqslant\ \|K\|\,\mathrm{e}^{c|\operatorname{Supp} K|}\ \mathrm{e}^{-(c-1)|\mathcal{A}_K|}. \tag{5.46}$$

Next

$$\operatorname{Tr} K\,\mathrm{e}^{-\beta\sum_{A\subset\Lambda}T^{\boldsymbol{\mu}}_A} = S^{|\Lambda|}\sum_{\mathcal{A}_K}\rho_K(\mathcal{A}_K)\sum_{\substack{\{\mathcal{A}_1,\dots\mathcal{A}_k\}\\ \mathcal{A}_i\not\pitchfork\mathcal{A}_K}}\prod_{i=1}^k\rho(\mathcal{A}_i), \tag{5.47}$$

and from cluster expansions we get

$$\langle K\rangle_\Lambda = \sum_{\mathcal{A}_K}\rho_K(\mathcal{A}_K)\exp\Bigl\{-\sum_{C,\operatorname{Supp} C\pitchfork\mathcal{A}_K}\Phi^{\mathrm{T}}(C)\Bigr\}; \tag{5.48}$$

in this expression, the sets $\mathcal{A}_K$ and clusters C are in the volume Λ. The thermodynamic limit clearly exists, since ρ_K and Φ^{T} have exponential decay.

CHAPTER 6

The Pirogov-Sinai theory of first-order phase transitions

1. Generalities

If we observe a thermodynamic system at a point of first-order phase transition, we see large domains with pure phases inside. Any local measurements would reveal one of the phases, i.e. there is *coexistence of different phases*. For instance, consider molecules H_2O at temperature 100^oC (and at atmospheric pressure); in a system close to equilibrium, we see bubbles of gas inside of the liquid, or dropplets of liquid inside of the gas.

Bubbles or dropplets are essentially spherical — or they would be in absence of gravitation; this means that the system tends to minimize the boundary between liquid and gas. More precisely, the surfaces that separate liquid and gas yield a *surface tension*.

Phase coexistence and surface tension are two phenomena related to first-order phase transitions.

In classical lattice models of Statistical Physics, there are mathematical objects leading to the existence of a surface tension at low temperatures, the *contours*. These objects are one of the main ingredients of the Pirogov-Sinai theory. We introduce in Section 4 an abstract contour model, i.e. a system of Statistical Physics where configurations are given in terms of sets of contours, and the weight of a configuration is a product of activities of contours.

Using two properties on the contours, namely an energy estimate: the activity of a contour is exponentially small with respect to its size, and an entropy estimate: the number of contours of given length, containing a given site, goes at most exponentially with its length, the free energy of the system can be expressed as a convergent serie of clusters of contours. While the second property is true independently of thermodynamic parameters, the first property can be generally proven only when the inverse temperature β is larger than some constant β_0.

Let us consider a system for which the thermodynamic parameters are β and $\boldsymbol{\mu} \in \mathcal{U} \subset \mathbb{R}^s$. $\boldsymbol{\mu}$ may be a chemical potential, or an external magnetic field, or both of them, or ... The relevant quantity for Thermodynamics is the free energy $f^{\boldsymbol{\mu},\beta}$ (more precisely: $f^{\boldsymbol{\mu},\beta}$ is the free energy per site in the infinite volume limit), and we are interested in its analytic properties. Indeed, non analyticity of $f^{\boldsymbol{\mu},\beta}$ is related to phase transitions — if $\frac{\partial}{\partial \mu_i} f^{\boldsymbol{\mu},\beta}$ is discontinuous at $\boldsymbol{\mu} = \boldsymbol{\mu}_c$, then $\boldsymbol{\mu}_c$ is a point of *first-order phase transition*.

$\mathcal{U}$ decomposes into regions where the free energy is analytic; such a decomposition is called a *phase diagram*. Hereafter we restrict our considerations to systems at low temperatures, starting the study by the zero-temperature case.

Zero-temperature phase diagram. The limit $\lim_{\beta\to\infty} f^{\boldsymbol{\mu},\beta} = e_0^{\boldsymbol{\mu}}$ is the *ground energy* of the system. In the framework of the Pirogov-Sinai theory, we give ourselves a set of *reference configurations* G, $|G| = p$, which are possible ground states of the system: for all $\boldsymbol{\mu} \in \mathcal{U}$, we suppose that the set of periodic ground states $G^{\boldsymbol{\mu}}$ is a subset of G. Therefore $e_0^{\boldsymbol{\mu}} = e^{\boldsymbol{\mu}}(g)$ with $g \in G^{\boldsymbol{\mu}}$. Thermodynamic quantities are associated with derivatives of

a thermodynamic potential, here $e_0^{\boldsymbol{\mu}}$. Assuming that the energy of a given configuration is analytic in $\boldsymbol{\mu}$ (often it is a linear function), we have that at zero temperature, the free energy $e_0^{\boldsymbol{\mu}}$ is analytic on each domain

$$\mathfrak{M}^\infty(g) = \{\boldsymbol{\mu} \in \mathcal{U} : g \in G^{\boldsymbol{\mu}}\}.$$

In Thermodynamics one often considers lines in the space of thermodynamic parameters, and the natural question is whether the changes of observables are smooth. Consider here a line $[t_1, t_2] \ni t \mapsto \boldsymbol{\mu}(t) \in \mathcal{U}$, such that there is $t_c \in (t_1, t_2)$:

$$G^{\boldsymbol{\mu}(t)} = \begin{cases} \{g^{(1)}\} & \text{if } t \in [t_1, t_c) \\ \{g^{(1)}, g^{(2)}\} & \text{if } t = t_c \\ \{g^{(2)}\} & \text{if } t \in (t_c, t_2]. \end{cases}$$

This describes a first-order phase transition: since $e^{\boldsymbol{\mu}(t)}(g^{(1)}) \neq e^{\boldsymbol{\mu}(t)}(g^{(2)})$ if $t \neq t_c$, we have in general a discontinuity of the derivatives of $e_0^{\boldsymbol{\mu}(t)} = \min(e^{\boldsymbol{\mu}(t)}(g^{(1)}), e^{\boldsymbol{\mu}(t)}(g^{(2)})$ at $\boldsymbol{\mu}_c = \boldsymbol{\mu}(t_c)$.

Low temperature phase diagram. The discussion above concerns the case of temperature zero, and its relevance for Physics is not obvious. The aim of the Pirogov-Sinai theory is to show that it remains true in a domain of (inverse) temperature $[\beta_0, \infty]$. Namely, we shall construct p different functions $f^{\boldsymbol{\mu},\beta}(g)$, $g \in G$, such that

- $\min_{g \in G} f^{\boldsymbol{\mu},\beta}(g)$ is the free energy of the system;
- $\lim_{\beta \to \infty} f^{\boldsymbol{\mu},\beta}(g) = e^{\boldsymbol{\mu}}(g)$, $g \in G$;
- $f^{\boldsymbol{\mu},\beta}(g)$ is analytic in the domain

$$\mathfrak{M}^\beta(g) = \{\boldsymbol{\mu} \in \mathcal{U} : f^{\boldsymbol{\mu},\beta}(g) = \min_{g' \in G} f^{\boldsymbol{\mu},\beta}(g')\}.$$

The discussion of the case of temperature zero then extends to small temperatures. Under the further assumptions that the zero-temperature phase diagram is linearly regular (see Chapter 2), it can be proven that the phase diagram at inverse temperature β is a small deformation of the zero-temperature one. Furthermore, if $f^{\boldsymbol{\mu},\beta}(g)$ is minimum, the typical configuration is g everywhere except for small islands. More precisely, the expectation value of observables is close to the value in the ground configuration g, and correlations decay exponentially fast.

The functions $f^{\boldsymbol{\mu},\beta}(g)$ are called *metastable free energies*, a name that comes from their construction. We shall consider restricted partition functions, where only "small" excitations are allowed. This "smallness" is a notion that depends on the difference $f^{\boldsymbol{\mu},\beta}(g) - \min_{g' \in G} f^{\boldsymbol{\mu},\beta}(g')$ — the smallest the difference, the weakest the condition. If $f^{\boldsymbol{\mu},\beta}(g)$ is minimum, there is no restriction and it coincides with the true free energy.

To explain the notion of metastability, let us suppose that some stochastic dynamics has been defined on our lattice system (for instance a Glauber one). Consider a line in the thermodynamic parameters $[t_1, t_2] \ni t \mapsto \boldsymbol{\mu}(t) \in \mathcal{U}$ as before, i.e. there is $t_c \in (t_1, t_2)$ with

$$\boldsymbol{\mu}(t) \in \begin{cases} \mathfrak{M}^\beta(\{g^{(1)}\}) & \text{if } t \in [t_1, t_c) \\ \mathfrak{M}^\beta(\{g^{(1)}, g^{(2)}\}) & \text{if } t = t_c \\ \mathfrak{M}^\beta(\{g^{(2)}\}) & \text{if } t \in (t_c, t_2]. \end{cases}$$

Here, for $Q \subset G$, $\mathfrak{M}^\beta(Q) \doteqdot \cap_{g \in Q} \mathfrak{M}^\beta(g) \setminus \cup_{g \notin Q} \mathfrak{M}^\beta(g)$, and $\mathfrak{M}^\beta(g)$ was defined above.

We start with $t = t_1$ and let the system evolve for a long time. The typical configuration is $g^{(1)}$ essentially everywhere. Increasing the value of t up to t_c, there is no substancial

change. Crossing t_c, however keeping $t - t_c$ small, the system remains for a while in the phase $g^{(1)}$, with small excitations appearing and disappearing. This is a metastable state, that will be eventually destroyed when a big excitation will appear; this excitation will not disappear, but on the contrary will continue to increase, to cover a large domain. The whole volume will no longer be in the state $g^{(1)}$ — actually, we shall obtain a phase close to $g^{(2)}$, after a sufficiently long time.

The name of "metastable free energy" for the energy of a model where only small excitations are allowed, the restriction depending on the "instability parameter" $f^{\boldsymbol{\mu},\beta}(g) - \min_{g' \in G} f^{\boldsymbol{\mu},\beta}(g')$, is judiciously chosen.

These ideas started with Peierls more than sixty years ago [Pei 1936]. He introduced the notion of contour for the Ising model, and showed that the magnetization is strictly positive at low temperature. Since it is zero at high temperature, this implies a phase transition with symmetry breaking when the temperature is decreased. Strangely, the controversy about the description of phase transitions did not make use of this result.[1] Peierls' ideas were ignored during thirty years, until Dobrushin and Griffiths [Dob 1965, Gri 1964]. The symmetry between the phases is that of spin flips. The situation when this symmetry is a translation was treated in [Dob 1968]. More involved is the case with reflection or rotation [Hei 1974].

The Peierls argument does not directly apply to systems where the ground states are not related with some symmetry. The generalization to this situation was done by Pirogov and Sinai [PS 1975, Sin 1982]. Actually, it is more than a technical extension — the notion of metastable free energies, for instance, acquires its full meaning when the thermal fluctuations are different for different phases. It also makes useless the complications of [Hei 1974].

The theory benefitted of improvements from the Prague School [KP 1984, Zah 1984, HKZ 1988]. The extension to systems with complex interactions was done in [BI 1989], in view of an application to fields theory; the paper is based on ideas of Zahradník [Zah 1984] and constitutes a useful working reference. There exist two reviews by Kotecký; [Kot 1994] is a pedagogical study of a simple model, while [Kot 1995] contains more general discussion.[2] A presentation of the Pirogov-Sinai theory with statements and explanations can be found in [EFS 1993].

Among the extensions of the Pirogov-Sinai theory, there are studies of interfaces [HKZ 1988, HZ 1998], potentials with long-range interactions [Park 1988], systems with degeneracies and residual entropy [GS 1988], systems with degeneracies for which the phases are stabilized by the thermal fluctuations [BS 1989], finite-size scaling [BK 1990, BK 1994], continuous spin models [Zah 1998]. Phase diagrams with an infinite number of ground states on a line of coexistence at temperature zero were considered in [BJK 1996, NOZ 1998]; in some situations, the line is absent at finite temperature, and the free energy is analytic.

In the domains of the phase diagram where a single state has minimal metastable free energy, the stability of the corresponding Gibbs state with respect to any boundary

[1] The relevance of lattice models for understanding phase transitions seems to have been considered as very poor. Kramers already noticed in 1936 that for different values of the magnetic field, the thermodynamic limit of the free energy may yield functions that cannot be joined analytically [H. A. Kramers, Commun. Kammerlingh Onnes Lab. **22**, suppl 83, 1 (1936)]. This is described in M. Dresden, *Kramers's contributions to Statistical Mechanics*, Physics Today, September 1988.

[2] It also includes a beautiful 3D picture, showing the magnetization of the Ising model as a function of temperature and magnetic field.

conditions was shown in [LM 1997]. Here we prove the "thermodynamic stability" of the Gibbs states with respect to small perturbations, periodic or not (see Theorem 6.4 for precise signification).

Finally, let us mention the applications to quantum systems, [Pir 1978, BKU 1996, DFF 1996, DFFR 1996, BKU 1997, KU 1998], that we discuss in Chapters 7 and 8.

2. The Ising model – notion of contours

The Ising model is the simplest model of Statistical Physics where a first-order phase transition occurs. At low enough temperature, this can be proven by the *Peierls argument* [Pei 1936, Dob 1965, Gri 1964].

The Ising model describes a system of spin $\frac{1}{2}$ on a lattice; for this reason we shall denote configurations of spins by s_Λ (rather than n_Λ). The single site state space is $\Omega = \{-1, +1\}$, and the Hamiltonian with "+" boundary conditions is

$$H^{\text{Ising}}_{\Lambda,+}(s_\Lambda) = -J \sum_{<x,y>\subset\Lambda} (s_x s_y - 1) - h \sum_{x\in\Lambda} s_x - J \sum_{x\in\partial_1\Lambda} s_x \tag{6.1}$$

where the first sum runs over pairs of nearest neighbours. The last term could also be written as nearest neighbour interactions between spins inside and outside of the volume. We restrict our interest to a two-dimensional system and $J \in \mathbb{C}$ must have positive real part. Actually, this model with complex interactions has not great physical relevance, but it constitutes an easy example that requires the use of cluster expansion techniques.

We introduce the contours as closed paths in the dual lattice that separates spins of opposite spins, see Fig. 6.1. Let us denote $\gamma_1, \ldots, \gamma_n$ the contours, and $\Gamma = \{\gamma_1, \ldots, \gamma_n\}$

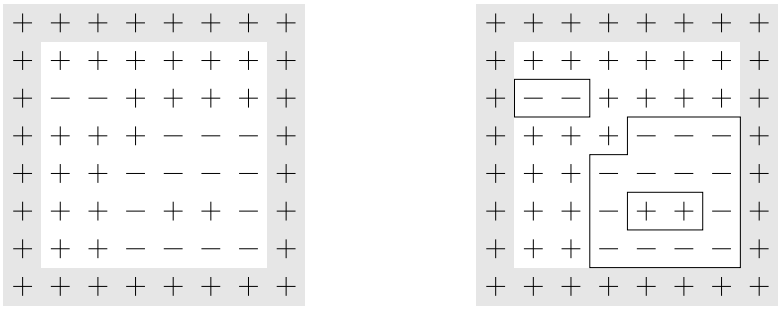


FIGURE 6.1. A configuration of the two-dimensional Ising model, and its contours.

an *admissible* set of contours, i.e. a set of mutually disjoint contours. To any configuration s_Λ corresponds a unique admissible set of contours $\Gamma(s_\Lambda)$, and when $h = 0$ the energy of a configuration can be expressed as

$$H^{\text{Ising}}_{\Lambda,+}(s_\Lambda) = 2J \sum_{\gamma\in\Gamma(s_\Lambda)} |\gamma|, \tag{6.2}$$

where $|\gamma|$ is the length of γ. The partition function takes the following form

$$Z_{\Lambda,+} = \sum_{\Gamma} \prod_{\gamma\in\Gamma} \mathrm{e}^{-2J\beta|\gamma|}\,. \tag{6.3}$$

If β is large enough, we can use the cluster expansion to compute the free energy. More interesting, let us focus to the magnetization at a given site $x \in \Lambda$:

$$\begin{aligned}\langle s_x \rangle_{\Lambda,+} &= \langle \mathbb{I}\left[s_x = +1\right]\rangle_{\Lambda,+} - \langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+} \\ &= 1 - 2\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}. \end{aligned} \tag{6.4}$$

Showing that $\mathrm{Re}\langle s_x \rangle_{\Lambda,+} \geqslant \varepsilon > 0$ (uniformly in Λ) amounts to show that $\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}$ is small. The condition $s_x = -1$ implies that x is surrounded by an odd number of contours; thus there is at least one, so that

$$\left|\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}\right| \leqslant \sum_{\gamma \circlearrowright x} \left| \mathrm{e}^{-2J\beta|\gamma|} \right| \left| \frac{\sum_{\Gamma:\Gamma\cup\{\gamma\} \text{ admissible}} \prod_{\gamma' \in \Gamma} \mathrm{e}^{-2J\beta|\gamma'|}}{\sum_{\Gamma} \prod_{\gamma' \in \Gamma} \mathrm{e}^{-2J\beta|\gamma'|}} \right|. \tag{6.5}$$

where $\gamma \circlearrowright x$ means that γ surrounds x.

If $J \in \mathbb{R}_+$ the fraction is smaller than 1, and we find a bound by omitting it. Then it is not hard to show that the sum over contours surrounding a given site, with a contribution $\mathrm{e}^{-2J\beta|\gamma|}$, is as small as we want by taking β large enough. From this we conclude that $\langle s_x \rangle_{\Lambda,+} > 0$ at sufficiently low temperature, hence the magnetization of the system is strictly positive. This concludes the usual Peierls argument.

Here, we have to deal with a complex J. Using Proposition 5.1, and with S denoting clusters (or swarms), we have

$$\sum_{\Gamma:\Gamma\cup\{\gamma\} \text{ admissible}} \prod_{\gamma' \in \Gamma} \mathrm{e}^{-2J\beta|\gamma'|} = \exp\Big\{ \sum_{S:\, \gamma'\cap\gamma=\varnothing \;\forall \gamma' \in S} \Phi^{\mathrm{T}}(S) \Big\} \tag{6.6}$$

and the same expression for the denominator, but without the restriction on clusters whose elements do not intersect γ. Therefore

$$\left|\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}\right| \leqslant \sum_{\gamma \circlearrowright x} \mathrm{e}^{-2\,\mathrm{Re}\, J\beta|\gamma|} \left| \exp\Big\{ - \sum_{S:\exists \gamma' \in S, \gamma'\cap\gamma\neq\varnothing} \Phi^{\mathrm{T}}(S) \Big\} \right|. \tag{6.7}$$

It is not hard to show that the sum over clusters intersecting a contour γ can be bounded by $\delta|\gamma|$, with δ as small as we need by choosing β large enough. See (5.25) for a related statement, which formally does not apply here because the contours are not subsets of $\mathbb{Z}^2$. Then

$$\left|\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}\right| \leqslant \sum_{\gamma \circlearrowright x} \mathrm{e}^{-\,\mathrm{Re}\, J\beta|\gamma|}. \tag{6.8}$$

The sum over contours can be estimated by first summing over the length ℓ of γ; second choosing an initial segment for the contours ($\leqslant \ell^2$); and third there are 3 choices for the next segment, then 3 again, ..., and this yields a bound 3^ℓ.

$$\left|\langle \mathbb{I}\left[s_x = -1\right]\rangle_{\Lambda,+}\right| \leqslant \sum_{\ell \geqslant 4} \ell^2 3^\ell \, \mathrm{e}^{-\beta\,\mathrm{Re}\, J\ell}. \tag{6.9}$$

If $\beta\,\mathrm{Re}\, J$ is large enough, this sum is small.

3. The Blume-Capel model – notion of metastable free energy

After this introduction to contours through the example of the Ising model, let us have an illustration of metastable free energies by considering the Blume-Capel model. This heuristical discussion can be found in [BL 1984] and [Sla 1987].

This model describes spin 1 particles on a two-dimensional square lattice. The single site state space is $\Omega = \{-1, 0, +1\}$, and the Hamiltonian (with free boundary conditions)

$$H_\Lambda^{\text{Blume-Capel}} = \sum_{<x,y>\subset\Lambda} (s_x - s_y)^2 - \mu_1 \sum_{x\in\Lambda} s_x^2 - \mu_2 \sum_{x\in\Lambda} s_x. \tag{6.10}$$

The zero temperature phase diagram has three domains, the ground states being the three translation invariant configurations $s^{(-1)}$, $s^{(0)}$, $s^{(+1)}$, with $s_x^{(j)} = j$ for all $x \in \mathbb{Z}^\nu$. This is a regular phase diagram, and the point of maximal coexistence is $\boldsymbol{\mu}_0 = (0, 0)$. It is given by the equation $e^{\boldsymbol{\mu}}(s^{(-1)}) = e^{\boldsymbol{\mu}}(s^{(0)}) = e^{\boldsymbol{\mu}}(s^{(+1)})$, i.e. it is the point where the energies of the three translation invariant configurations are equal.

To understand the physics of the low temperatures, we have to look on excitations. Consider the configuration $s^{(+1)}$; the difference of energy when one spin is flipped into 0 is 4 (the number of neighbours of a site). Let us neglect all other excitations, since they cost more energy, and define $f_\Lambda^\beta(s^{(+1)})$ as the logarithm of a restricted partition function, with a sum over configurations containing only this type of excitations (which can appear many times):

$$f_\Lambda^\beta(s^{(+1)}) \simeq -\frac{1}{\beta|\Lambda|} \log \sum_{k\geqslant 0} \frac{1}{k!} \Big(|\Lambda|\, \mathrm{e}^{-4\beta} \Big)^k = -\frac{1}{\beta}\, \mathrm{e}^{-4\beta}\,.$$

For symmetry reasons $f_\Lambda^\beta(s^{(-1)})$ is the same. It is however different for $f_\Lambda^\beta(s^{(0)})$, because there are two types of excitations, namely the flip of a spin 0 into $+1$, or into -1.

$$\begin{aligned} f_\Lambda^\beta(s^{(0)}) &\simeq -\frac{1}{\beta|\Lambda|} \log \sum_{k_1\geqslant 0} \frac{1}{k_1!} \Big(|\Lambda|\, \mathrm{e}^{-4\beta} \Big)^{k_1} \sum_{k_2\geqslant 0} \frac{1}{k_2!} \Big(|\Lambda|\, \mathrm{e}^{-4\beta} \Big)^{k_2} \\ &= -\frac{2}{\beta}\, \mathrm{e}^{-4\beta}\,. \end{aligned}$$

Therefore we have $f_\Lambda^\beta(s^{(0)}) < f_\Lambda^\beta(s^{(\pm 1)})$ if $\beta < \infty$, so we expect that the point $\boldsymbol{\mu} = (0, 0)$ belongs to the domain of the phase "$s^{(0)}$" at low temperature. This heuristic discussion can be continued to take into account the parameter $\boldsymbol{\mu} = (\mu_1, \mu_2)$; the equation $f_\Lambda^\beta(s^{(-1)}) = f_\Lambda^\beta(s^{(0)}) = f_\Lambda^\beta(s^{(\pm 1)})$ characterizes the point $\boldsymbol{\mu}_0(\beta)$, the intersection of the three domains, while the coexistence lines may be obtained by equalling the corresponding $f_\Lambda^\beta(\cdot)$. These functions are good approximations of the metastable free energies that are defined in the sequel.

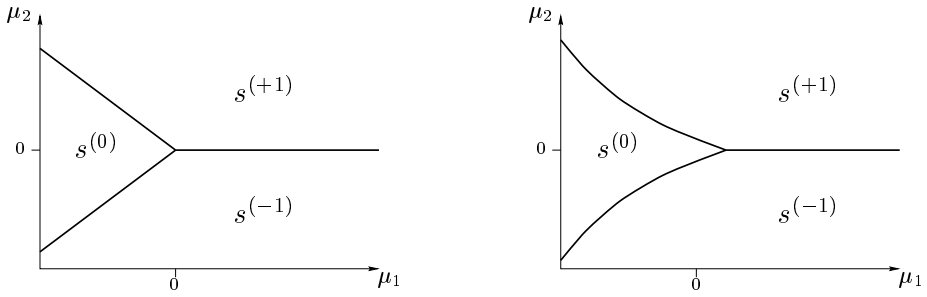


FIGURE 6.2. Phase diagrams of the Blume-Capel model, at zero and low temperature.

4. Setting and properties

We now generalize the considerations of the previous section and formulate a theory valid for a large class of models, that can be put into a contour one. The following definitions are rather abstract, since no Hamiltonian is ever mentioned.[3] The reader can however keep in mind concrete models, as for instance the Blume-Capel one.

Let $G = \{g^{(1)}, \dots, g^{(p)}\}$ a set of periodic configurations that we call *reference states*. $\mathcal{U} \subset \mathbb{R}^{p-1}$ is the space of $(p-1)$ thermodynamic parameters $\boldsymbol{\mu} = (\mu_1, \dots, \mu_{p-1})$. The energies of the reference states are $e^{\boldsymbol{\mu}}(g^{(1)}), \dots, e^{\boldsymbol{\mu}}(g^{(p)})$; they are analytic functions of $\boldsymbol{\mu}$ in $\mathcal{U}$. We set $e_0^{\boldsymbol{\mu}} = \min_{g\in G} e^{\boldsymbol{\mu}}(g)$. The zero-temperature phase diagram is given by the homeomorphism described in Chapter 2, Section 2.4. The degeneracy breaking condition in its stronger form (2.26) is assumed to hold (i.e. the phase diagram is linearly regular), and

$$\left|\frac{\partial}{\partial\mu_i} e^{\boldsymbol{\mu}}(g)\right| \leqslant 1. \tag{6.11}$$

Classical lattice models are living on lattices that are subsets of $\mathbb{Z}^\nu$. However, our expansion of quantum models (see Chapter 7) yields a contour model on a lattice $\Lambda \times \{1, 2, \dots, M\}^{\mathrm{per}}$, $\Lambda \subset \mathbb{Z}^\nu$; there is one more dimension, which is finite and periodic. This motivates to consider the following lattice; with $\bar\nu \geqslant \nu$ (and $\nu \geqslant 2$),

$$\boldsymbol{\Lambda} = \Lambda \times \{1, \dots, M_1\}^{\mathrm{per}} \times \cdots \times \{1, \dots, M_{\bar\nu-\nu}\}^{\mathrm{per}}.$$

$\boldsymbol{\Lambda} \subset \mathbb{Z}^{\bar\nu}$ is finite. The thermodynamic limit will still be denoted $\lim_{\Lambda\nearrow\mathbb{Z}^\nu}$, and means a sequence of increasing volumes $(\boldsymbol{\Lambda}_n)$ with fixed $M_1, \dots, M_{\bar\nu-\nu}$. $\boldsymbol{\Lambda}^{\mathrm{per}}$ is the torus $\Lambda^{\mathrm{per}} \times \{1, \dots, M_1\}^{\mathrm{per}} \times \cdots \times \{1, \dots, M_{\bar\nu-\nu}\}^{\mathrm{per}}$.

A *contour* is a pair $(\operatorname{supp} Y, \alpha_Y)$; the finite, connected set $\operatorname{supp} Y \subset \mathbb{Z}^{\bar\nu}$ is the *support* of Y. Let $C(x) \subset \mathbb{R}^{\bar\nu}$ be the unit cell centered on $x \in \mathbb{R}^{\bar\nu}$. The *boundary* of Y is $\partial Y = \partial \operatorname{Supp} Y$, where for $B \subset \mathbb{Z}^{\bar\nu}$, $\partial B \doteqdot \partial \cup_{x\in B} C(x)$ (if $A \subset \mathbb{R}^{\bar\nu}$, $\partial A \doteqdot \overline{A} \cap \overline{A^{\mathrm{c}}}$). α_Y is then a labelling that attributes an element $g \in G$ to each connected component of ∂Y. $|\partial B| \in \mathbb{N}$ is the number of $(\bar\nu - 1)$-dimensional faces in ∂B.

A *contour configuration*, or *admissible set of contours*, is a set $\mathfrak{Y} = \{Y_1, \dots, Y_n\}$ such that $(\operatorname{Supp}\mathfrak{Y} \doteqdot \cup_{Y\in\mathfrak{Y}} \operatorname{Supp} Y)$

- $\operatorname{Supp} Y_i \not\owedge \operatorname{supp} Y_j$ if $i \neq j$,
- the boundary of each connected component of $(\operatorname{Supp}\mathfrak{Y})^{\mathrm{c}}$ has constant labelling.

An example of a contour configuration is displayed in Fig. 6.3. Remark that the contours of the Ising model, as defined in Section 2, do not agree with the definition. However, if we really want to put the Ising model into this framework, a standard way is to define the set of excitations of a configuration, $E(s) = \{x \in \mathbb{Z}^\nu : \exists y, |y - x| = 1, \text{ and } s_x \neq s_y\}$; then the contours are connected components of $E(s)$, together with the information on which phases are on their boundaries.

We need a few more definitions. The *exterior* $\operatorname{Ext} Y$ of a contour Y is the unique infinite connected component of $(\operatorname{Supp} Y)^{\mathrm{c}}$. The *g-interior* $\operatorname{Int}_g Y$ is the union of the finite components of $(\operatorname{Supp} Y)^{\mathrm{c}}$ which have labels $\alpha = g$; the *interior* of Y is $\operatorname{Int} Y = \cup_{g\in G} \operatorname{Int}_g Y$.

[3] It is not only true that different models would lead to different definitions of contours; a given model can by itself have different interpretations. This point was noted in a presentation of M. Zahradník in Churaňov (October 1995): at the end of the talk, there was a little confusion;

Christian Borgs: – Miloš, what is now a contour?

M. Z. : – Well, I would say, it's a matter of personal choice...

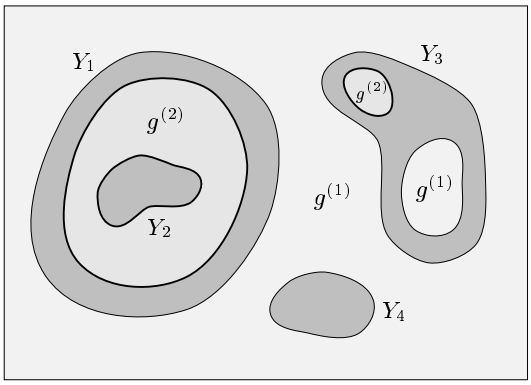


FIGURE 6.3. Schematic picture for an admissible set of four contours. The boundaries of the supports of contours are thin, resp. thick, when $\alpha = g^{(1)}$, resp. $g^{(2)}$.

The *volume* is $\operatorname{Vol} Y = \operatorname{Supp} Y \cup \operatorname{Int} Y \subset \mathbb{Z}^{\bar\nu}$ and the *diameter* is $\operatorname{diam} Y = \operatorname{diam} \operatorname{Supp} Y$. Finally, Y is a *g-contour* if $\operatorname{Ext} Y$ has label g.

Given a contour configuration $\mathfrak{Y}$ in a finite volume $\mathbf{\Lambda}$, we define $\operatorname{Supp} \mathfrak{Y} = \cup_{Y\in\mathfrak{Y}} \operatorname{Supp} Y$, and $\mathfrak{W}_g(\mathfrak{Y})$ as the union of the connected components of $(\operatorname{Supp} \mathfrak{Y})^{\mathrm{c}}$ that have labels $\alpha = g$ on their boundaries. With these definitions, the following relations are valid: $\cup_g \mathfrak{W}_g(\mathfrak{Y}) \cup \operatorname{Supp} \mathfrak{Y} = \mathbf{\Lambda}$, $\mathfrak{W}_g(\mathfrak{Y}) \cap \operatorname{Vol} Y = \operatorname{Int}_g Y$, ...

$\beta \in [\beta_0, \infty]$ is as before the inverse temperature. We give ourselves a weight for the contours; $z^{\boldsymbol{\mu},\beta}$ is a mapping from the set of contours into $\mathbb{C}$, that is analytic in $\boldsymbol{\mu}$ and β in the domain $\mathcal{U} \times [\beta_0, \infty]$. It is translation invariant [that is, $z^{\boldsymbol{\mu},\beta}(\mathfrak{t}_x Y) = z^{\boldsymbol{\mu},\beta}(Y)$], and we have uniform exponential bounds:

$$\left|z^{\boldsymbol{\mu},\beta}(Y)\right| \;\leqslant\; \mathrm{e}^{-\beta e_0^{\boldsymbol{\mu}} |\operatorname{Supp} Y|}\, \mathrm{e}^{-\gamma |\operatorname{Supp} Y|}, \tag{6.12}$$

$$\left|\frac{\partial}{\partial \mu_i} z^{\boldsymbol{\mu},\beta}(Y)\, \mathrm{e}^{\beta e_0^{\boldsymbol{\mu}} |\operatorname{Supp} Y|}\right| \;\leqslant\; \mathrm{e}^{-\gamma |\operatorname{Supp} Y|}, \tag{6.13}$$

for a large enough constant γ, and

$$\lim_{\beta\to\infty} z^{\boldsymbol{\mu},\beta}(Y) = 0. \tag{6.14}$$

The first inequality is usually referred to as the *Peierls condition*. In the sequel we shall often write $O(\mathrm{e}^{-\gamma})$ for a number that is bounded by $C \cdot \mathrm{e}^{-\gamma}$, the constant C depending on $\bar\nu$ and p only.

The partition function of a contour model with boundary conditions $g_0 \in G$ is by definition

$$Z_{g_0}(\mathbf{\Lambda}) = \sum_{\substack{\mathfrak{Y} \\ \alpha(\partial \operatorname{Vol} \mathfrak{Y}) = g_0}} \prod_{g\in G} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g) |\mathfrak{W}_g(\mathfrak{Y})|} \prod_{Y\in\mathfrak{Y}} z^{\boldsymbol{\mu},\beta}(Y) \tag{6.15}$$

where the sum is over all contour configurations in $\mathbf{\Lambda}$, compatible with the boundary condition. In particular, $Z_{g_0}(\varnothing) = 1$.

We summarize the results of the Pirogov-Sinai theory in the following theorem, the proof of which will be described in the next sections.

THEOREM 6.1. **Stability of the phase diagram.**

Assume that for all $(\boldsymbol{\mu}, \beta) \in \mathcal{U} \times [\beta_0, \infty]$ *our contour model satisfies all the assumptions in this section, with* $\gamma \geqslant \gamma_0$, γ_0 *being a constant that depends on* $\bar{\nu}$ *and* p *only. Then there exist* p *continuously differentiable functions* $f^{\boldsymbol{\mu},\beta}(g)$, $g \in G$, *with the properties*

- $\lim_{\beta\to\infty} f^{\boldsymbol{\mu},\beta}(g) = e^{\boldsymbol{\mu}}(g)$, $g \in G$.
- *If* $\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g_0) = \min_{g\in G} \operatorname{Re} f^{\boldsymbol{\mu},\beta}(g)$, *then* $f^{\boldsymbol{\mu},\beta}(g_0)$ *is the free energy of the system.*
- $f^{\boldsymbol{\mu},\beta}(g)$ *is analytic on the domain*

$$\mathfrak{M}(g) = \big\{(\boldsymbol{\mu}, \beta) \in \mathcal{U} \times [\beta_0, \infty] : \operatorname{Re} f^{\boldsymbol{\mu},\beta}(g) = \min_{g' \in G} \operatorname{Re} f^{\boldsymbol{\mu},\beta}(g')\big\}. \tag{6.16}$$

- *For all* $\beta \in [\beta_0, \infty]$, *there exists* $\boldsymbol{\mu}_0(\beta) \in \mathcal{U}$ *such that* $\operatorname{Re} f^{\boldsymbol{\mu}_0(\beta),\beta}(g) = \operatorname{Re} f^{\boldsymbol{\mu}_0(\beta),\beta}(g')$, $g, g' \in G$, *and the matrix of derivatives*

$$\Big(\frac{\partial}{\partial \mu_i}\big[f^{\boldsymbol{\mu},\beta}(g^{(j)}) - f^{\boldsymbol{\mu},\beta}(g^{(p)})\big]\Big)_{1 \leqslant i,j \leqslant p-1}$$

has an inverse that is uniformly bounded in $\boldsymbol{\mu} \in \mathcal{U}$.

As a consequence, the phase diagram at inverse temperature β has the same topological structure as the zero-temperature one. Furthermore, the point of maximal coexistence $\boldsymbol{\mu}_0(\beta)$ is C^1 in β, by the inverse function theorem.

Correlation functions and order parameters play an important role in Statistical Physics, so that results about the expectation values of local observables in the thermodynamic limit merit a discussion. Let us include them into our general contour model.

Here the name "observables" does not refer to a function on the phase space — we rather have in mind observables in the original spin model. Hence it is necessary to precise the meaning in the context of the contour model. The structure is as follows.

We are given a finite set $\{K_i\}_{i\in I}$ of observables with disjoint supports.

- K_i, $i \in I$, is a function $G \to \mathbb{C}$; we associate to it a finite number[4] C_{K_i} and we set $C_K = \prod_{i\in I} C_{K_i}$.
- They have supports: $\operatorname{Supp} K_i \subset \mathbb{Z}^{\bar{\nu}}$, $|\operatorname{Supp} K_i| < \infty$, $\operatorname{Supp} K_i \not\cap \operatorname{Supp} K_j$ if $i \neq j$.
- A K-contour Y_K is such that there exists $J \subset I$ ($J \neq \varnothing$): $\operatorname{Supp} Y_K \supset \cup_{i\in J} \operatorname{Supp} K_i$ and $\operatorname{Supp} Y_K \not\cap \cup_{i\notin J} \operatorname{Supp} K_i$; there is a weight $z_K : \{Y_K\} \to \mathbb{C}$, satisfying the bound

$$|z_K(Y_K)| \leqslant \mathrm{e}^{-\beta e_0^{\boldsymbol{\mu}} |\operatorname{Supp} Y_K|}\, \mathrm{e}^{-\gamma |\operatorname{Supp} Y_K|} \prod_{i\in J} C_{K_i}.$$

The expectation value of $K = \prod_{i\in I} K_i$ with boundary conditions g_0 ($g_0 \in G$) — in the context of the general contour model — is defined as

$$\Big\langle \prod_{i\in I} K_i \Big\rangle_{\boldsymbol{\Lambda},g_0} = \frac{1}{Z_{g_0}(\boldsymbol{\Lambda})} \sum_{\mathcal{Y}_K} \sum_{\mathcal{Y}:\mathcal{Y}_K,K} \prod_{g\in G} \Big[\mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g) |\mathfrak{W}_g(\mathcal{Y}_K \cup \mathcal{Y})|} \prod_{i\in I:\operatorname{Supp} K_i \subset \mathfrak{W}_g(\mathcal{Y}_K\cup\mathcal{Y})} K_i(g) \Big] \prod_{Y_K \in \mathcal{Y}_K} z_K(Y_K) \prod_{Y\in\mathcal{Y}} z^{\boldsymbol{\mu},\beta}(Y). \tag{6.17}$$

The first sum is over sets $\mathcal{Y}_K$ of K-contours; the second sum is over sets of usual contours, such that $\mathcal{Y}_K \cup \mathcal{Y}$ is admissible and compatible with the boundary condition g_0 and $\operatorname{Supp} Y \not\cap \operatorname{Supp} K$. The contribution of K_i is either with a factor $K_i(g)$, if $\operatorname{Supp} K_i \subset \mathfrak{W}_g(\mathcal{Y}_K \cup \mathcal{Y})$, or with a K-contour Y_K, if $\operatorname{Supp} K_i \subset Y_K$.

[4] Think on the norm of K_i.

Classical lattice models can be put into this setting, and also quantum models, as we shall see in the next two chapters. Typical applications are when $|I| = 1$ (order parameters) and $|I| = 2$ (correlation functions).

The Pirogov-Sinai theory brings the following properties.

THEOREM 6.2. **Local observables.**

For all $\delta > 0$, there exists $\gamma_0 < \infty$ such that if the assumptions of this section hold with $\gamma \geqslant \gamma_0$ for all $(\boldsymbol{\mu}, \beta) \in \mathcal{U} \times [\beta_0, \infty]$, then if $\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g_0) = \min_{g \in G} \operatorname{Re} f^{\boldsymbol{\mu},\beta}(g)$,

- *the thermodynamic limit of the expectation value of local observables with boundary conditions g_0,*
$$\langle K \rangle_{g_0} = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \langle K \rangle_{\boldsymbol{\Lambda}, g_0},$$
exists;
- *$\langle \cdot \rangle_{g_0}$ represents a "g_0-phase": for all K,*
$$\big| \langle K \rangle_{g_0} - K(g_0) \big| \leqslant \delta C_K;$$
- *this state is exponentially clustering: let*
$$d(K) = \min_{i,j \in I, i \neq j} \operatorname{dist}(\operatorname{Supp} K_i, \operatorname{Supp} K_j);$$
then there exists $\xi = \xi^{\boldsymbol{\mu},\beta}(g_0) > 0$ such that
$$\Big| \Big\langle \prod_{i \in I} K_i \Big\rangle_{g_0} - \prod_{i \in I} \langle K_i \rangle_{g_0} \Big| \leqslant c(|I|) C_K \exp\big(-d(K)/\xi\big),$$
with $c(|I|)$ a constant that depends only on the number of local observables.

Periodic boundary conditions are often considered, because corresponding volumes have no boundary and this may bring many technical simplifications. The partition function of the contour model with periodic boundary conditions is given by

$$Z_{\mathrm{per}}(\boldsymbol{\Lambda}) = \sum_{\mathfrak{Y}} \prod_{g \in G} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g) |\mathfrak{W}_g(\mathfrak{Y})|} \prod_{Y \in \mathfrak{Y}} z^{\boldsymbol{\mu},\beta}(Y) \tag{6.18}$$

where $\boldsymbol{\Lambda}$ has periodic boundary conditions in all $\bar{\nu}$ directions; $\mathfrak{Y}$ must be admissible. The expectation value of a local observable K is defined by (6.17) with the following modifications: the supports of the contours are subsets of the $\bar{\nu}$-dimensional torus $\boldsymbol{\Lambda}$; the normalization factor is $1/Z_{\mathrm{per}}(\boldsymbol{\Lambda})$; and $\mathfrak{Y}_K \cup \mathfrak{Y}$ must be admissible.

Let $\mathfrak{M}(Q) = \cap_{g \in Q} \mathfrak{M}(g) \setminus \cup_{g \notin Q} \mathfrak{M}(g)$ with $\mathfrak{M}(g)$ given in (6.16). $\mathfrak{M}(Q)$ is the set of thermodynamic parameters $(\beta, \boldsymbol{\mu})$ where the set of pure phases is Q.

THEOREM 6.3. **Periodic boundary conditions.**

Under the same assumptions as in Theorem 6.2, the expectation values of a local observable with periodic boundary conditions exists in the thermodynamic limit; moreover, if $(\boldsymbol{\mu}, \beta) \in \mathfrak{M}(Q)$,

$$\langle K \rangle_{\mathrm{per}} = \frac{1}{|Q|} \sum_{g \in Q} \langle K \rangle_g.$$

An important assumption for Theorems 6.2 and 6.3 is that the weights are translation invariant. This means that the original spin model is also translation invariant. In fact, periodic systems can be transformed into translation invariant ones by considering a lattice of parallelipipeds in $\mathbb{Z}^\nu$, the dimensions of the parallelipipeds being equal to the periods of the interaction. We can define a new model with larger single site state space (and

smaller range), that has translation invariance. However, the bigger the period, the bigger the constant γ_0 for the assumption on the bound of the weights.

This brings problems when considering models with a small perturbation, not necessarily periodic — this situation occurs when defining thermodynamically stable states, see Section 3.3, Chapter 2. This is the reason why we need the following complement to Theorems 6.2 and 6.3.

THEOREM 6.4. **Thermodynamic stability**

Consider a contour model with weights $z^{\boldsymbol{\mu},\beta,\alpha}$ and $z_K^{\boldsymbol{\mu},\beta,\alpha}$, analytic in $(\boldsymbol{\mu},\beta,\alpha) \in \mathcal{U} \times [\beta_0,\infty] \times [0,\alpha_0]$, and with uniform Peierls condition and bounds on derivatives. $z^{\boldsymbol{\mu},\beta,\alpha}$ and $z_K^{\boldsymbol{\mu},\beta,\alpha}$ are not necessarily translation invariant. We suppose that for each contours Y and Y_K,

$$z^{\boldsymbol{\mu},\beta}(Y) \equiv \lim_{\alpha\to 0} z^{\boldsymbol{\mu},\beta,\alpha}(Y)$$
$$z_K^{\boldsymbol{\mu},\beta}(Y_K) \equiv \lim_{\alpha\to 0} z_K^{\boldsymbol{\mu},\beta,\alpha}(Y_K)$$

are translation invariant.

Let $f^{\boldsymbol{\mu},\beta}(g)$, $g \in G$, be the functions given by Theorem 6.1. Then for all $g \in G$, and all $(\boldsymbol{\mu},\beta) \in \mathfrak{M}(\{g\})$, there exists $\bar\alpha > 0$ such that

$$\langle K\rangle_{\rm per}^{\boldsymbol{\mu},\beta,\alpha} = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \langle K\rangle_{\boldsymbol{\Lambda}\,{\rm per}}^{\boldsymbol{\mu},\beta,\alpha}$$

exists for all $\alpha \in [0,\bar\alpha]$. Furthermore

$$\lim_{\alpha\to 0} \langle K\rangle_{\rm per}^{\boldsymbol{\mu},\beta,\alpha} = \langle K\rangle_g^{\boldsymbol{\mu},\beta}.$$

Notice that we did not define metastable free energies with non-translation invariant weights — their thermodynamic limits do not exist in general. But there is no problem with expectation values of local observables, since these are local quantities, up to terms with exponential decay.

States at coexistence points are *not* thermodynamically stable. However, we would need such a notion in order, for instance, to exclude superfluidity in the chessboard phase of the Bose-Hubbard model. This would be achieved by the following property, which is certainly true.

CONJECTURE. *Consider weights $z^{\boldsymbol{\mu},\beta,\alpha}$, $z_K^{\boldsymbol{\mu},\beta,\alpha}$ which are periodic*[5] *with respect to lattice translations (with arbitrary period). Then, if $(\boldsymbol{\mu},\beta) \in \mathfrak{M}(Q)$,*

$$\lim_{\alpha\to 0} \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{1}{|\boldsymbol{\Lambda}|} \sum_{x\in\boldsymbol{\Lambda}} \big\langle \mathrm{t}_x K\big\rangle_{\boldsymbol{\Lambda},\,\rm per}^{\alpha} = \sum_{g\in Q} c_g \langle K\rangle_g$$

with $c_g \geqslant 0$, $\sum_{g\in Q} c_g = 1$; these coefficients depend on the weights.

In the case of the superfluidity order parameter, we have $K = c_0^\dagger$, and the weights $z^{\boldsymbol{\mu},\beta,\alpha}$, $z_K^{\boldsymbol{\mu},\beta,\alpha}$ are those of a system with external field $\alpha\sum_{x\in\Lambda}(c_x^\dagger + c_x)$. In this case $K(g) = 0$ for any x, g, and $\lim_{\alpha\to 0} z_K^{\boldsymbol{\mu},\beta,\alpha}(Y) = 0$. This implies [see (6.17)] that $\langle c_0^\dagger\rangle_g = 0$; from the conjecture, we can conclude that there is no off-diagonal long-range order in the chessboard phases of the Bose-Hubbard model.

[5] To allow interfaces, it would be nice not to need periodicity.

5. Positive weights: a discussion

The physics of the Pirogov-Sinai theory is that of classical lattice systems, where the weights $z^{\boldsymbol{\mu},\beta}$ take real positive values. In view of the application to quantum models, we have to allow complex values, but this brings some extra difficulties; moreover, it loses its physical meaning. It is then a moral duty to present first the theory in a restricted but conceptually meaningful form, and to postpone the general case to a later section. In the following, $\boldsymbol{\Lambda}'$, $\boldsymbol{\Lambda}''$ are any simply connected subsets of $\boldsymbol{\Lambda}$.

The basic mathematical tool for the Pirogov-Sinai theory is cluster expansions. However it is impossible to apply directly Proposition 5.1, because the compatibility relation between the contours is rather complicated; the condition with the labels can be viewed as a long-range interaction between the contours. The idea to solve this problem is to define new weights for g_0-contours by

$$\mathfrak{z}(Y) = z^{\boldsymbol{\mu},\beta}(Y)\, \mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp} Y|} \prod_{g\in G} \frac{Z_g(\operatorname{Int}_g Y)}{Z_{g_0}(\operatorname{Int}_g Y)}. \tag{6.19}$$

A contour Y is *external* if $\operatorname{Supp} Y \cap \operatorname{Vol} Y' = \varnothing$ for all $Y' \in \mathfrak{Y}$. The partition function can be written as

$$Z_{g_0}(\boldsymbol{\Lambda}') = \sum_{\substack{\{Y_1,\dots,Y_k\} \\ \text{external } g_0\text{-contours}}} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\boldsymbol{\Lambda}'\setminus\cup_j \operatorname{Vol} Y_j|} \prod_{j=1}^{k} \Big[z^{\boldsymbol{\mu},\beta}(Y_j) \prod_{g\in G} Z_g(\operatorname{Int}_g Y_j)\Big] \tag{6.20}$$

where the sum is over non-intersecting, external g_0-contours. Dividing and multiplying $Z_g(\operatorname{Int}_g Y_j)$ by $Z_{g_0}(\operatorname{Int}_g Y_j)$, and iterating, we obtain

$$Z_{g_0}(\boldsymbol{\Lambda}') = \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\boldsymbol{\Lambda}'|} \sum_{\{Y_1,\dots,Y_n\}} \prod_{j=1}^{n} \mathfrak{z}(Y_j), \tag{6.21}$$

where the sum is over sets of disjoints g_0-contours. The compatibility condition is now exactly that of polymers, so we can apply cluster expansion, provided the decay is still strong.

Equations (6.19) and (6.21) propose a nice viewpoint on the theory. So let us make a heuristical break.

If the weights $\mathfrak{z}(Y)$ have sufficiently strong exponential decay with respect to the size of Y, it can be shown that they are rare; this means that the system is in the "g_0-phase", with typical configurations being equal to g_0 except for some small islands. With $\tilde{f}(g_0)$ the free energy of this phase,[6] we have

$$Z_{g_0}(\boldsymbol{\Lambda}') \simeq \mathrm{e}^{-\beta \tilde{f}(g_0)|\boldsymbol{\Lambda}'|}$$

(with a correction due to boundary effects of the order $\mathrm{e}^{O(\mathrm{e}^{-\gamma})|\partial\boldsymbol{\Lambda}'|}$).

But a different scenario may also happen. Suppose that the system should be in the g-phase, and we are looking at $Z_{g_0}(\boldsymbol{\Lambda}')$. Then if $\boldsymbol{\Lambda}'$ is large enough, typical configurations will have a large contour Y' with a large interior $\operatorname{Int}_g Y' \simeq \boldsymbol{\Lambda}'$. In this case, since $z^{\boldsymbol{\mu},\beta}(Y') \simeq \mathrm{e}^{-\gamma|\operatorname{Supp} Y'|}$ (here in the discussion we set $e_0^{\boldsymbol{\mu}} = 0$),

$$\begin{aligned} Z_{g_0}(\boldsymbol{\Lambda}') &\simeq \mathrm{e}^{-\gamma|\partial\boldsymbol{\Lambda}'|}\, \mathrm{e}^{-\beta\tilde{f}(g)|\boldsymbol{\Lambda}'|} \\ &> \mathrm{e}^{-\beta\tilde{f}(g_0)|\boldsymbol{\Lambda}'|}. \end{aligned} \tag{6.22}$$

[6] To be precisely defined below.

If such a scenario takes place, then a contour Y that has a sufficiently large interior $\operatorname{Int}_g Y$ will have a g_0-weight

$$\begin{aligned}\mathfrak{z}(Y) &\simeq z^{\boldsymbol{\mu},\beta}(Y)\frac{\mathrm{e}^{-\beta\tilde f(g)|\operatorname{Int} Y|}}{\mathrm{e}^{-\gamma|\operatorname{Supp} Y|}\ \mathrm{e}^{-\beta\tilde f(g)|\operatorname{Int} Y|}}\\ &\simeq 1.\end{aligned}$$

Equation (6.22) suggests that $\mathfrak{z}$ has sufficient decay if $f(g_0) < f(g)$, or if Y is not too big:

$$\begin{aligned}\mathrm{e}^{-\gamma|\operatorname{Supp} Y|}\ \mathrm{e}^{-\beta\tilde f(g)|\operatorname{Vol} Y|} &< \mathrm{e}^{-\beta\tilde f(g_0)|\operatorname{Vol} Y|}\\ \iff \tilde f(g_0)-\tilde f(g) &< \frac{\gamma}{\beta}\frac{|\operatorname{Supp} Y|}{|\operatorname{Vol} Y|} \simeq \frac{\gamma}{\beta}\frac{1}{\operatorname{diam} Y}.\end{aligned} \tag{6.23}$$

This shows that the size of the contours may play a role, and that a natural parameter to characterize the instability due to contours is $\beta(\tilde f(g_0)-\tilde f(g))$. The conclusion of this discussion is that a contour may destabilize a phase if it creates a large domain with a phase that has lower free energy inside; such a contour pays on its boundary but gains on its volume, and if the latter is big compared to the former, it is likely to occur.

Let us end this break now and go on with mathematics.

We define truncated g_0-weights

$$\tilde{\mathfrak{z}}(Y) = \begin{cases}\mathfrak{z}(Y) & \text{if } \mathfrak{z}(Y) \leqslant \mathrm{e}^{-(\gamma-2\bar\nu)|\operatorname{Supp} Y|}\\ 0 & \text{if } \mathfrak{z}(Y) > \mathrm{e}^{-(\gamma-2\bar\nu)|\operatorname{Supp} Y|}.\end{cases} \tag{6.24}$$

If γ is large enough, these new weights satisfy the assumptions for the use of the cluster expansion. The *metastable free energies* are defined as

$$\tilde f^{\boldsymbol{\mu},\beta}(g_0) = -\frac{1}{\beta}\lim_{\Lambda\nearrow\mathbb{Z}^\nu}\frac{1}{|\boldsymbol{\Lambda}|}\log\mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\boldsymbol{\Lambda}|}\sum_{\substack{\{Y_1,\dots,Y_n\}\\ g_0\text{-contours}}}\prod_{j=1}^n\tilde{\mathfrak{z}}(Y_j). \tag{6.25}$$

[Notice that $\lim_{\beta\to\infty}\tilde f^{\boldsymbol{\mu},\beta}(g) = e^{\boldsymbol{\mu}}(g)$ because of (6.14).]

Let us define $\tilde a_g = \beta\tilde f^{\boldsymbol{\mu},\beta}(g) - \min_{g'\in G}\beta\tilde f^{\boldsymbol{\mu},\beta}(g')$.

Proposition 6.5 (**Stability of small contours**). *There exists $\gamma_0 < \infty$ (depending on $\bar\nu$ and p only) such that if (6.12) holds with $\gamma \geqslant \gamma_0$, then the metastable free energies exist. Furthermore if $\tilde a_{g_0}\operatorname{diam}\boldsymbol{\Lambda}' \leqslant 1$, we have*

$$\frac{Z_g(\boldsymbol{\Lambda}')}{Z_{g_0}(\boldsymbol{\Lambda}')} \leqslant \mathrm{e}^{|\partial\boldsymbol{\Lambda}'|}$$

We say that a phase $g\in G$ is *stable* if $\tilde f^{\boldsymbol{\mu},\beta}(g)$ is minimum, i.e. if $\tilde a_g = 0$. Proposition 6.5 implies that $\mathfrak{z}(Y) \leqslant \mathrm{e}^{-(\gamma-2\bar\nu)|\operatorname{Supp} Y|}$ for all g-contours Y, therefore $\tilde f^{\boldsymbol{\mu},\beta}(g)$ is the free energy of the system. Furthermore the phase diagram at inverse temperature β can be constructed using the metastable free energies: the domain of the phase g is the set $\{\boldsymbol{\mu} : \tilde a_g = 0\}$, i.e. all $\boldsymbol{\mu}$ where $\tilde f^{\boldsymbol{\mu},\beta}(g)$ is minimum.

Equation (6.19) makes sense when interiors of contours are disconnected from exterior. In some models this does not hold, although it is clear that phases are charaterized by rarety of contours. Studying such models requires a reformulation of Pirogov-Sinai theory, which is currently being pursued [HZ 1998, Zah 1996].

To help in the study of the phase diagram, we define in the next section different metastable free energies, which are differentiable functions of $\boldsymbol{\mu}, \beta$.

6. Differentiable metastable free energies

The definition (6.24) is slightly inconvenient, because the metastable free energies in (6.25) are discontinuous functions. A remedy could be to proceed as in [Zah 1984] and to define

$$\tilde{\mathfrak{z}}(Y) = \min(\mathfrak{z}(Y),\, \mathrm{e}^{-(\gamma-2\bar{\nu})|\operatorname{Supp} Y|}).$$

These functions are continuous, but not differentiable. Another problem is that when the weights take complex values, the corresponding partition functions can be zero and the definition (6.19) does not make sense.

A procedure that leads to differentiable metastable free energies in the complex case was proposed in [HKZ 1988, BK 1990]. The iterative method that we employ here follows [BK 1994]; actually, [BKU 1996] contains a simplified form of [BK 1994] which is enough for our purpose.

We choose a smooth characteristic function χ with the following properties:

- χ is a C^1 function.
- $\chi(x) = 0$ if $x \leqslant -1$; $\chi(x) = 1$ if $x \geqslant 1$.
- $0 \leqslant \frac{\mathrm{d}\chi}{\mathrm{d}x}(x) \leqslant 1$ for all x.

We define $\hat{Z}_{g_0}(\varnothing) = 1$, $f^{(0)}(g_0) = e^{\boldsymbol{\mu}}(g_0)$ for all $g_0 \in G$, $f_0^{(0)} = e_0^{\boldsymbol{\mu}}$, and set the counter n to 1. Then we enter the iterative procedure.

$\triangleright\triangleright\triangleright$ For all $g_0 \in G$, and all g_0-contours Y with $\operatorname{diam} Y = n$, let

$$\hat{\chi}(Y) = \prod_{g\in G} \chi\big(2 - 4n\beta[\operatorname{Re} f^{(n-1)}(g_0) - \operatorname{Re} f^{(n-1)}(g)]\big) \tag{6.26}$$

and

$$\hat{\mathfrak{z}}(Y) = \hat{\chi}(Y) z^{\boldsymbol{\mu},\beta}(Y)\, \mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp} Y|} \prod_{g\in G} \frac{Z_g(\operatorname{Int}_g Y)}{\hat{Z}_{g_0}(\operatorname{Int}_g Y)}. \tag{6.27}$$

Next we define the partition functions for volumes $\boldsymbol{\Lambda}'$ with $\operatorname{diam} \boldsymbol{\Lambda}' = n$:

$$\hat{Z}_{g_0}(\boldsymbol{\Lambda}') = \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\boldsymbol{\Lambda}'|} \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j), \tag{6.28}$$

where the sum is over disjoint g_0-contours in $\boldsymbol{\Lambda}'$.

At this stage it is useful to observe the following properties

LEMMA 6.6. **Iterative lemma.**

There exists γ_0 (that depends on $\bar{\nu}$ and p only) such that if (6.12)–(6.13) *hold with $\gamma > \gamma_0$, then for all Y with* $\operatorname{diam} Y = n$ *and all $\boldsymbol{\Lambda}'$ with* $\operatorname{diam} \boldsymbol{\Lambda}' = n$,

(a) $|\hat{\mathfrak{z}}(Y)| \leqslant \mathrm{e}^{-(\gamma-2)|\operatorname{Supp} Y|}$;

(b) $|\frac{\partial}{\partial \mu_i}\hat{\mathfrak{z}}(Y)| \leqslant (8\beta p + 1)|\operatorname{Vol} Y|\, \mathrm{e}^{-(\gamma-2)|\operatorname{Supp} Y|}$;

(c) $\hat{Z}_{g_0}(\boldsymbol{\Lambda}') \neq 0$ *for all* $\boldsymbol{\Lambda}'$, $\operatorname{diam} \boldsymbol{\Lambda}' = n$;

(d) $|Z_{g_0}(\boldsymbol{\Lambda}')| \leqslant \exp(-\beta f_0^{(n-1)}|\boldsymbol{\Lambda}'|)\, \mathrm{e}^{\frac{1}{8\bar{\nu}}|\partial\boldsymbol{\Lambda}'|}$;

(e) $|\frac{\partial}{\partial \mu_i} Z_{g_0}(\boldsymbol{\Lambda}')| \leqslant a\beta|\boldsymbol{\Lambda}'| \exp(-\beta f_0^{(n-1)}|\boldsymbol{\Lambda}'|)\, \mathrm{e}^{\frac{1}{8\bar{\nu}}|\partial\boldsymbol{\Lambda}'|}$.

Notice that point (c) allows to define $\hat{\mathfrak{z}}(Y)$ with (6.27) in the next loop of the iteration, i.e. for Y with $\operatorname{diam} Y = n + 1$.

The final step of the iteration is to define

$$f^{(n)}(g) = e^{\boldsymbol{\mu}}(g) + \lim_{\boldsymbol{\Lambda}\nearrow\mathbb{Z}^\nu} -\frac{1}{\beta|\boldsymbol{\Lambda}|}\log \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j) \tag{6.29}$$

with the sum over disjoint g-contours in $\boldsymbol{\Lambda}$, with diameter smaller or equal to n. We write

$$f_0^{(n)} = \min_{g\in G} \operatorname{Re} f^{(n)}(g). \tag{6.30}$$

The iterative procedure ends here. ▷▷▷

Proof of the iterative lemma. *Proof of (a):* $\hat{\mathfrak{z}}(Y)$ is given by (6.27); since $\operatorname{diam}\operatorname{Int}_g Y < n$, we can use the claim (d) of the iterative lemma to bound $Z_g(\operatorname{Int}_g Y)$. We need a lower bound for $\hat{Z}_{g_0}(\operatorname{Int}_g Y)$, which we obtain from cluster expansions. Namely, from (6.28),

$$\log \hat{Z}_{g_0}(\operatorname{Int}_g Y) = -\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Int}_g Y| + \log \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j) \tag{6.31}$$

where the sum is over disjoint g_0-contours in $\operatorname{Int}_g Y$; $|\hat{\mathfrak{z}}(Y_j) \leqslant \mathrm{e}^{-(\gamma-2)|\operatorname{Supp} Y_j|}$ by the lemma, since $\operatorname{diam} Y_j < n$. Therefore we can use cluster expansions to get

$$\log \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j) = \sum_{x\in\operatorname{Int}_g Y} \sum_{C,\operatorname{Supp}\ni x} \frac{\Phi^{\mathrm{T}}(C)}{|\operatorname{Supp} C|}; \tag{6.32}$$

all contours of the clusters are inside $\operatorname{Int}_g Y$. In particular, their diameters are smaller or equal to $n-1$; then

$$\log \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j) = -\beta|\operatorname{Int}_g Y|\big(f^{(n-1)}(g_0) - e^{\boldsymbol{\mu}}(g_0)\big) - \sum_{C,\operatorname{Supp} C\not\subset\operatorname{Int}_g Y} \Phi^{\mathrm{T}}(C)\frac{|\operatorname{Supp} C\cap\operatorname{Int}_g Y|}{|\operatorname{Supp} C|}. \tag{6.33}$$

The last sum may be bounded by (5.22); this leads to the bound for $\hat{Z}_{g_0}(\operatorname{Int}_g Y)$

$$\prod_{g\in G} |\hat{Z}_{g_0}(\operatorname{Int}_g Y)| \geqslant \mathrm{e}^{-\beta \operatorname{Re} f^{(n-1)}(g_0)|\operatorname{Int} Y|}\, \mathrm{e}^{-\frac{1}{8\bar{\nu}}|\operatorname{Supp} Y|}. \tag{6.34}$$

If $\beta(\operatorname{Re} f^{(n-1)}(g_0) - f_0^{(n-1)}) > \frac{1}{2n}$, then $\hat{\chi}(Y) = 0$ and also $\hat{\mathfrak{z}}(Y) = 0$; otherwise, we have

$$\begin{aligned} |\hat{\mathfrak{z}}(Y)| &\leqslant \mathrm{e}^{-\gamma|\operatorname{Supp} Y|}\, \mathrm{e}^{-\beta(e^{\boldsymbol{\mu}}(g_0)-e_0^{\boldsymbol{\mu}})|\operatorname{Supp} Y|} \prod_{g\in G} \mathrm{e}^{\frac{1}{4\bar{\nu}}|\partial\operatorname{Int}_g Y|}\, \mathrm{e}^{\frac{1}{2n}|\operatorname{Int}_g Y|} \\ &\leqslant \mathrm{e}^{-(\gamma-1)|\operatorname{Supp} Y|}\, \mathrm{e}^{-\beta(e^{\boldsymbol{\mu}}(g_0)-e_0^{\boldsymbol{\mu}})|\operatorname{Supp} Y|}. \end{aligned} \tag{6.35}$$

For the last inequality, we used $\sum_{g\in G}|\partial\operatorname{Int}_g Y| \leqslant 2\bar{\nu}|\operatorname{Supp} Y|$ and $\operatorname{diam} Y|\operatorname{Supp} Y| \geqslant |\operatorname{Vol} Y|$.

Finally, $e^{\boldsymbol{\mu}}(g_0)$ cannot be much larger than $e_0^{\boldsymbol{\mu}}$. Indeed, from $\beta(\operatorname{Re} f^{(n-1)}(g_0) - \operatorname{Re} f^{(n-1)}(g) \leqslant \frac{1}{2n}$ for all $g\in G$, and

$$\beta\big|e^{\boldsymbol{\mu}}(g) - f^{(n-1)}(g)\big| \leqslant \frac{1}{4}$$

by (5.25) with $c=0$ and $\delta=\frac{1}{4}$, we have $\beta(e^{\boldsymbol{\mu}}(g_0) - e_0^{\boldsymbol{\mu}}) \leqslant 1$.

Proof of (b):

$$\Big|\frac{\partial}{\partial\mu_i}\hat{\mathfrak{z}}(Y)\Big| \leqslant \Big|\frac{\partial}{\partial\mu_i}\hat{\chi}(Y)\Big|\big|z^{\boldsymbol{\mu},\beta}(Y)\,\mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp}Y|}\big|\prod_{g\in G}\Big|\frac{Z_g(\operatorname{Int}_g Y)}{Z_{g_0}(\operatorname{Int}_g Y)}\Big| \tag{6.36a}$$

$$+\hat{\chi}(Y)\Big|\frac{\partial}{\partial\mu_i}z^{\boldsymbol{\mu},\beta}(Y)\,\mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp}Y|}\big|\prod_{g\in G}\Big|\frac{Z_g(\operatorname{Int}_g Y)}{Z_{g_0}(\operatorname{Int}_g Y)}\Big| \tag{6.36b}$$

$$+\hat{\chi}(Y)\big|z^{\boldsymbol{\mu},\beta}(Y)\,\mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp}Y|}\big|\sum_{g\in G}\Big|\frac{\partial}{\partial\mu_i}\frac{Z_g(\operatorname{Int}_g Y)}{Z_{g_0}(\operatorname{Int}_g Y)}\Big|\prod_{g'\in G\setminus\{g\}}\Big|\frac{Z_{g'}(\operatorname{Int}_{g'} Y)}{Z_{g_0}(\operatorname{Int}_{g'} Y)}\Big| \tag{6.36c}$$

By the definition of $\chi(Y)$, we have

$$|\frac{\partial}{\partial\mu_i}\hat{\chi}(Y)| \leqslant \sum_{g\in G}4\beta n|\frac{\partial}{\partial\mu_i}f^{(n-1)}(g_0)-\frac{\partial}{\partial\mu_i}f^{(n-1)}(g)|. \tag{6.37}$$

Since $\beta f^{(n-1)}(g)$ has an expansion in terms of clusters, we can use the bounds (5.24) and (6.11) to get

$$|\frac{\partial}{\partial\mu_i}f^{(n-1)}(g)| \leqslant 2. \tag{6.38}$$

We obtain the bound for (6.36a), namely $8\beta p\operatorname{diam}Y\,\mathrm{e}^{-(\gamma-2)|\operatorname{Supp}Y|}$. The bound for (6.36b) is immediate from (6.13) and the bound for the ratio of partition functions; we find $(1+2\beta)\,\mathrm{e}^{-(\gamma-2)|\operatorname{Supp}Y|}$.

Finally we consider

$$\frac{\partial}{\partial\mu_i}\frac{Z_g(\operatorname{Int}_g Y)}{\hat{Z}_{g_0}(\operatorname{Int}_g Y)}=\frac{\frac{\partial}{\partial\mu_i}Z_g(\operatorname{Int}_g Y)}{\hat{Z}_{g_0}(\operatorname{Int}_g Y)}+Z_g(\operatorname{Int}_g Y)\frac{\partial}{\partial\mu_i}\frac{1}{\hat{Z}_{g_0}(\operatorname{Int}_g Y)}. \tag{6.39}$$

For the first term we combine the bound (e) of the lemma with (6.34); for the second term we have from (6.33)

$$\big[\hat{Z}_{g_0}(\operatorname{Int}_g Y)\big]^{-1} = \mathrm{e}^{\beta f^{(n-1)}(g_0)|\operatorname{Int}_g Y|}\,\mathrm{e}^{h_{g_0}(\operatorname{Int}_g Y)} \tag{6.40}$$

where $h_{g_0}(\boldsymbol{\Lambda}')$ is a sum over clusters of g_0-contours that intersect the boundary of $\boldsymbol{\Lambda}'$; $|h_{g_0}(\boldsymbol{\Lambda}')|+|\frac{\partial}{\partial\mu_i}h_{g_0}(\boldsymbol{\Lambda}')| \leqslant \frac{1}{8\bar{\nu}}|\partial\boldsymbol{\Lambda}'|$. Collecting the four bounds, we obtain

$$|\frac{\partial}{\partial\mu_i}\hat{\mathfrak{z}}(Y)| \leqslant \mathrm{e}^{-(\gamma-2)|\operatorname{Supp}Y|}\Big[8\beta p\operatorname{diam}Y+1+2\beta+(a+2)\beta|\operatorname{Int}Y|+|\operatorname{Supp}Y|\Big], \tag{6.41}$$

yielding the desired bound.

Proof of (c): Cluster expansion can be used to obtain an expansion for the logarithm. It is bounded, therefore $\hat{Z}_{g_0}$ cannot be zero.

Proof of (d): Let $a_{g_0}^{(n-1)}=\beta(\operatorname{Re}f^{(n-1)}(g_0)-f_0^{(n-1)})$; a g_0-contour is *small* if $a_{g_0}^{(n-1)}\operatorname{diam}Y \leqslant 1$, otherwise it is *big*. We write the partition function as

$$Z_{g_0}(\boldsymbol{\Lambda}')=\sum_{\{Y_1,\dots,Y_k\}}Z_{g_0}^{\mathrm{small}}(\mathrm{Ext})\prod_{j=1}^{k}z^{\boldsymbol{\mu},\beta}(Y_j)\prod_{g\in G}Z_g(\operatorname{Int}_g Y_j) \tag{6.42}$$

where the sum is over disjoint, big, external g_0-contours in $\mathbf{\Lambda}'$. $\mathrm{Ext} = \cap_{j=1}^n \mathrm{Ext}\, Y_j$ and $Z_{g_0}^{\mathrm{small}}(\mathrm{Ext})$ is the partition function that takes only into account small contours; more precisely,

$$Z_{g_0}^{\mathrm{small}}(\mathrm{Ext}) = \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\,\mathrm{Ext}\,|} \sum_{\{Y_1,\dots,Y_k\}} \prod_{j=1}^{k} \mathfrak{z}(Y_j), \tag{6.43}$$

the sum being over small, disjont g_0-contours in Ext.

Let $f^{\,\mathrm{small}}(g_0)$ be the free energy corresponding to $Z_{g_0}^{\mathrm{small}}$. We show that $f^{\,\mathrm{small}}(g_0)$ is close to $f^{(n-1)}(g_0)$; with x any site of $\mathbb{Z}^{\bar{\nu}}$,

$$\begin{aligned} f^{(n-1)}(g_0) - f^{\,\mathrm{small}}(g_0) &= \sum_{C, \mathrm{Supp}\, C \ni x} \frac{\Phi^{\mathrm{T}}(C)}{|\,\mathrm{Supp}\, C|} - \sum_{C, \mathrm{Supp}\, C \ni x,\, \mathrm{small}} \frac{\Phi^{\mathrm{T}}(C)}{|\,\mathrm{Supp}\, C|} \\ &= \sum_{C, \mathrm{Supp}\, C \ni x,\, \mathrm{big}} \frac{\Phi^{\mathrm{T}}(C)}{|\,\mathrm{Supp}\, C|}, \end{aligned} \tag{6.44}$$

and all the contours in the clusters have diameter smaller or equal to $n-1$. Big clusters contain at least one contour with diameter bigger than $1/a_{g_0}^{(n-1)}$; from (5.25), choosing $c = 2$,

$$|f^{(n-1)}(g_0) - f^{\,\mathrm{small}}(g_0)| \;\leqslant\; \mathrm{e}^{-2/a_{g_0}^{(n-1)}} \;\leqslant\; \frac{a_{g_0}^{(n-1)}}{2}. \tag{6.45}$$

We obtain the bound

$$\begin{aligned} |Z_{g_0}^{\mathrm{small}}(\mathrm{Ext})| &\leqslant \mathrm{e}^{-\beta\,\mathrm{Re}\, f^{(n-1)}(g_0)|\,\mathrm{Ext}\,|}\, \mathrm{e}^{\frac{a_{g_0}^{(n-1)}}{2}|\,\mathrm{Ext}\,|}\, \mathrm{e}^{\frac{1}{16\bar{\nu}}|\partial\,\mathrm{Ext}\,|} \\ &= \mathrm{e}^{-\beta f_0^{(n-1)}|\,\mathrm{Ext}\,|}\, \mathrm{e}^{-\frac{a_{g_0}^{(n-1)}}{2}|\,\mathrm{Ext}\,|}\, \mathrm{e}^{\frac{1}{16\bar{\nu}}|\partial\,\mathrm{Ext}\,|}. \end{aligned} \tag{6.46}$$

By the iterative lemma at steps before n, we know that

$$|Z_g(\mathrm{Int}_g\, Y)| \;\leqslant\; \mathrm{e}^{-\beta f_0^{(n-2)}|\,\mathrm{Int}_g\, Y|}\, \mathrm{e}^{\frac{1}{8\bar{\nu}}|\partial\,\mathrm{Int}_g\, Y|}. \tag{6.47}$$

We have to check that $f_0^{(n-2)}$ and $f_0^{(n-1)}$ are close. From (5.25) with $c = 1$ and $\delta = 1/\mathrm{e}$, we have for any $g_0 \in G$

$$\beta|f^{(n-1)}(g_0) - f^{(n-2)}(g_0)| \;\leqslant\; \mathrm{e}^{-(n-1)} \;\leqslant\; \frac{1}{n}. \tag{6.48}$$

Let g and g' such that $f_0^{(n-1)} = \mathrm{Re}\, f^{(n-1)}(g)$ and $f_0^{(n-2)} = \mathrm{Re}\, f^{(n-2)}(g')$ (possibly $g = g'$). Then

$$\begin{aligned} 0 - \frac{1}{n} \;\leqslant\; \beta\Big[\mathrm{Re}\, f^{(n-2)}(g) - \mathrm{Re}\, f^{(n-2)}(g')\Big] + \beta\Big[\mathrm{Re}\, f^{(n-1)}(g) - \mathrm{Re}\, f^{(n-2)}(g)\Big] = \\ = f_0^{(n-1)} - f_0^{(n-2)} = \\ = \beta\Big[\mathrm{Re}\, f^{(n-1)}(g) - \mathrm{Re}\, f^{(n-1)}(g')\Big] + \beta\Big[\mathrm{Re}\, f^{(n-1)}(g') - \mathrm{Re}\, f^{(n-2)}(g')\Big] \;\leqslant\; 0 + \frac{1}{n}. \end{aligned}$$

Recall that $\mathrm{diam}\,\mathrm{Int} \;\leqslant\; n$; we see here that

$$\beta|f_0^{(n-1)} - f_0^{(n-2)}||\,\mathrm{Int}\,| \;\leqslant\; |\partial\,\mathrm{Int}\,| \;\leqslant\; \sum_{j=1}^{k} 2\bar{\nu}|\,\mathrm{Supp}\, Y_j|.$$

At this stage, we have

$$|Z_{g_0}(\mathbf{\Lambda}')| \leqslant \mathrm{e}^{-\beta f_0^{(n-1)}|\mathbf{\Lambda}'|}\, \mathrm{e}^{\frac{1}{16\bar\nu}|\partial\mathbf{\Lambda}'|} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{external, big } g_0\text{-contours}}} \mathrm{e}^{-\frac{a g_0^{(n-1)}}{2}|\operatorname{Ext}|} \prod_{j=1}^{k} z^{\boldsymbol{\mu},\beta}(Y_j)\, \mathrm{e}^{\beta e_0^{\boldsymbol{\mu}}|\operatorname{Supp} Y_j|}\, \mathrm{e}^{-\beta(e_0^{\boldsymbol{\mu}}-f_0^{(n-1)})|\operatorname{Supp} Y_j|}\, \mathrm{e}^{2\bar\nu|\operatorname{Supp} Y_j|}. \quad (6.49)$$

If $e_0^{\boldsymbol{\mu}} = e^{\boldsymbol{\mu}}(g)$,

$$-\beta\big(e_0^{\boldsymbol{\mu}} - f_0^{(n-1)}\big) \leqslant -\beta\big(e^{\boldsymbol{\mu}}(g) - f^{(n-1)}(g)\big) \leqslant 1. \quad (6.50)$$

$$|Z_{g_0}(\mathbf{\Lambda}')| \leqslant \mathrm{e}^{-\beta f_0^{(n-1)}|\mathbf{\Lambda}'|}\, \mathrm{e}^{\frac{1}{16\bar\nu}|\partial\mathbf{\Lambda}'|} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{external, big } g_0\text{-contours}}} \mathrm{e}^{-\frac{a g_0^{(n-1)}}{2}|\operatorname{Ext}|} \prod_{j=1}^{k} \mathrm{e}^{-(\gamma-2\bar\nu-1)|\operatorname{Supp} Y_j|}. \quad (6.51)$$

Let $\tilde f$ be the free energy corresponding to a polymer model with weights $z(Y) = \mathrm{e}^{-(\gamma-2\bar\nu-2)|\operatorname{Supp} Y|}$ when Y is big, 0 otherwise, and let $\tilde Z$ be its partition function (with $\beta = 1$). We introduce

$$1 \leqslant \mathrm{e}^{\tilde f|\operatorname{Vol} Y_j|+|\operatorname{Supp} Y_j|}\, \tilde Z(\operatorname{Int} Y_j) \quad (6.52)$$

in the product of (6.51). Since only big contours are present in $\tilde Z$, again using (5.25) with $c = 2$,

$$-\tilde f \leqslant \mathrm{e}^{-2/a_g^{(n-1)}} \leqslant a_g^{(n-1)}/2 \quad (6.53)$$

if γ is large enough. Therefore

$$|Z_{g_0}(\mathbf{\Lambda}')| \leqslant \mathrm{e}^{-\beta f_0^{(n-1)}|\mathbf{\Lambda}'|}\, \mathrm{e}^{\frac{1}{16\bar\nu}|\partial\mathbf{\Lambda}'|}\, \mathrm{e}^{\tilde f|\mathbf{\Lambda}'|} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{external, big } g_0\text{-contours}}} \prod_{j=1}^{k} \mathrm{e}^{-(\gamma-2\bar\nu-2)|\operatorname{Supp} Y_j|}\, \tilde Z(\operatorname{Int} Y_j)$$
$$\leqslant \mathrm{e}^{-\beta f_0^{(n-1)}|\mathbf{\Lambda}'|}\, \mathrm{e}^{\frac{1}{8\bar\nu}|\partial\mathbf{\Lambda}'|}. \quad (6.54)$$

Proof of (e): Because of lack of time, the proof is not written here. I apologize and refer to the appendix of [BKU 1996].

□

7. Proofs of the theorems

Proof of Theorem 6.1. We use the functions $f^{(n)}(g_0)$ constructed by iteration to define the metastable free energies. We set, for all $g \in G$,

$$f^{\boldsymbol{\mu},\beta}(g) = \lim_{n\to\infty} f^{(n)}(g). \quad (6.55)$$

The limit exists, as well as the limit of derivatives; indeed, it follows from cluster expansions, that we can use because of Lemma 6.6 (a) and (b).

We check now that $\hat\chi(Y)=1$ for all g_0-contours Y, when $\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g_0)=\min_{g\in G}\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g)$. For all $n\geqslant 0$,

$$\beta\big|f^{(n-1)}(g_0)-f^{\boldsymbol{\mu},\beta}(g_0)\big|=\Big|\sum_{\substack{C,\operatorname{Supp}\ni x\\ C:\,\geqslant n}}\frac{\Phi^{\mathrm{T}}(C)}{|\operatorname{Supp}C|}\Big|\ \leqslant\ \frac{1}{8n}. \tag{6.56}$$

The sum is over clusters containing at least one contour with diameter bigger or equal to n; the last inequality follows from (5.25) with $c=1$ and $\delta=\frac{1}{8}$. Therefore, if $\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g_0)$ is minimum,

$$\beta\big(\operatorname{Re} f^{(n-1)}(g)-\operatorname{Re} f^{(n-1)}(g_0)\big)\ \geqslant\ -\frac{1}{4n}, \tag{6.57}$$

for all $g\in G$, and $\hat\chi(Y)=1$ in (6.26).

As a consequence, $\hat Z_{g_0}(\boldsymbol{\Lambda})=Z_{g_0}(\boldsymbol{\Lambda})$ for all $\boldsymbol{\Lambda}$, and the metastable free energy $f^{\boldsymbol{\mu},\beta}(g_0)$ is equal to the free energy of the system.

The analyticity of $f^{\boldsymbol{\mu},\beta}(g_0)$, in the domain where its real part is minimum, is true because it has an expansion in terms of clusters with polymers having analytic weights [when $\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g_0)$ is not minimum, the weights are C^1 but not analytic, because so is the function $\hat\chi(Y)$].

The last claim is a consequence of the inverse function theorem.

□

Proof of Theorem 6.2. The expectation value of local observables has an expansion in terms of contours, see (6.17). K-contours have various external labels, but we would prefer them to have external label g_0.

Consider observables K, and a contour configuration $\mathfrak{Y}_K\cup\mathfrak{Y}$. We gather together a contour $Y_K\in\mathfrak{Y}_K$ with contours that surround it. We also consider collections of contours surrounding supports of observables. Whenever a contour belongs to two different collections, we take the union of the collections. See Fig. 6.4 for a concrete example. We denote by $\mathcal{Y}_K$ a collection of contours and observables such that one contour surround all others (this contour can be a usual contour, or a K-contour).

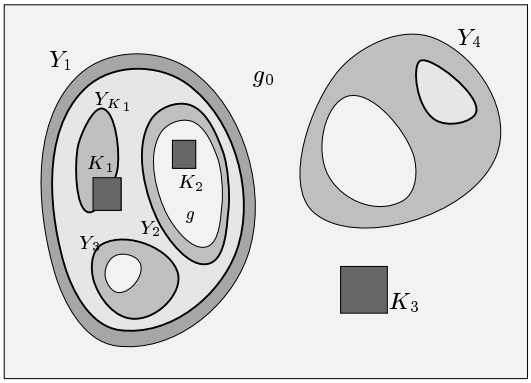


Figure 6.4. Five contours and three observables. $\mathfrak{Y}_K=\{Y_{K_1}\}$, $\mathfrak{Y}=\{Y_1,Y_2,Y_3,Y_4\}$; then $\mathfrak{Y}'_K=\{\mathcal{Y}_K\}$ with $\mathcal{Y}_K=\{Y_{K_1},Y_1,Y_2\}$ and $\mathfrak{Y}'=\{Y_3,Y_4\}$. Here $z_K(\mathcal{Y}_K)=z_K(Y_{K_1})z(Y_1)z(Y_2)K_2(g)$; the contribution of K_3 is a factor $K_3(g_0)$.

We define the weight $z_K(\mathcal{Y}_K)$ to be

$$z_K(\mathcal{Y}_K) = \prod_{Y_K \in \mathcal{Y}_K} z_K(Y_K) \prod_{Y \in \mathcal{Y}_K} z(Y) \prod K_i(g_i) \tag{6.58}$$

The last product is over those observables K_i such that $\operatorname{Supp} K_i \subset \operatorname{Vol} \mathcal{Y}_K$, but K_i does not belong to any K-contour of $\mathcal{Y}_K$. The configuration $g_i \in G$ is chosen according to the labels of contours of $\mathcal{Y}_K$. We define

$$\operatorname{Supp} \mathcal{Y}_K = \bigcup_{Y_K \in \mathcal{Y}_K} \operatorname{Supp} Y_K \bigcup_{Y \in \mathcal{Y}_K} \operatorname{Supp} Y \bigcup_{i : \operatorname{Supp} K_i \subset \operatorname{Vol} \mathcal{Y}_K} \operatorname{Supp} K_i.$$

Let $J \subset I$ denote the observables concerned by $\mathcal{Y}_K$. We have the bound for $z_K(\mathcal{Y}_K)$

$$|z_K(\mathcal{Y}_K)| \leqslant \mathrm{e}^{-\beta e_0^{\boldsymbol{\mu}} |\operatorname{Supp} \mathcal{Y}_K|} \, \mathrm{e}^{-\gamma |\operatorname{Supp} \mathcal{Y}_K|} \prod_{i \in J} C_{K_i} \, \mathrm{e}^{\gamma |\operatorname{Supp} K_i|}. \tag{6.59}$$

It is possible to rewrite Equation (6.17) by first summing over sets $\mathfrak{Y}'_K$ of collections of contours, then over compatible sets of contours, namely

$$\left\langle \prod_i K_i \right\rangle_{\boldsymbol{\Lambda}, g_0} = \frac{1}{Z_{g_0}(\boldsymbol{\Lambda})} \sum_{\mathfrak{Y}'_K} \sum_{\mathfrak{Y}' : \mathfrak{Y}'_K} \prod_{i \in I : \operatorname{Supp} K_i \not\subset \operatorname{Vol}(\mathfrak{Y}'_K \cup \mathfrak{Y}')} K_i(g_0) \prod_{g \in G} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g) |\mathfrak{W}_g(\mathfrak{Y}'_K \cup \mathfrak{Y}')|} \prod_{\mathcal{Y}_K \in \mathfrak{Y}'_K} z_K(\mathcal{Y}_K) \prod_{Y \in \mathfrak{Y}'} z^{\boldsymbol{\mu}, \beta}(Y). \tag{6.60}$$

The constraint $\mathfrak{Y}' : \mathfrak{Y}'_K$ means that $\mathfrak{Y}'_K \cup \mathfrak{Y}'$ is admissible and compatible with the boundary conditions g_0, and moreover that $\operatorname{Vol} Y \not\Subset \operatorname{Supp} \mathcal{Y}_K$ for all $Y \in \mathfrak{Y}'$ and $\mathcal{Y}_K \in \mathfrak{Y}'_K$.

The next step consists in defining

$$\mathfrak{z}_K(\mathcal{Y}_K) = z_K(\mathcal{Y}_K) \, \mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0) |\operatorname{Supp} \mathcal{Y}_K|} \prod_{g \in G} \frac{Z_g(\operatorname{Int}_g \mathcal{Y}_K)}{Z_{g_0}(\operatorname{Int}_g \mathcal{Y}_K)}. \tag{6.61}$$

This makes sense, since $Z_{g_0}(\boldsymbol{\Lambda}') \neq 0$ when $\operatorname{Re} f^{\boldsymbol{\mu}, \beta}(g_0)$ is minimum. Furthermore, we have the bound

$$|\mathfrak{z}_K(\mathcal{Y}_K)| \leqslant \mathrm{e}^{-(\gamma - 2) |\operatorname{Supp} \mathcal{Y}_K|}. \tag{6.62}$$

Remark that in (6.61) interiors of $\mathcal{Y}_K$ are not necessarily simply connected sets, and the contours in $Z_\cdot(\operatorname{Int}_g \mathcal{Y}_K)$ are required to have simply connected volumes. This makes the situation slightly different to that of the previous section. However, it is clear that all the steps can be repeated almost without any change.

The expectation value of local observables can be rewritten using (6.61)

$$\left\langle \prod_i K_i \right\rangle_{\boldsymbol{\Lambda}, g_0} = \frac{1}{Z_{g_0}(\boldsymbol{\Lambda})} \, \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0) |\boldsymbol{\Lambda}|} \sum_{\mathfrak{Y}'_K} \prod_{i \in I : \operatorname{Supp} K_i \not\subset \operatorname{Vol} \mathfrak{Y}'_K} K_i(g_0) \prod_{\mathcal{Y}_K \in \mathfrak{Y}'_K} \mathfrak{z}_K(\mathcal{Y}_K) \sum_{\substack{\{Y_1, \dots, Y_k\} \\ g_0\text{-contours}, Y_j \sim \mathfrak{Y}'_K}} \prod_{j=1}^{k} \hat{\mathfrak{z}}(Y_j) \tag{6.63}$$

where the last sum is restricted to contours Y_j such that $\operatorname{Vol} Y_j \not\Subset (\operatorname{Supp} \mathfrak{Y}'_K \cup \operatorname{Supp} K)$. We can use cluster expansion for the logarithm of the last sum, as well as for $Z_{\boldsymbol{\Lambda}, g_0}$, so as

to obtain

$$\Big\langle \prod_i K_i \Big\rangle_{\mathbf{\Lambda},g_0} = \sum_{\mathfrak{Y}'_K} \prod_{i\in I:\mathrm{Supp}\, K_i \not\subset \mathrm{Vol}\, \mathfrak{Y}'_K} K_i(g_0) \prod_{\mathcal{Y}_K\in\mathfrak{Y}'_K} \mathfrak{z}_K(\mathcal{Y}_K) \exp\Big(\sum_{C:\mathfrak{Y}'_K,K} \Phi^{\mathrm{T}}(C)\Big). \quad (6.64)$$

Here, the constraint $C:\mathfrak{Y}'_K,K$ means that at least one g_0-contour of C has volume that intersects $\mathrm{Supp}\,\mathfrak{Y}_K \cup \mathrm{Supp}\, K$.

The above expression is absolutely convergent, uniformly in $\mathbf{\Lambda}$. This proves the first claim of Theorem 6.2.

For the second claim, we note that, in (6.64), the case $\mathfrak{Y}'_K = \varnothing$ yields $\prod_i K_i(g_0)$; consequently, the difference between $\langle K\rangle_{g_0}$ and $K(g_0)$ is as in (6.64), but with a sum over non-empty $\mathfrak{Y}'_K$. Because of the bound (6.59), and bounds on clusters, we get the claim.

To prove the last claim, we write

$$\langle \prod_i K_i\rangle_{g_0} = \langle \prod_i K_i\rangle^{\mathrm{short}}_{g_0} + \langle \prod_i K_i\rangle^{\mathrm{big}}_{g_0}, \quad (6.65)$$

where $\langle \prod_i K_i\rangle^{\mathrm{short}}_{g_0}$ is given by (6.64), except for a restriction on the sizes of elements in $\mathfrak{Y}'_K$ and clusters. Namely, only collections $\mathcal{Y}_K$ with $|\,\mathrm{Supp}\,\mathcal{Y}_K| < \frac{1}{4}d(K)$ and clusters C with $|\,\mathrm{Supp}\, C| < \frac{1}{4}d(K)$ are considered.

$\langle \prod_i K_i\rangle^{\mathrm{big}}_{g_0}$ involves a sum over $\mathfrak{Y}'_K$ where at least one $\mathcal{Y}_K \in \mathfrak{Y}'_K$ has bigger support, and a sum over all $\mathfrak{Y}'_K$, but with a contribution of clusters

$$\exp\Big(\sum_{C:\mathfrak{Y}'_K,K} \Phi^{\mathrm{T}}(C)\Big) - \exp\Big(\sum_{\substack{C:\mathfrak{Y}'_K,K\\ \mathrm{short}}} \Phi^{\mathrm{T}}(C)\Big) =$$
$$= \exp\Big(\sum_{\substack{C:\mathfrak{Y}'_K,K\\ \mathrm{short}}} \Phi^{\mathrm{T}}(C)\Big)\Big[\exp\Big(\sum_{\substack{C:\mathfrak{Y}'_K,K\\ \mathrm{big}}} \Phi^{\mathrm{T}}(C)\Big) - 1\Big]. \quad (6.66)$$

It is clear that we have exponential decay, namely that there exists ξ such that

$$|\langle \prod_i K_i\rangle^{\mathrm{big}}_{g_0}| \;\leqslant\; \mathrm{e}^{-d(K)/\xi} \prod_{i\in I} C_{K_i}. \quad (6.67)$$

The proof can be completed by expanding each $\langle K_i\rangle_{g_0}$ as above, and writing $\langle K_i\rangle_{g_0} = \langle K_i\rangle^{\mathrm{short}}_{g_0} + \langle K_i\rangle^{\mathrm{big}}_{g_0}$. Since

$$\langle \prod_i K_i\rangle^{\mathrm{short}}_{g_0} = \prod_i \langle K_i\rangle^{\mathrm{short}}_{g_0}, \quad (6.68)$$

and each $\langle K_i\rangle^{\mathrm{big}}_{g_0}$ having exponential decay, we obtain the bound of Theorem 6.2.

□

Because of lack of time, no proof for Theorem 6.3 (expectation values of local observables with periodic boundary conditions) is provided here; we refer to e.g. [BKU 1996].

Before entering the proof of Theorem 6.4, let us observe that the weights $z^{\boldsymbol{\mu},\beta,\alpha}(Y)$ converge to $z^{\boldsymbol{\mu},\beta}(Y)$ uniformly in Y:

Lemma 6.7.

For any $\varepsilon > 0$, there exists $\bar\alpha > 0$ such that if $\alpha \leqslant \bar\alpha$,

$$|z^{\boldsymbol{\mu},\beta,\alpha}(Y) - z^{\boldsymbol{\mu},\beta}(Y)| \;\leqslant\; \varepsilon\, \mathrm{e}^{-\frac{\gamma}{2}|\,\mathrm{Supp}\, Y|}$$

for all contours Y.

PROOF. Let us fix ε. For any Y such that $|\operatorname{Supp} Y| \geqslant \frac{2}{\gamma}\log\frac{2}{\varepsilon}$, we have

$$|z^{\boldsymbol{\mu},\beta,\alpha}(Y) - z^{\boldsymbol{\mu},\beta}(Y)| \leqslant 2\,\mathrm{e}^{-\gamma|\operatorname{Supp} Y|} \leqslant \varepsilon\,\mathrm{e}^{-\frac{\gamma}{2}|\operatorname{Supp} Y|}. \tag{6.69}$$

On the other hand, for any Y there exists $\bar\alpha(Y) > 0$ such that

$$|z^{\boldsymbol{\mu},\beta,\alpha}(Y) - z^{\boldsymbol{\mu},\beta}(Y)| \leqslant \varepsilon\,\mathrm{e}^{-\frac{\gamma}{2}|\operatorname{Supp} Y|} \tag{6.70}$$

for $\alpha \leqslant \bar\alpha(Y)$. Therefore we can choose

$$\bar\alpha = \min_{Y,|\operatorname{Supp} Y| \leqslant \frac{2}{\gamma}\log\frac{2}{\varepsilon}} \bar\alpha(Y). \tag{6.71}$$

□

PROOF OF THEOREM 6.4. Let us define

$$\tilde z(Y) = z^{\boldsymbol{\mu},\beta,\alpha}(Y) - z^{\boldsymbol{\mu},\beta}(Y). \tag{6.72}$$

From the lemma, we know that $|\tilde z(Y)| \leqslant \varepsilon\,\mathrm{e}^{-\frac{\gamma}{2}|\operatorname{Supp} Y|}$ for all Y, if α is small enough. First let us see that, if $a_{g_0}\operatorname{diam}\boldsymbol{\Lambda} \leqslant 1$,

$$\mathrm{e}^{-O(\alpha)|\boldsymbol{\Lambda}|} \leqslant \Big|\frac{Z^\alpha_{g_0}(\boldsymbol{\Lambda})}{Z_{g_0}(\boldsymbol{\Lambda})}\Big| \leqslant \mathrm{e}^{O(\alpha)|\boldsymbol{\Lambda}|}, \tag{6.73}$$

with $Z^\alpha_{g_0}(\boldsymbol{\Lambda})$ the partition function with weights $z^{\boldsymbol{\mu},\beta,\alpha}$.

$$\begin{aligned} Z^\alpha_{g_0}(\boldsymbol{\Lambda}) &= \sum_{\{Y_1,\dots,Y_k\}} \prod_{g\in G} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g)|\mathfrak{W}_g(\{Y_1,\dots,Y_k\})|} \prod_{j=1}^k \big(\tilde z(Y_j) + z^{\boldsymbol{\mu},\beta}(Y_j)\big) \\ &= \sum_{\{Y_1,\dots,Y_\ell\}} \Big[\prod_{j=1}^\ell \tilde z(Y_j)\Big] Z_{g_0}(\boldsymbol{\Lambda} \setminus \cup_j \operatorname{Supp} Y_j). \end{aligned} \tag{6.74}$$

It is not hard to check[7] that the ratio

$$\frac{Z_{g_0}(\boldsymbol{\Lambda} \setminus \cup_j \operatorname{Supp} Y_j)}{Z_{g_0}(\boldsymbol{\Lambda})}$$

may be bounded by $\prod_j \mathrm{e}^{|\operatorname{Supp} Y_j|}$. Therefore

$$\Big|\frac{Z^\alpha_{g_0}(\boldsymbol{\Lambda})}{Z_{g_0}(\boldsymbol{\Lambda})}\Big| \leqslant \sum_{\{Y_1,\dots,Y_\ell\}} \prod_{j=1}^\ell |\tilde z(Y_j)|\,\mathrm{e}^{|\operatorname{Supp} Y_j|}. \tag{6.75}$$

The bound (6.73) is now immediate.

Since $Z^\alpha_{g_0}(\boldsymbol{\Lambda}) \neq 0$, the expectation value of K in the model with weights $z^{\boldsymbol{\mu},\beta,\alpha}$ is well defined at finite volume and is given by (6.63). We can use the standard trick of Pirogov-Sinai theory, namely to define new weights

$$\mathfrak{z}^\alpha(Y) = z^{\boldsymbol{\mu},\beta,\alpha}(Y)\,\mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp} Y|} \prod_{g\in G} \frac{Z^\alpha_g(\operatorname{Int}_g Y)}{Z^\alpha_{g_0}(\operatorname{Int}_g Y)} \tag{6.76}$$

$$\mathfrak{z}^\alpha_K(\mathcal{Y}_K) = z^{\boldsymbol{\mu},\beta,\alpha}_K(\mathcal{Y}_K)\,\mathrm{e}^{\beta e^{\boldsymbol{\mu}}(g_0)|\operatorname{Supp}\mathcal{Y}_K|} \prod_{g\in G} \frac{Z^\alpha_g(\operatorname{Int}_g \mathcal{Y}_K)}{Z^\alpha_{g_0}(\operatorname{Int}_g \mathcal{Y}_K)}. \tag{6.77}$$

[7] The idea is, of course, to use cluster expansions. The only difficulty is that the volume is not necessarily simply connected; however, the contribution of the contours that surround the holes of the volumes can be easily estimated.

We prove in Lemma 6.8 below that the ratio of partition functions satisfy a bound that allows to use cluster expansions. Therefore we have an expression similar to that of (6.64). This expansion is absolutely convergent, uniformly in $\mathbf{\Lambda}$, which proves the first claim of Theorem 6.4. Furthermore, since $|\mathfrak{z}^\alpha(Y)| \leqslant \mathrm{e}^{-\gamma'|\operatorname{Supp} Y|}$, and similarly for $\mathfrak{z}^\alpha_K(\mathcal{Y}_K)$, we have by Lemma 6.7 that $\mathfrak{z}^\alpha(Y) \to \mathfrak{z}(Y)$ uniformly in Y, so that we get the second claim. □

Recall that we defined $a_g = \beta(\operatorname{Re} f^{\boldsymbol{\mu},\beta}(g) - f_0^{\boldsymbol{\mu},\beta})$.

Lemma 6.8.

Assume that the set $\{g \in G : \operatorname{Re} f^{\boldsymbol{\mu},\beta}(g) = f_0^{\boldsymbol{\mu},\beta}\}$ *has only one element. Then there exists* $\bar\alpha > 0$ *such that if* $\alpha \leqslant \bar\alpha$ *and* $a_{g_0} \operatorname{diam} \mathbf{\Lambda} \leqslant 1$,

- $Z^\alpha_{g_0}(\mathbf{\Lambda}) \neq 0$,
- $\left|\frac{Z^\alpha_g(\mathbf{\Lambda})}{Z^\alpha_{g_0}(\mathbf{\Lambda})}\right| \leqslant \mathrm{e}^{5|\partial\mathbf{\Lambda}|}$.

Proof. We proceed by induction on the size of $\mathbf{\Lambda}$. The statements are clear when $\mathbf{\Lambda} = \varnothing$, and we look now to the situation where $\operatorname{diam}\mathbf{\Lambda} = n$.

By the induction hypothesis, $Z^\alpha_{g_0}(\operatorname{Int}_g Y) \neq 0$ if Y is a contour in $\mathbf{\Lambda}$; the definition (6.76) makes sense, and

$$Z^\alpha_{g_0}(\mathbf{\Lambda}) = \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g_0)|\mathbf{\Lambda}|} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ g_0\text{-contours}}} \prod_{j=1}^k \mathfrak{z}^\alpha(Y_j). \tag{6.78}$$

$\mathfrak{z}^\alpha(Y_j)$ has exponential decay; hence $Z^\alpha_{g_0}(\mathbf{\Lambda})$ differs from 0 by the cluster expansion.

The bound for the ratio of partition functions is proven in a similar way as Lemma 6.6 (d). We call "small" a g-contour Y with $a_g \operatorname{diam} Y \leqslant 1$, Y is "big" otherwise.

$$\frac{Z^\alpha_g(\mathbf{\Lambda})}{Z^\alpha_{g_0}(\mathbf{\Lambda})} = \frac{1}{Z^\alpha_{g_0}(\mathbf{\Lambda})} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{big, external}}} Z^{\alpha,\,\text{small}}_g(\operatorname{Ext}) \prod_{j=1}^k \Big\{ z^{\boldsymbol{\mu},\beta,\alpha}(Y_j) \prod_{g'\in G} Z^\alpha_{g'}(\operatorname{Int}_{g'} Y_j)\Big\}. \tag{6.79}$$

Here, $\operatorname{Ext} = \cap_j \operatorname{Ext} Y_j$ and

$$Z^{\alpha,\,\text{small}}_g(\mathbf{\Lambda}') \doteq \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{small, external}}} \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g)|\operatorname{Ext}|} \prod_{j=1}^k \Big\{ z^{\boldsymbol{\mu},\beta,\alpha}(Y_j) \prod_{g'\in G} Z^\alpha_{g'}(\operatorname{Int}_{g'} Y_j)\Big\}. \tag{6.80}$$

For small g-contour Y_j, and if $\operatorname{diam}\mathbf{\Lambda}' \leqslant n-1$, we can use the induction hypothesis so as to write

$$Z^{\alpha,\,\text{small}}_g(\mathbf{\Lambda}') = \mathrm{e}^{-\beta e^{\boldsymbol{\mu}}(g)|\mathbf{\Lambda}'|} \sum_{\substack{\{Y_1,\dots,Y_k\}\\ \text{small}}} \prod_{j=1}^k \mathfrak{z}^\alpha(Y_j) \tag{6.81}$$

with $|\mathfrak{z}^\alpha(Y_j)| \leqslant \mathrm{e}^{-(\gamma-10\bar\nu)|\operatorname{Supp} Y_j|}$. Proceeding as in the proof for the bound (6.73), we get

$$\begin{aligned} |Z^{\alpha,\,\text{small}}_g(\mathbf{\Lambda}')| &\leqslant |Z^{\text{small}}_g(\mathbf{\Lambda}')|\, \mathrm{e}^{O(\alpha)|\mathbf{\Lambda}'|} \\ &\leqslant \mathrm{e}^{-\beta[\operatorname{Re} f^{\text{small}}(g)+O(\alpha)]|\mathbf{\Lambda}'|}\, \mathrm{e}^{|\partial\mathbf{\Lambda}'|}. \end{aligned} \tag{6.82}$$

Furthermore $f^{\,\mathrm{small}}(g)$ is close to $f^{\boldsymbol{\mu},\beta}(g)$:

$$\beta|f^{\,\mathrm{small}}(g) - f^{\boldsymbol{\mu},\beta}(g)| \;\leqslant\; \sum_{\substack{C,\mathrm{Supp}\,C\ni x\\ \mathrm{big}}} \frac{|\Phi^{\mathrm{T}}(C)|}{|\,\mathrm{Supp}\,C|} \;\leqslant\; a_g/4. \tag{6.83}$$

Let us come back to (6.79); let $\mathrm{Supp} = \cup_{j=1}^{k} \mathrm{Supp}\,Y_j$, and observe that

$$|Z^{\alpha}_{g_0}(\boldsymbol{\Lambda})| \;\geqslant\; |Z^{\alpha}_{g_0}(\mathrm{Ext})|\,\mathrm{e}^{-\,\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0)|\,\mathrm{Supp}\,|}\;\mathrm{e}^{-|\partial\boldsymbol{\Lambda}|-|\,\mathrm{Supp}\,|}\prod_{j=1}^{k}|Z^{\alpha}_{g_0}(\mathrm{Int}\,Y_j)|. \tag{6.84}$$

Therefore

$$\begin{aligned}
\Big|\frac{Z^{\alpha}_{g}(\boldsymbol{\Lambda})}{Z^{\alpha}_{g_0}(\boldsymbol{\Lambda})}\Big| \;&\leqslant\; \mathrm{e}^{|\partial\boldsymbol{\Lambda}|}\sum_{\substack{\{Y_1,\dots,Y_k\}\\ \mathrm{big,\ external}}}\Big|\frac{Z^{\alpha,\,\mathrm{small}}_{g}(\mathrm{Ext})}{Z^{\alpha}_{g_0}(\mathrm{Ext})}\Big|\\
&\qquad\prod_{j=1}^{k}\Big\{|z^{\boldsymbol{\mu},\beta,\alpha}(Y_j)|\,\mathrm{e}^{[\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0)+1]|\,\mathrm{Supp}\,Y_j|}\prod_{g'\in G}\Big|\frac{Z^{\alpha}_{g'}(\mathrm{Int}_{g'}\,Y_j)}{Z^{\alpha}_{g_0}(\mathrm{Int}_{g'}\,Y_j)}\Big|\Big\}\\
&\leqslant\; \mathrm{e}^{2|\partial\boldsymbol{\Lambda}|}\sum_{\substack{\{Y_1,\dots,Y_k\}\\ \mathrm{big,\ external}}}\mathrm{e}^{-\beta[\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g)-\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0)]|\,\mathrm{Ext}\,|}\;\mathrm{e}^{[O(\alpha)+\frac{a_g}{4}]|\,\mathrm{Ext}\,|}\\
&\qquad\prod_{j=1}^{k}\mathrm{e}^{-(\gamma-1-10\bar{\nu})|\,\mathrm{Supp}\,Y_j|}\;\mathrm{e}^{-\beta[e_0^{\boldsymbol{\mu}}-\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0)]|\,\mathrm{Supp}\,Y_j|}.
\end{aligned}$$

First we observe that

$$\begin{aligned}
-\beta\big(\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g) - \mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0)\big) + O(\alpha) &= -a_g + a_{g_0} + O(\alpha)\\
&\leqslant\; -\tfrac{1}{2}a_g + 2a_{g_0}
\end{aligned}$$

if α is small enough — we use here the fact that a_g and a_{g_0} cannot be zero at the same time when $g \neq g_0$. Second we estimate $e_0^{\boldsymbol{\mu}} - f^{\boldsymbol{\mu},\beta}(g_0)$. $\beta|e_0^{\boldsymbol{\mu}} - f_0^{\boldsymbol{\mu},\beta}| \;\leqslant\; 1$ from cluster expansion, and $\beta(\mathrm{Re}\,f^{\boldsymbol{\mu},\beta}(g_0) - f_0^{\boldsymbol{\mu},\beta}) = a_{g_0}$. We obtain

$$\Big|\frac{Z^{\alpha}_{g}(\boldsymbol{\Lambda})}{Z^{\alpha}_{g_0}(\boldsymbol{\Lambda})}\Big| \;\leqslant\; \mathrm{e}^{2|\partial\boldsymbol{\Lambda}|}\sum_{\substack{\{Y_1,\dots,Y_k\}\\ \mathrm{big,\ external}}}\mathrm{e}^{-\frac{1}{4}a_g|\,\mathrm{Ext}\,|}\;\mathrm{e}^{2a_{g_0}(|\,\mathrm{Ext}\,|+|\,\mathrm{Supp}\,|)}\prod_{j=1}^{k}\mathrm{e}^{-(\gamma-2-10\bar{\nu})|\,\mathrm{Supp}\,Y_j|}. \tag{6.85}$$

Let $\check{Z}$ be a partition function with big g-contours Y having weights $\mathrm{e}^{-(\gamma-3-10\bar{\nu})|\,\mathrm{Supp}\,Y|}$ and $\check{f}$ be the corresponding free energy with $\beta = 1$. Since

$$1 \;\leqslant\; \mathrm{e}^{\check{f}|\,\mathrm{Vol}\,Y|}\;\mathrm{e}^{|\,\mathrm{Supp}\,Y|}\,\check{Z}(\mathrm{Int}\,Y),$$

we can write

$$\Big|\frac{Z^{\alpha}_{g}(\boldsymbol{\Lambda})}{Z^{\alpha}_{g_0}(\boldsymbol{\Lambda})}\Big| \;\leqslant\; \mathrm{e}^{2|\partial\boldsymbol{\Lambda}|}\;\mathrm{e}^{2a_{g_0}|\boldsymbol{\Lambda}|}\sum_{\substack{\{Y_1,\dots,Y_k\}\\ \mathrm{big,\ external}}}\mathrm{e}^{-\frac{1}{4}a_g|\,\mathrm{Ext}\,|}\prod_{j=1}^{k}\mathrm{e}^{\check{f}|\,\mathrm{Vol}\,Y_j|}\;\mathrm{e}^{-(\gamma-3-10\bar{\nu})|\,\mathrm{Supp}\,Y_j|}\,\check{Z}(\mathrm{Int}\,Y_j). \tag{6.86}$$

We obtain the desired bound by using $a_{g_0}|\boldsymbol{\Lambda}| \;\leqslant\; |\partial\boldsymbol{\Lambda}|$, and $-\frac{1}{4}a_g \;\leqslant\; \check{f}$. □

CHAPTER 7

Contour representation for quantum models

The idea to expand a quantum model around its potential part is not new at all. It was proposed by Ginibre thirty years ago, as a tool to establish the existence of phase transitions in different quantum lattice models [Gin 1969]. The proof combined Trotter formula and Peierls argument. A different approach, that does not make use of the Trotter formula but also rely on the Peierls argument, was simultaneously proposed by Robinson [Rob 1969]. This more algebraic method was used to show that the lattice gas with nearest-neighbour repulsion (antiferromagnetic Ising model) is stable against small kinetic moves [LM 1993].

The Trotter formula was used for various studies of quantum lattice models. Kennedy [Ken 1985] proved long-range order in the anisotropic Heisenberg ferromagnet;[1] it should be noticed that his method is perturbative in the temperature, but not in the anisotropy coefficient — for all anisotropy, it is possible to be at low enough temperature and to observe the chessboard structure. Again with the Trotter formula, the Ising model with strong transverse magnetic field can be shown to have Ornstein-Zernike decay of the two-point function [Ken 1991]. A boson model with nearest-neighbour interaction was proposed in [MS 1996] and the low temperature phases were established; the ground state has a finite degeneracy, that is removed by mixed thermal-quantum fluctuations (our results, from this chapter and the next one, are not sufficient to cover this situation). The Falicov-Kimball was investigated in [MM 1996]; the degeneracy of the ground states of the classical model was shown to be removed by the quantum fluctuations. One-dimensional spin systems were studied by [AN 1994]; using a functional integral representation, the quantum spin chain is mapped onto a two-dimensional Potts model, and studied in a random-cluster representation.

The extension of Pirogov-Sinai theory to quantum lattice models was proposed in [Pir 1978], but was realized only 20 years later [BKU 1996, DFF 1996]. Both papers apply to spin systems, but the latter also deals with fermion systems. An extension to bosons can be found in [BKU 1997] (with a discussion of the incompressibility of the ground states). A class of models where the ground states of the classical part are infinitely degenerated was studied in [DFFR 1996, FR 1996, KU 1998]; see Chapter 8. Interfaces in quantum models are discussed in [BCF 1997] (see also [DMN 1998]).

1. Duhamel expansion

We consider a system with Hamiltonian $H_\Lambda = T_\Lambda + V_\Lambda$, where V_Λ is an operator that is the quantum equivalent of a classical interaction. T_Λ is a quantum perturbation, as for instance a small kinetic matrix. Our aim is to obtain expansions of the operator $\mathrm{e}^{-\beta T_\Lambda - \beta V_\Lambda}$; recall that this operator plays a role in the definition of the free energy of the system.

[1] A page devoted to the Heisenberg model, and results of Mathematical Physics around, exists on internet [KN 1994–].

Our starting point is the Duhamel formula

$$\mathrm{e}^{-\beta V_\Lambda - \beta T_\Lambda} \;=\; \mathrm{e}^{-\beta V_\Lambda} \;+\; \int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{-\tau V_\Lambda}\,(-T_\Lambda)\,\mathrm{e}^{-(\beta-\tau)(V_\Lambda+T_\Lambda)}\,. \tag{7.1}$$

(It can be proved by showing that both sides satisfy the differential equation $\frac{\mathrm{d}}{\mathrm{d}\beta}[\cdot] = -[\cdot][V_\Lambda + T_\Lambda]$.) Iterating, we obtain

$$\mathrm{e}^{-\beta V_\Lambda - \beta T_\Lambda} \;=\; \mathrm{e}^{-\beta V_\Lambda} \;+\; \sum_{m\,\geqslant\,1} \int_{0<\tau_1<\ldots<\tau_m<\beta} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_m \\ \mathrm{e}^{-\tau_1 V_\Lambda}\,(-T_\Lambda)\,\mathrm{e}^{-(\tau_2-\tau_1)V_\Lambda}\;\ldots\,(-T_\Lambda)\,\mathrm{e}^{-(\beta-\tau_m)V_\Lambda}\,. \tag{7.2}$$

T_Λ is a quantum interaction, i.e. $T_\Lambda = \sum_{\boldsymbol{A},A\subset\Lambda} T_{\boldsymbol{A}}$. Inserting the expansion of unity $\mathbb{1} = \sum_{n_\Lambda\in\Omega^\Lambda} |n_\Lambda\rangle\langle n_\Lambda|$ on the right of each operator $(-T_\Lambda)$, we obtain an expression for the trace, namely

$$\mathrm{Tr}\;\mathrm{e}^{-\beta V_\Lambda - \beta T_\Lambda} = \mathrm{Tr}\;\mathrm{e}^{-\beta V_\Lambda} + \sum_{m\,\geqslant\,1} (-1)^m \sum_{\boldsymbol{A}_1,\ldots,\boldsymbol{A}_m} \sum_{n_\Lambda^{(1)},\ldots,n_\Lambda^{(m)}} \int_{0<\tau_1<\ldots<\tau_m<\beta} \mathrm{d}\tau_1\ldots\mathrm{d}\tau_m \\ \mathrm{e}^{-\tau_1 V_\Lambda(n_\Lambda^{(1)})}\,\langle n_\Lambda^{(1)}|\,T_{\boldsymbol{A}_1}\,|n_\Lambda^{(2)}\rangle\,\mathrm{e}^{-(\tau_2-\tau_1)V_\Lambda(n_\Lambda^{(2)})}\;\ldots\,\langle n_\Lambda^{(m)}|\,T_{\boldsymbol{A}_m}\,|n_\Lambda^{(1)}\rangle\,\mathrm{e}^{-(\beta-\tau_m)V_\Lambda(n_\Lambda^{(1)})}\,, \tag{7.3}$$

where we used $V_\Lambda(n_\Lambda)$ instead of $\langle n_\Lambda|\,V_\Lambda\,|n_\Lambda\rangle$.

Remark that a similar expansion can be done using Trotter formula:

$$\mathrm{e}^{-\beta V_\Lambda - \beta T_\Lambda} \;=\; \lim_{N\to\infty}\Big(\,\mathrm{e}^{-V_\Lambda/N}\;\mathrm{e}^{-T_\Lambda/N}\,\Big)^{\beta N} \;=\; \lim_{N\to\infty}\Big(\,\mathrm{e}^{-V_\Lambda/N}\,\big[1-\frac{T_\Lambda}{N}\big]\Big)^{\beta N}. \tag{7.4}$$

Proceeding in the same way as with the Duhamel expansion, we obtain a discrete analogous of (7.3)

$$\mathrm{Tr}\;\mathrm{e}^{-\beta V_\Lambda - \beta T_\Lambda} = \mathrm{Tr}\;\mathrm{e}^{-\beta V_\Lambda} + \lim_{N\to\infty} \sum_{m=1}^{\beta N} (-1)^m \sum_{\boldsymbol{A}_1,\ldots,\boldsymbol{A}_m} \sum_{n_\Lambda^{(1)},\ldots,n_\Lambda^{(m)}} \sum_{1\,\leqslant\,\tau_1<\ldots<\tau_m\,\leqslant\,\beta N} \\ \mathrm{e}^{-\frac{\tau_1}{N}V_\Lambda(n_\Lambda^{(1)})}\,\langle n_\Lambda^{(1)}|\,\frac{T_{\boldsymbol{A}_1}}{N}\,|n_\Lambda^{(2)}\rangle\,\mathrm{e}^{-\frac{\tau_2-\tau_1}{N}V_\Lambda(n_\Lambda^{(2)})}\;\ldots\,\langle n_\Lambda^{(m)}|\,\frac{T_{\boldsymbol{A}_m}}{N}\,|n_\Lambda^{(1)}\rangle\,\mathrm{e}^{-\frac{\beta N-\tau_m}{N}V_\Lambda(n_\Lambda^{(1)})}\,. \tag{7.5}$$

The two expansions are totally equivalent for our purpose. Actually, our choice to use the Duhamel formula is motivated mainly by esthetic considerations.

2. Models with local interactions

When the potential V is an on-site interaction, i.e. when it is of the form (3.1), we can show that the domain of the high temperature phase extends to very low temperatures, provided the quantum perturbation T is small enough.

The idea is to combine the Duhamel expansion with a polymer representation of the partition function; the result will be then immediate from Chapter 5.

To a given choice of $\boldsymbol{A}_1,\ldots,\boldsymbol{A}_m$, corresponds a set $\{\mathcal{A}_1,\ldots,\mathcal{A}_\ell\}$ of mutually disjoint connected subsets of Λ, such that $\cup_{j=1}^m A_j = \cup_{j=1}^\ell \mathcal{A}_j$. We call these connected subsets

polymers and define their weight,

$$\rho(\mathcal{A}) = \mathrm{e}^{\beta f_0(\beta,\boldsymbol{\mu})|\mathcal{A}|} \sum_{m \geqslant 1} (-1)^m \sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m \\ \cup_j A_j = \mathcal{A}}} \sum_{n_{\mathcal{A}}} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_m$$
$$\langle n_{\mathcal{A}}| \, \mathrm{e}^{-\tau_1 V_{\mathcal{A}}} \, T_{\boldsymbol{A}_1} \, \mathrm{e}^{-(\tau_2-\tau_1)V_{\mathcal{A}}} \, \dots T_{\boldsymbol{A}_m} \, \mathrm{e}^{-(\beta-\tau_m)V_{\mathcal{A}}} \, |n_{\mathcal{A}}\rangle \quad (7.6)$$

where $f_0(\beta, \boldsymbol{\mu})$ is the free energy of the classical model, i.e. when $H = V$. The partition function takes the form

$$Z_\Lambda = \mathrm{e}^{-\beta f_0(\beta,\boldsymbol{\mu})|\Lambda|} \sum_{\substack{\{\mathcal{A}_1,\dots,\mathcal{A}_\ell\} \\ \mathcal{A}_i \not\sim \mathcal{A}_j}} \prod_{j=1}^{\ell} \rho(\boldsymbol{A}_j). \quad (7.7)$$

With $e_0 = \min_{n_x} \langle n_x| \, V_{\{x\}} \, |n_x\rangle$, $x \in \mathbb{Z}^\nu$, we have

$$|\langle n_{\mathcal{A}}| \, \mathrm{e}^{-\tau_1 V_{\mathcal{A}}} \, T_{\boldsymbol{A}_1} \, \mathrm{e}^{-(\tau_2-\tau_1)V_{\mathcal{A}}} \, \dots T_{\boldsymbol{A}_m} \, \mathrm{e}^{-(\beta-\tau_m)V_{\mathcal{A}}} \, |n_{\mathcal{A}}\rangle| \leqslant \mathrm{e}^{-\beta e_0|\mathcal{A}|} \, \|T_{\boldsymbol{A}_1}\| \dots \|T_{\boldsymbol{A}_m}\|. \quad (7.8)$$

$f_0(\beta, \boldsymbol{\mu}) \leqslant e_0$, and the integral over times τ_j brings a factor $\beta^m/m!$. We find a bound

$$|\rho(\mathcal{A})| \leqslant S^{|\mathcal{A}|} \, \mathrm{e}^{-c|\mathcal{A}|} \sum_{m \geqslant 1} \frac{1}{m!} \Big(\beta|\mathcal{A}| \sum_{A \ni x} \|T_A\| \, \mathrm{e}^{c|A|} \Big)^m. \quad (7.9)$$

Theorem 3.2 is a direct consequence of Proposition 5.3.

3. Derivation of the classical contour representation

The excitations of a classical lattice model can be (generally) expressed as contours. The study of the low temperature behaviour, and more precisely the proof that the features of the ground states survive at low temperatures, is related to the rarety of the contours. Our aim is analogous here, where we consider a quantum perturbation of a nice classical model. We want to show that the fluctuations due to the small quantum term are rare, and hence the expectation value of observables is close to the matrix element in the (classical) ground state. The procedure follows [BKU 1996, DFF 1996], see also [BKU 1997]. Actually, there is an important technical difference between [BKU 1996] and [DFF 1996], namely that in the previous paper one introduces a discretization of the additional dimension, so as to obtain a classical lattice model; in the second paper, the contour model is in a semi-continuous space, and it is necessary to reformulate the Pirogov-Sinai theory in this case. However, the basic idea, namely to control the fluctuations by showing that contours are rare, is the same in both papers.

We immediately describe the result of this section — the contour representation of the quantum model — in Proposition 7.1 below, and therefore we recall some notation.

Let $M \in \mathbb{N}$ and $\tilde{\beta} > 0$ be such that $M\tilde{\beta} = \beta$ — the discretization of the additional continuous dimension, as we shall see. We introduce the lattice $\mathbb{L}_\Lambda = \Lambda \times \{1, 2, \dots, M\} \subset \mathbb{Z}^{\nu+1}$.

We view $\mathbb{L}_\Lambda$ as a cylinder by imposing periodic boundary conditions along the extra dimension (i.e. we assume that for all $x \in \Lambda$, $(x, 1)$ and (x, M) are neighbours). We define contours as in Section 4, Chapter 6; a *contour* Y is a pair $(\mathrm{Supp}\, Y, \alpha_Y)$, where $\mathrm{Supp}\, Y \subset \mathbb{L}_\Lambda$ is a (non-empty) connected set and α_Y is a labelling of elementary faces F of $\partial\, \mathrm{Supp}\, Y$, $\alpha_Y(F) = g^{(1)}, \dots, g^{(p)}$, that is constant on the boundary of each connected component of $\mathbb{L}_\Lambda \setminus \mathrm{Supp}\, Y$. A set of contours $\{Y_1, \dots, Y_k\}$ is *admissible* if the contours are mutually

disjoint and if the labelling is constant on the boundary of each connected component of $\left[\cup_{i=1}^{k} \operatorname{Supp} Y_i\right]^{\mathrm{c}}$. This set is said to be *compatible with the boundary conditions* g_0 if the external connected components (those touching $\mathbb{Z}^{\nu+1} \setminus \mathbb{L}_\Lambda$) of $\left[\cup_{i=1}^{k} \operatorname{Supp} Y_i\right]^{\mathrm{c}}$ have the label equal to g_0. The horizontal faces centered at (x,τ) will be referred to as $P(x,\tau)$ (P for "plaquette").

Let K be a local operator, with $\operatorname{Supp} K \subset \Lambda$. We define $\mathbb{L}_\Lambda^K$, with periodic boundary conditions along the time direction for all $x \in \Lambda$ not belonging to $\operatorname{Supp} K$ (i.e. we assume that for all $x \in \Lambda \setminus \operatorname{Supp} K$: $(x,1)$ and (x,M) are neighbours). In other words, think of $\mathbb{L}_\Lambda^K$ as the cylinder $\mathbb{L}_\Lambda$ that is cut along $\operatorname{Supp} K$ at $t = \frac{1}{2}$. The "boundary" $S(K) \subset \mathbb{T}_\Lambda^K$ in time direction is

$$S(K) = \bigcup_{x \in \operatorname{Supp} K} P(x, \tfrac{1}{2});$$

notice that $P(x,0) \equiv P(x,M)$ whenever $x \notin \operatorname{Supp} K$. The admissibility and compatibility with the boundary conditions of a set of contours in $\mathbb{T}_\Lambda$ is defined in the same way as above.

A *K-contour* Y_K now is a triple $(S(K), \operatorname{Supp} Y_K, \alpha_{Y_K})$ where $\operatorname{Supp} Y_K \subset \mathbb{L}_\Lambda^K$ is such that each connected component intersects $S(K)$, possibly $\operatorname{Supp} Y_K = \varnothing$, and the labelling α_{Y_K} is constant on boundary faces of each connected components of the complement $[\operatorname{Supp} Y_K]^{\mathrm{c}}$.

We are now ready for the definition of the equivalent classical contour model.

PROPOSITION 7.1. **Contour model for quantum system.**
Let $H^{\boldsymbol{\mu}} = T^{\boldsymbol{\mu}} + V^{\boldsymbol{\mu}}$ a quantum interaction, with $T^{\boldsymbol{\mu}} \in \mathcal{Q}$ and $V^{\boldsymbol{\mu}} \in \mathcal{C}(R_0, G, \Delta_0, a, b)$.

i) *There exists a function ρ: $\{Y \mid \operatorname{Supp} Y \subset \mathbb{L}_\Lambda\} \longrightarrow \mathbb{C}$ such that the partition function of $H^{\boldsymbol{\mu}}_{\Lambda,g_0}$ can be written as*

$$Z_\Lambda^{g_0} = \sum_{\{Y_1,\dots,Y_k\}} \prod_{i=1}^{k} \rho(Y_i) \prod_{g \in G} \mathrm{e}^{-\tilde{\beta} e^{\boldsymbol{\mu}}(g)|W_g|}, \tag{7.10}$$

where the sum is over admissible sets of contours in $\mathbb{L}_\Lambda$ compatible with the boundary conditions g_0; the set W_g is the union of the connected components of $\left[\cup_{i=1}^{k} \operatorname{Supp} Y_i\right]^{\mathrm{c}}$ with labels g on its boundaries.

ii) *For any $c \in \mathbb{R}$, there exist $\tilde{\beta}_0 < \infty$ and $\varepsilon_0 > 0$ such that if $\tilde{\beta} \in [\tilde{\beta}_0, 2\tilde{\beta}_0]$ and $\|T^{\boldsymbol{\mu}}\| \leqslant \varepsilon_0$ the following bound is valid for any Y:*

$$|\rho(Y)| \leqslant \mathrm{e}^{-(\tilde{\beta} e_0^{\boldsymbol{\mu}} + c)|Y|}. \tag{7.11}$$

iii) *For any $c \in \mathbb{R}$, there exist $\tilde{\beta}_0' < \infty$ and $\varepsilon_0' > 0$ such that if $\tilde{\beta} \in [\tilde{\beta}_0', 2\tilde{\beta}_0']$ and $\|T^{\boldsymbol{\mu}}\| + \sum_{i=1}^{p} \|\frac{\partial}{\partial \mu_i} T^{\boldsymbol{\mu}}\| \leqslant \varepsilon_0'$ we have*

$$\left|\frac{\partial}{\partial \mu_i} \rho(Y)\right| \leqslant (C_0 \tilde{\beta} + 1)\, \mathrm{e}^{-(\tilde{\beta} e_0^{\boldsymbol{\mu}} + c)|Y|}. \tag{7.12}$$

iv) *If $K \in \mathcal{L}(0)$, or if $K \in \mathcal{L}(c)$ and $[T_{\boldsymbol{A}}, N_A] = 0$ for all $\boldsymbol{A}$, there exists a function ρ_K: $\{Y_K \mid \operatorname{Supp} Y_K \subset \mathbb{L}_\Lambda^K\} \longrightarrow \mathbb{C}$ such that*

$$\operatorname{Tr} K\, \mathrm{e}^{-\beta H_\Lambda^{\boldsymbol{\mu} g_0}} = \sum_{\{Y_K, Y_1, \dots, Y_k\}} \rho_K(Y_K) \prod_{i=1}^{k} \rho(Y_i) \prod_{g \in G} \mathrm{e}^{-\tilde{\beta} e^{\boldsymbol{\mu}}(g)|W_m|}. \tag{7.13}$$

As before, the sum is over admissible sets of contours, compatible with the boundary condition g_0; ρ is the same function as in i); W_m is the union of the connected components of $\left[\cup_{i=1}^k \operatorname{Supp} Y_i \cup \operatorname{Supp} Y_K\right]^{\mathrm{c}}$ with labels m on their boundaries.

v) *For any $\gamma_K \in \mathbb{R}$ there exist $\tilde\beta_{0,K} < \infty$ and $\varepsilon_{0,K} > 0$ such that if $\tilde\beta \in [\tilde\beta_{0,K}, 2\tilde\beta_{0,K}]$ and $\|T\| \leqslant \varepsilon_{0,K}$ we have*

$$|\rho_K(Y_K)| \leqslant C_K \, \mathrm{e}^{-(\tilde\beta e_0^{\boldsymbol{\mu}} + \gamma_K)|Y_K|} \tag{7.14}$$

with $C_K < \infty$.

The rest of the section is the proof of this proposition. We begin by expanding $\operatorname{Tr} K \, \mathrm{e}^{-\beta H_\Lambda^{\boldsymbol{\mu} g_0}}$ to obtain explicit expressions for ρ_K and ρ; hence part iv) will be proven, and also part i) that can be viewed as a special case of iv) with $K = \mathbb{1}$ [i.e., formally, $\operatorname{Supp} K = \varnothing$ and there is no summation over Y_K in (7.13)]. Similarly v) implies ii) and therefore the following proofs of iv), v), and iii) are sufficient. For sake of clarity we drop out the dependance in $\boldsymbol{\mu}$ in the proofs of points iv) and v).

Proof of Proposition 7.1 iv). Our Hamiltonian has periodicity $\ell_0 < \infty$. Without loss of generality, however, one can consider only translation invariant Hamiltonians, applying the standard trick. Namely, if Ω is the single site phase space, we let $\Omega' = \Omega^{\{1,\dots,\ell_0\}^\nu}$. Then we consider the torus $\Lambda' \subset \mathbb{Z}^\nu$, $\ell_0^\nu |\Lambda'| = |\Lambda|$, each point of which is representing a block of sites in Λ of size ℓ_0^ν, and identify

$$\Omega'^{\Lambda'} \simeq \Omega^\Lambda.$$

Constructing $\mathcal{H}'$ as the Hilbert space spanned by the elements of $\Omega'^{\Lambda'}$, it is clear that $\mathcal{H}'$ is isomorphic to $\mathcal{H}$. The new translation invariant interactions Φ' and T' are defined by resumming, for each $A \subset \Lambda'$, the corresponding contributions with supports in the union of corresponding blocks. Notice the change in range of interactions. Namely, it decreased to $\lceil R/\ell_0 \rceil$ (the lowest integer bigger or equal to R/ℓ_0).

From now on, keeping the original notation $\mathcal{H}$, S, ... , we suppose that the Hamiltonian is translation invariant.

We expand $\operatorname{Tr} K \, \mathrm{e}^{-\beta H_\Lambda^{g_0}}$ with Duhamel formula, and we find [compare with (7.3)]

$$\operatorname{Tr} K \, \mathrm{e}^{-\beta H_\Lambda^{g_0}} = \sum_{m \geqslant 0} \sum_{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m} \sum_{n_\Lambda^{(0)},\dots,n_\Lambda^{(m)}} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_m \langle n_\Lambda^{(0)}| \, K \, |n_\Lambda^{(1)}\rangle$$

$$\mathrm{e}^{-\tau_1 V_\Lambda^{g_0}(n_\Lambda^{(1)})} \, \langle n_\Lambda^{(1)}| \, (-T_{\boldsymbol{A}_1}) \, |n_\Lambda^{(2)}\rangle \, \mathrm{e}^{-(\tau_2-\tau_1) V_\Lambda^{g_0}(n_\Lambda^{(2)})} \, \dots \, \langle n_\Lambda^{(m)}| \, (-T_{\boldsymbol{A}_m}) \, |n_\Lambda^{(0)}\rangle \, \mathrm{e}^{-(\beta-\tau_m) V_\Lambda^{g_0}(n_\Lambda^{(0)})} . \tag{7.15}$$

Let us introduce the *space-time configuration* $\boldsymbol{n}_\Lambda : [0,\beta]_{\mathrm{per}} \to \Omega^\Lambda$ and the *quantum configuration* $\boldsymbol{\omega}_\Lambda = (\boldsymbol{n}_\Lambda; \boldsymbol{A}_1, \dots, \boldsymbol{A}_m; \tau_1, \dots, \tau_m)$, where the mapping $\boldsymbol{n}_\Lambda$ is constant except for $(m+1)$ discontinuities at times $0, \tau_1, \dots, \tau_m$. The previous equation can be summarized with

$$\operatorname{Tr} K \, \mathrm{e}^{-\beta H_\Lambda^{g_0}} = \int_{\mathcal{W}_{g_0,\Lambda}} \mathrm{d}\boldsymbol{\omega}_\Lambda \langle \boldsymbol{n}_\Lambda(-0)| \, K \, |\boldsymbol{n}_\Lambda(+0)\rangle \, \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau V_\Lambda^{g_0}(\boldsymbol{n}_\Lambda(\tau))}$$

$$\prod_{\boldsymbol{A} \in \boldsymbol{\omega}_\Lambda} \langle \boldsymbol{n}_\Lambda(\tau_{\boldsymbol{A}} - 0)| \, (-T_{\boldsymbol{A}}) \, |\boldsymbol{n}_\Lambda(\tau_{\boldsymbol{A}} + 0)\rangle \tag{7.16}$$

where $\int_{\mathcal{W}_{g_0,\Lambda}} \mathrm{d}\boldsymbol{\omega}_\Lambda$ is a shorthand for a sum over $m \geqslant 0$, over m transitions (in Λ), over m configurations, and integration over m ordered times; we denoted with $\tau_{\boldsymbol{A}_i}$ the time τ_i

at which occurs the transition $\boldsymbol{A}_i$. $\mathcal{W}_{g_0,\Lambda}$ is the space of all quantum configurations on the infinite volume $\mathbb{Z}^\nu \times [0,\beta]_{\mathrm{per}}$ with a finite number of transitions (all inside Λ), and such that $\boldsymbol{n}_x(\tau) = (g_0)_x$ for all $x \notin \Lambda$ and all τ. In other words, $\mathcal{W}_{g_0,\Lambda}$ represents all the quantum configurations with boundary conditions g_0.

A configuration $n \in \boldsymbol{\Omega}$ is said to be in the sate $g \in G$ at x whenever $n_{U(x)} = g_{U(x)}$. If there is no such $g \in G$, the configuration is said to be *classically excited* at x. Let $E(n)$ be the set of excitations of n, i.e.

$$E(n) = \{x \in \mathbb{Z}^\nu : n_{U(x)} \neq g_{U(x)} \ \forall g \in G\}. \tag{7.17}$$

Similarly, we define the excitations of a quantum configuration $\boldsymbol{\omega}$ to be

$$\boldsymbol{E}(\boldsymbol{\omega}) = \bigcup_{\boldsymbol{A}\in\boldsymbol{\omega}} (\bar{A} \times \tau_{\boldsymbol{A}}) \cup \bigcup_{\tau\in[0,\beta]_{\mathrm{per}}} (E(\boldsymbol{n}(\tau)) \times \tau). \tag{7.18}$$

We need a notion of connectedness on $\mathbb{T} = \mathbb{Z}^\nu \times [0,\beta]_{\mathrm{per}}$ and we choose the most intuitive one; a subset $B \subset \mathbb{T}$ is *connected* if for any $(x,\tau),(x',\tau') \in B$, there exists a sequence $\big((x_0,\tau_0),(x_1,\tau_1),\dots,(x_k,\tau_k)\big)$ with $(x_0,\tau_0) = (x,\tau)$, $(x_k,\tau_k) = (x',\tau')$, $(x_j,\tau_j) \in B$, $0 \leqslant j \leqslant k$, and for all j: either $[|x_j - x_{j-1}| = 1$ and $\tau_j = \tau_{j-1}]$ or $[x_j = x_{j-1}$ and one of the segments $x_j \times [\tau_{j-1},\tau_j]$, $x_j \times [\tau_j,\tau_{j-1}]$ is included in $B]$.

Then for all $\boldsymbol{\omega} \in \mathcal{W}_{g_0,\Lambda}$, $\boldsymbol{E}(\boldsymbol{\omega})$ decomposes in a unique way into a finite number of connected components. We define a *quantum contour* γ to be a pair $(B,\boldsymbol{\omega}_B)$ with $B \subset \mathbb{T}$ connected and $\boldsymbol{\omega}_B$ is the restriction of a quantum configuration to B (we suppose here that $\boldsymbol{\omega}$ is such that no transition intersects both B and its complement; we do not define $\boldsymbol{\omega}$ in this case).

A set Γ of quantum contours is *admissible* and compatible with the boundary condition g_0 if there exists a $\boldsymbol{\omega} \in \mathcal{W}_{g_0,\Lambda}$ that has Γ as set of quantum contours. Let $\mathcal{G}_{g_0,\Lambda}$ be the space of all such Γ. Since there is a bijection between $\mathcal{W}_{g_0,\Lambda}$ and $\mathcal{G}_{g_0,\Lambda}$, we can rewrite (7.16),

$$\operatorname{Tr} K\, \mathrm{e}^{-\beta H_{g_0,\Lambda}} = \int_{\mathcal{G}_{g_0,\Lambda}} \mathrm{d}\Gamma\, \rho_K(\Gamma), \tag{7.19}$$

where

$$\rho_K(\Gamma) = \langle \boldsymbol{n}^\Gamma(-0)|\, K\, |\boldsymbol{n}^\Gamma(+0)\rangle\, \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau V_\Lambda^{g_0}(\boldsymbol{n}^\Gamma(\tau))} \prod_{\boldsymbol{A}\in\boldsymbol{\omega}^\Gamma} \langle \boldsymbol{n}^\Gamma(\tau_{\boldsymbol{A}}-0)|\, (-T_{\boldsymbol{A}})\, |\boldsymbol{n}^\Gamma(\tau_{\boldsymbol{A}}+0)\rangle \tag{7.20}$$

(the product over transitions is ordered according to the times at which they occur). We denote by $\boldsymbol{\omega}^\Gamma$ (resp. $\boldsymbol{n}^\Gamma$) the quantum contour (resp. the space-time configuration) that corresponds to Γ. We also introduce the shorthand $\int \mathrm{d}(x,\tau)$ for $\int \mathrm{d}\tau \sum_x$.

LEMMA 7.2. *The contribution of an admissible set of contours Γ factorizes into contributions of its elements; more precisely,*

$$\rho_K(\Gamma) = \prod_{g\in G} \mathrm{e}^{-e^{\boldsymbol{\mu}}(g)|\tilde{W}_g|}\, \rho_K(\gamma_K) \prod_{\gamma\in\Gamma\setminus\{\gamma_K\}} \rho(\gamma) \tag{7.21}$$

where

$$\tilde{W}_g = \{(x,\tau) \in \mathbb{Z}^\nu \times [0,\beta]_{\mathrm{per}} : \boldsymbol{n}^\Gamma_{U(x)}(\tau) = g_{U(x)}\}; \tag{7.22}$$

since $\boldsymbol{n}^\Gamma_{U(x)}$ is constant except for a finite number of discontinuities, $\tilde{W}_g$ is a union of vertical segments; we define its length $|\tilde{W}_g|$ as the sum of the lengths of the vertical segments.

The weights of the contour $\gamma = (B, \boldsymbol{\omega}_B)$ *is*

$$\rho(\gamma) = \prod_{\boldsymbol{A}\in\boldsymbol{\omega}_B} \langle \boldsymbol{n}^{\gamma}(\tau_{\boldsymbol{A}} - 0)| \, (-T_{\boldsymbol{A}}) \, |\boldsymbol{n}^{\gamma}(\tau_{\boldsymbol{A}} + 0)\rangle \exp\Big\{ - \int_B \mathrm{d}(x,\tau) \Phi_x(\boldsymbol{n}^{\gamma}_{U(x)}(\tau)) \Big\} \tag{7.23}$$

and, for a K-contour $\gamma_K = (B, \boldsymbol{\omega}_B)$,

$$\rho_K(\gamma_K) = \langle \boldsymbol{n}^{\gamma_K}(-0)| \, K \, |\boldsymbol{n}^{\gamma_K}(+0)\rangle \prod_{\boldsymbol{A}\in\boldsymbol{\omega}_B} \langle \boldsymbol{n}^{\gamma_K}(\tau_{\boldsymbol{A}} - 0)| \, (-T_{\boldsymbol{A}}) \, |\boldsymbol{n}^{\gamma_K}(\tau_{\boldsymbol{A}} + 0)\rangle$$
$$\exp\Big\{ - \int_B \mathrm{d}(x,\tau) \Phi_x(\boldsymbol{n}^{\gamma_K}_{U(x)}(\tau)) \Big\}. \tag{7.24}$$

The proof of this lemma is not hard in the case of spin or boson systems, using the fact that two operators with disjoint supports commute. In the case of fermion systems there is an additional sign due to the anticommutation relations between creation and annihilation operators, and the factorization of this sign is not obvious. Ideas how to solve this problem were proposed in [MM 1996] in the case of the Falicov-Kimball model. However, the first full proof in the general case is in Section 4.2 of [DFF 1996]. It is nicely written, and rather than reproducing it *verbatim* here, we present a geometric argument that works in most of the situations, although it is less general.

Argument for the factorization of the fermionic sign :

Let J denote a "jump", i.e. a pair $(<x, y>, \sigma)$, where $x, y \in \mathbb{Z}^{\nu}$, and σ represents an internal degree of freedom of our fermion, for instance a spin. We set $T_J = c^{\dagger}_{y\sigma} c_{x\sigma}$. We give ourselves a set $\mathcal{J}_\Lambda$ of sets of jumps, and consider an interaction T that is given by

$$T_\Lambda = \sum_{\{J_1,\dots,J_m\}\in\mathcal{J}_\Lambda} t_{J_1} \dots t_{J_m} T_{J_1} \dots T_{J_m}, \qquad t_{J_i} \in \mathbb{C}. \tag{7.25}$$

Expanding the partition function of a model with this quantum interaction, we arrive at a space-time picture with contours. Except for the sign, we can factorize the contribution $\rho(\Gamma)$ of a set of contours Γ, namely,

$$Z_{g_0}(\Lambda) = \int_{\mathcal{G}_{g_0,\Lambda}} \mathrm{d}\Gamma \prod_{g\in G} \mathrm{e}^{-e\boldsymbol{\mu}(g)|W_g|} \, \varepsilon(\Gamma) \prod_{\gamma\in\Gamma} \tilde{\rho}(\gamma) \tag{7.26}$$

with

$$\tilde{\rho}(\gamma) = \Big(\prod_{J\in\gamma} (-t_J) \Big) \exp\Big\{ - \int_B \mathrm{d}(x,\tau) \Phi_x(\boldsymbol{n}^{\gamma}_{U(x)}(\tau)) \Big\}. \tag{7.27}$$

A natural notion here is that of *trajectories*. The trajectory of a particle of spin σ is a sequence $\theta = (\sigma; x_0, x_1, \dots, x_m; \tau_1, \dots, \tau_m)$; $x_0, \dots, x_m$ are the successive positions in space; τ_j, $1 \leqslant j \leqslant m$, is the time at which a jump from x_{j-1} to x_j occurs. The final position is the site x_m, which is not necessarily equal to x_1. To any quantum configuration corresponds an (admissible) set of trajectories $\Theta = (\theta_1, \dots, \theta_k)$. Let $\mathcal{T}_{g_0,\Lambda}$ denote the space of admissible sets of trajectories with jumps in Λ (as before, g_0 is the boundary condition). The partition function (7.26) can be written in terms of trajectories

$$Z_{g_0}(\Lambda) = \int_{\mathcal{T}_{g_0,\Lambda}} \mathrm{d}\Theta \exp\Big\{ - \int_{\mathbb{T}_\Lambda} \mathrm{d}(x,\tau) \Phi_x(\boldsymbol{n}^{\Theta}_{U(x)}(\tau)) \Big\} \varepsilon(\Theta) \prod_{\theta\in\Theta} \prod_{J\in\theta} (-t_J). \tag{7.28}$$

If Γ and Θ represents the same quantum configuration, then $\varepsilon(\Gamma) = \varepsilon(\Theta)$. Moreover, if we view $\boldsymbol{n}^{\Theta}_{\Lambda}(0)$ as a (finite) sequence of particles, ordered according to some predefinite order on sites and spins, then Θ describes a permutation of this sequence. Namely, the image

of an element (x, σ) is the the element (x', σ) such that there is $\theta \in \Theta$ with $\theta = (\sigma; x_1 = x, x_2, \ldots, x_m = x'; \tau_1, \ldots, \tau_m)$. The sign of this permutation is equal to $\varepsilon(\Theta)$.[2]

The idea behind this argument is to replace a set Θ of trajectories by an equivalent set Θ', that has identical trajectories outside of contours, and that defines the same permutation. This is illustrated in Fig. 7.1. The new set of trajectories allows to define *transpositions*, that depends on the contours only, and such that the total permutation is a (time-ordered) product of these transpositions. The sign attributed to each contour is thus $+1$ for a contour with an even number of transpositions, and -1 if this number is odd.

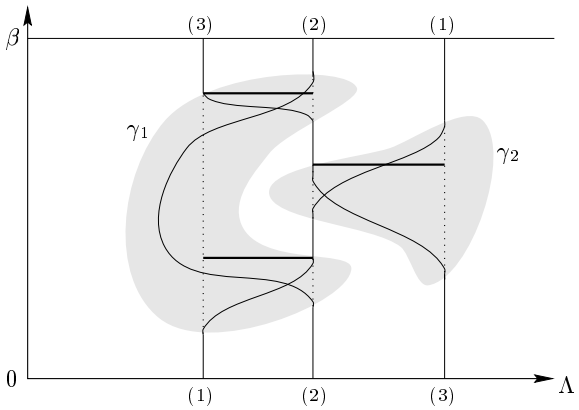


FIGURE 7.1. Symbolic picture with two contours γ_1 and γ_2, and three trajectories. Original trajectories (full lines) are equivalent with new trajectories (dotted lines inside contours) with transpositions (dark horizontal lines). Resulting signs are $\varepsilon(\gamma_1) = +1$ and $\varepsilon(\gamma_2) = -1$.

To define the new trajectories, we first consider the vertical lines obtained by the prolongation of all segments of trajectories outside of the contours. Intersections between trajectories and boundaries of contours form the "entrances" $(n_1, \ldots, n_m)$ and "exits" $(x_1, \ldots, x_n)$. Remark that intersections between the new vertical lines and the boundaries of contours yield the same entrances and exits. Entrances and exits are ordered in increasing times. In the new trajectories all the particles are supposed to go straightway, until the first exit x_1 occurs. We check which particle is leaving the contour at x_1. If this particle is supposed to be on another trajectory, then we define a bridge (i.e. a transposition) between the other trajectory, and the one that is leaving.

Then the particles are again supposed to go straightway, until the time when x_2 occurs. Again, we check whether a new bridge has to be defined. We repeat this procedure until the last exit of the contour has been met (notice that no transposition is ever defined with the last exit). An important remark is that the decision to define a bridge depends only on the given contour, since only a particle that previously entered, can leave.

As a result, we have that the total permutation stemming from Θ is given by a time-ordered product on the transpositions. This permutation clearly does not factorize with respect to the contours, but its sign does. This concludes the argument for the factorization of the sign.

So far we have obtained a contour model which is a suitable starting point for applying Pirogov-Sinai theory, except that the contours have support in a continuous space. One

[2]In fact, this is certainly true, but not mathematically obvious; this would require a proof, if this discussion pretended to be more than an argument.

way is to extend the Pirogov-Sinai theory to this situation; this is done in [DFF 1996]. However we proceed here as in [BKU 1996]; we discretize the continuous direction by introducing $\tilde{\beta}, M$ with $\beta = \tilde{\beta}M$, and we obtain the lattice $\mathbb{L}_\Lambda$.

For a given quantum configuration $\boldsymbol{\omega} \in \mathcal{W}_{g_0,\Lambda}$, we introduce *quantum* and *classical excitations*:

$$E_Q(\boldsymbol{\omega}) = \Big\{(x,t) \in \mathbb{L} : \big[\bigcup_{\boldsymbol{A}\in\boldsymbol{\omega}} (\bar{A} \times \tau_{\boldsymbol{A}})\big] \cap C(x,t) \neq \varnothing\Big\} \tag{7.29}$$

$$E_C(\boldsymbol{\omega}) = \Big\{(x,t) \in \mathbb{L} \setminus E_Q : \boldsymbol{n}_{U(x)}(\tilde{\beta}t) \neq g_{U(x)} \forall g \in G\Big\}. \tag{7.30}$$

Decomposing $E_Q(\boldsymbol{\omega}) \cup E_C(\boldsymbol{\omega})$ into connected components, we obtain the supports of the contours; the component touching $\operatorname{Supp} K \times 0$ yields Y_K. The labelling is determined by the configurations on the complements of the supports of the contours.

The weight of these contours $\rho(Y)$ is a complicated but well-defined expression, that is an integral over all sets of quantum contours having supports on $\cup_{(x,t)\in\operatorname{Supp} Y} C(x,t)$, and compatible with the labelling. The weight $\rho_K(Y_K)$ contains moreover a contribution of the local operator K.

This concludes the proof of the point iv) of the proposition.

□

Proof of Proposition 7.1 v). Let us start by the part of the contours with quantum transitions. We consider a connected set $A \subset \Lambda$ and a time $t \in \{1, \dots, M\}$ such that $(A \times t) \subset \operatorname{Supp} Y$, where Y is a contour. We have to show that

$$\mathrm{e}^{c|A|} \sum_{m \geqslant 1} \sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m \\ \cup_j \bar{A}_j = A}} \sum_{n^{(1)}_{A_1},\dots,n^{(m)}_{A_m}} \int_{0<\tau_1<\dots\tau_m<\tilde{\beta}} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_m \, \mathrm{e}^{-\tau_1 \sum_{x\in A} \Phi_x(n^{(0)}_{U(x)})}$$

$$\mathrm{e}^{-(\tau_2-\tau_1)\sum_{x\in A} \Phi_x(n^{(1)}_{U(x)})} \dots \mathrm{e}^{-(\tilde{\beta}-\tau_m)\sum_{x\in A} \Phi_x(n^{(m)}_{U(x)})} \left|\langle n^{(0)}| T_{\boldsymbol{A}_1} |n^{(1)}\rangle \dots \langle n^{(m-1)}| T_{\boldsymbol{A}_m} |n^{(m)}\rangle\right|$$

is a small quantity, uniformly in the initial configuration $n^{(0)}$. Remark that the configurations are such that $n^{(1)}_{A_1^{\mathrm{c}}} = n^{(0)}_{A_1^{\mathrm{c}}}$, $\dots$, $n^{(m)}_{A_m^{\mathrm{c}}} = n^{(m-1)}_{A_m^{\mathrm{c}}}$.

A geometrical representation of this sum is useful, see Fig. 7.2. Let $x \in A$. To each choice of A_1, $\dots$, A_m and τ_1, $\dots$, τ_m corresponds a "bush" $\mathfrak{b}$, that is, a collection of sets A'_1, $\dots$ A'_m and vertical segments ℓ_1, $\dots$, $\ell_m \subset \mathbb{T}_A$, such that

- $(A'_1, \dots, A'_m)$ is a permutation of $(A_1, \dots, A_m)$;
- $\bar{A}'_1 \ni x$, and ℓ_1 has one end at $x \times 0$ and the other on $\bar{A}'_1 \times \tau_{A'_1}$; x is the *root* of the bush;
- if there is a vertical segment ℓ_i between $\bar{A}'_i$ and $\bar{A}'_j$, then $\bar{A}'_i \Cap \bar{A}'_j$;
- the graph of m vertices with an edge between i and j whenever a vertical segment connects $\bar{A}'_i$ and $\bar{A}'_j$, is connected (or equivalently, this graph is a tree);
- if $\bar{A}'_i$ and $\bar{A}'_j$ are connected by a vertical segment, say ℓ_j, then no other transition intersects the set $(\bar{A}'_i \cap \bar{A}'_j) \times \ell_j$.

We obtain a bound by considering the (continuous) sum over all bushes. If τ'_j is the length of the segment ℓ_j, and denoting by $\check{n}^{(j)}_{A'_j}$ the configuration immediately before the transition j if ℓ_j lies below A'_j, otherwise $\check{n}^{(j)}_{A'_j}$ is the configuration immediately after, we

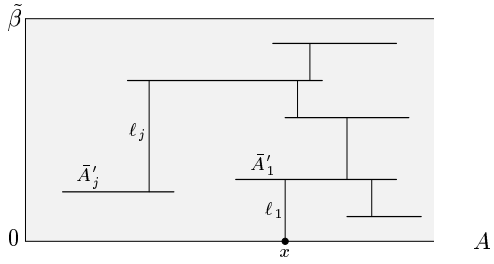


FIGURE 7.2. A "bush" with 6 transitions and 6 vertical segments.

have the inequality

$$\begin{aligned}
\mathrm{e}^{-\tau_1 \sum_{x\in A}\Phi_x(n^{(0)}_{U(x)})} \dots \mathrm{e}^{-(\tilde\beta-\tau_m)\sum_{x\in A}\Phi_x(n^{(m)}_{U(x)})} &\leqslant \\
&\leqslant \mathrm{e}^{-\tilde\beta|A|e_0^\Phi}\ \mathrm{e}^{\tilde\beta(a+b)|A|}\ \mathrm{e}^{-\tau_1 b(|n^{(0)}_A|+1)} \dots \mathrm{e}^{-(\tilde\beta-\tau_m)b(|n^{(m)}_A|+1)} \\
&\leqslant \mathrm{e}^{-\tilde\beta|A|e_0^\Phi}\ \mathrm{e}^{\tilde\beta(a+b)|A|}\ \mathrm{e}^{-\frac12\tau'_1 b(|\check n^{(1)}_{A'_1}|+1)} \dots \mathrm{e}^{-\frac12\tau'_m b(|\check n^{(m)}_{A'_m}|+1)} \qquad (7.31)
\end{aligned}$$

The first inequality holds because $\Phi\in\mathcal{C}(R_0,G,\Delta_0,a,b)$.

Denoting $\mathcal{B}_{m,x}$ the space of all bushes with root x and at most m transitions, and $\int_{\mathcal{B}_{m,x}}\mathrm{d}\mathfrak{b}$ a shorthand for the sum over sets $A'_1,\dots A'_m$ and time intervals $\tau'_1,\dots\tau'_m$, with corresponding restrictions and combinatorics, we have to estimate

$$\lim_{m\to\infty}\max_{n^{(0)}\in\mathbf{\Omega}}\int_{\mathcal{B}_{m,x}}\mathrm{d}\mathfrak{b}\check z(\mathfrak{b})$$

with

$$\check z(\mathfrak{b}) = \sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m\\ A_j=A'_j}}\ \sum_{n^{(1)}_{A'_1},\dots,n^{(m)}_{A'_m}}\ \prod_{j=1}^m \left|\langle\hat n^{(j)}|\,T_{\boldsymbol{A}_j}\,|n^{(j)}\rangle\right| \mathrm{e}^{c(2R_0)^\nu|A_j|}\ \mathrm{e}^{-\frac12\tau'_j b(1+|\check n^{(j)}_{A_j}|)},$$

where $\hat n^{(j)}$ is the configuration just before the j-th transition (possibly $\hat n^{(j)}=\check n^{(j)}$).

We proceed by induction on m. First,

$$\begin{aligned}
\max_{n^{(0)}}\int_{\mathcal{B}_{1,x}}\mathrm{d}\mathfrak{b}\sum_{\boldsymbol{A}_1:A_1=A'_1}\ \sum_{n^{(1)}_{A'_1}}&\left|\langle n^{(0)}|\,T_{\boldsymbol{A}_1}\,|n^{(1)}\rangle\right| \mathrm{e}^{c(2R_0)^\nu|A'_1|}\ \mathrm{e}^{-\frac12\tau'_1 b(1+|n^{(0)}_{A'_1}|)} \\
&\leqslant \frac{2}{b}\sum_{A'_1:\bar A'_1\ni x}\ \max_{n^{(0)}}\ \sum_{\boldsymbol{A}_1:A_1=A'_1}\ \sum_{n^{(1)}_{A'_1}}\frac{\left|\langle n^{(0)}|\,T_{\boldsymbol{A}_1}\,|n^{(1)}\rangle\right|}{1+|n^{(0)}_{A'_1}|}\,\mathrm{e}^{c(2R_0)^\nu|A'_1|} \\
&\leqslant \frac{2}{b}\sum_{A'_1:\bar A'_1\ni x}\Big[\|T\|\,\mathrm{e}^{c(2R_0)^\nu}\Big]^{|A'_1|} \\
&\leqslant \frac{2}{b}(2R_0)^\nu\frac{\beth\|T\|\,\mathrm{e}^{c(2R_0)^\nu}}{1-\beth\|T\|\,\mathrm{e}^{c(2R_0)^\nu}}. \qquad (7.32)
\end{aligned}$$

Let $\varepsilon=\frac{4}{b}(2R_0)^\nu\beth\|T\|\,\mathrm{e}^{c(2R_0)^\nu}$; the bound above is smaller than ε if $\|T\|$ is small enough.

We consider now the integration over bushes with at most m transitions.

$$\max_{n^{(0)}} \int_{\mathcal{B}_{m,x}} \mathrm{d}\mathfrak{b}\check{z}(\mathfrak{b}) \leqslant \max_{n^{(0)}} \sum_{A_1':\bar{A}_1'\ni x} \sum_{\boldsymbol{A}_1:A_1=A_1'} \sum_{n^{(1)}_{A_1'}} \int_0^\infty \mathrm{d}\tau_1' \, \mathrm{e}^{-\frac{1}{2}\tau_1' b(1+|n^{(0)}_{A_1'}|)}$$

$$\big|\langle n^{(0)}|\, T_{\boldsymbol{A}_1}\, |n^{(1)}\rangle\big|\, \mathrm{e}^{c(2R_0)^\nu|A_1'|} \sum_{k\geqslant 0} \frac{1}{k!} \prod_{j=1}^{k} \Big[2 \sum_{x_j\in\bar{A}_1'} \max_{n^{(0)}} \int_{\mathcal{B}_{m-1,x_j}} \mathrm{d}\mathfrak{b}\check{z}(\mathfrak{b})\Big]$$

$$\leqslant \frac{2}{b} \max_{n^{(0)}} \sum_{A_1':\bar{A}_1'\ni x} \sum_{\boldsymbol{A}_1:A_1=A_1'} \sum_{n^{(1)}_{A_1'}} \frac{\big|\langle n^{(0)}|\, T_{\boldsymbol{A}_1}\, |n^{(1)}\rangle\big|}{1+|n^{(0)}_{A_1'}|}\, \mathrm{e}^{c(2R_0)^\nu|A_1'|}\, \mathrm{e}^{2(2R_0)^\nu|A_1'|\varepsilon} \tag{7.33}$$

and we find a bound

$$\frac{2}{b}(2R_0)^\nu \frac{\beth\|T\|\, \mathrm{e}^{(2R_0)^\nu(c+2\varepsilon)}}{1-\beth\|T\|\, \mathrm{e}^{(2R_0)^\nu(c+2\varepsilon)}} \leqslant \varepsilon$$

if $\|T\|$ is small enough.

We have to discuss the effect of the local operator K. If $K\in\mathcal{L}(0)$, it yields a factor involving $\|K\|<\infty$, and we are done. But if $K\in\mathcal{L}(c)$, more caution is needed. A term $\exp(c_K|n_{\mathrm{Supp}\,K}|)$ appears and acts on the cells just below $\mathrm{Supp}\,K\times 0$. Let A connected such that $A\times M\subset \mathrm{Supp}\,Y_K$, $A\cap\mathrm{Supp}\,K\neq\varnothing$. For any choice of quantum transitions $(\boldsymbol{A}_i,\tau_i)$, the space-time configuration $\boldsymbol{n}$ in the cells centered on the sites of $A\times M$ has constant number of particles. Therefore

$$\exp\Big(c_K|\boldsymbol{n}_A(\tilde{\beta})|\Big) = \exp\Big(\frac{c_K}{\tilde{\beta}}\int_0^{\tilde{\beta}} \mathrm{d}\tau|\boldsymbol{n}_A(\tau)|\Big). \tag{7.34}$$

The only effect is to change b into $b-c_K/\tilde{\beta}$ in (7.31). It is bigger than 0 if $\tilde{\beta}$ is large enough (depending on c_K).

Having checked that the contribution of the quantum excitations has exponential decay, there remains to verify the same for the classical excitations. It is a much easier task.

Let $E_C\subset\mathrm{Supp}\,Y$. The space-time configuration is constant on E_C, and moreover it has to be classically excited. Since $\Phi\in\mathcal{C}(R_0,G,\Delta_0,a,b)$, properties (2.12) and (2.13) are valid, and we obtain a bound, for each site of E_C,

$$\mathrm{e}^{-\tilde{\beta}e_0^\Phi}\Big[\sum_{n_x:|n_x|\leqslant 2a/b} \mathrm{e}^{-\tilde{\beta}\Delta_0} + \sum_{n_x:|n_x|>2a/b} \mathrm{e}^{-\tilde{\beta}(b|n_x|-a)}\Big]$$

and this is as small as we may need by choosing $\tilde{\beta}$ large enough. If the local operator $K\in\mathcal{L}(c)$ occurs, then we have to choose $\tilde{\beta}$ large enough, depending on c_K, so as the expression above remains small.

□

Proof of Proposition 7.1 iii). This proof is not hard, but tedious, and rather than bothering the reader we simply refer to [BKU 1997] — the bound is true because of the assumptions on the derivatives of the classical energy and on the norm of the quantum interactions $\|\frac{\partial}{\partial\mu_i}T^{\boldsymbol{\mu}}\|$.

□

Theorems 3.3 and 3.4 are now consequences of the Pirogov-Sinai theory (Chapter 6) applied to the contour model specified in Proposition 7.1. As for the expectation value of local observables, there is a difference between the equations (6.17) and (7.13). It could be possible to modify Proposition 7.1 iv); it is a tedious but straightforward task. However, since everything is already written down, we content ourselves by observing that small adaptations of the Pirogov-Sinai theory allow to consider the contour model as it is specified in Proposition 7.1.

CHAPTER 8

Effective potential due to quantum fluctuations

A partition function is a sum over configurations, with some weight. All the configurations have to be considered, because all of them have a weight that differs from 0 (in general). However, it is useful to imagine that only *typical configurations* are important; these typical configurations all look the same (i.e. macroscopic observables take the same value on all of them), and their total weight is much bigger then the total weight of the non-typical configurations. In the previous chapter, the typical (space-time) configurations consisted in a classical ground state, that is constant along the time direction, with rare contours here and there. We showed that the effect of these contours was unimportant, but it has to be understood that they were present, and they brought a small correction to the partition function. Our aim now is to compute the contribution of the contours, at least the smallest and the most frequent ones, and to show that it can be rewritten as a new classical interaction.

The motivation to go beyond the study of the previous chapter has multiple origins.

- This allows to compute some thermodynamic quantities where quantum effects are important. For instance, take an Ising model in a transverse magnetic field: the Hilbert space $\mathcal{H}_\Lambda$ is the one spanned by the classical configurations $\sigma_\Lambda \in \{-1,+1\}^\Lambda$, and the Hamiltonian is

$$H_\Lambda = \sum_{<x,y>\subset\Lambda} S_x^{(3)} S_y^{(3)} - h \sum_{x\in\Lambda} S_x^{(1)}. \tag{8.1}$$

  The susceptibility in the direction 1,

$$\chi^{(j1)} = \frac{\partial}{\partial h} \langle S_x^{(j)} \rangle_\Lambda, \tag{8.2}$$

  may be considered as a measure of the quantum fluctuations.
- For models that are stable with respect to the quantum fluctuations, we know that the low temperature phase diagram is a small deformation of the zero temperature phase diagram of the corresponding classical model. We may be interested in how the quantum perturbation moves the coexistence lines.
- The quantum fluctuations may totally modify the features of the low temperature phases; there are models where the classical interaction has degenerate ground states, and for which the quantum fluctuations remove the degeneracy.

Actually, we shall concentrate on the last point. Another consequence of this effective potential is the stabilization of interfaces, see [DMN 1998].

Systematic approaches to models with degeneracies were proposed first in [DFFR 1996], then in [KU 1998]. Of course, we shall follow here the last method, but let us begin with a quick look on the first one.

Starting from a Hamiltonian $H(t) = H^{(0)} + tV$, $H^{(0)}$ being a diagonal operator with infinitely many ground states, and V the quantum perturbation, the idea is to define an

antisymmetric matrix $S = tS^{(1)} + t^2 S^{(2)}$ and to consider

$$H^{(2)}(t) = \mathrm{e}^{S}\, H(t)\, \mathrm{e}^{-S}\,.$$

Denoting $\mathrm{ad}_{H^{(0)}} S = [H^{(0)}, S] = -\mathrm{ad}_S H^{(0)}$, $H^{(2)}(t)$ is expanded using Lie-Schwinger series

$$H^{(2)}(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathrm{ad}_S^n H(t).$$

At order t^1 in this expansion we find tV and $t\,\mathrm{ad}_{S^{(1)}} H^{(0)}$, and we choose $S^{(1)}$ such that these terms cancel. At order t^2 we have $t^2[\mathrm{ad}_{S^{(2)}} H^{(0)} + \mathrm{ad}_{S^{(1)}} V + \frac{1}{2}\mathrm{ad}^2_{S^{(1)}} H^{(0)}]$. $S^{(2)}$ is chosen so as the off-diagonal terms disappear at this order, and as a result $H^{(2)}(t)$ is diagonal, up to terms of order t^3 or higher. If the diagonal part of $H^{(2)}(t)$ has a finite number of ground states, and if the excitations cost strictly positive energy, then it can be shown that these ground states are stable. It is possible to include higher orders in this perturbation scheme. See [DFFR 1996] for additional information.

1. The asymmetric Hubbard model

Before beginning the full developments in the general situation, we present a heuristical derivation of the effective potential in the case of the asymmetric Hubbard model. Recall that the local configuration space is $\{0, \uparrow, \downarrow, 2\}$; the classical interaction is the on-site term ($R_0 = 0$).

$$\Phi_x(n_x) = \tfrac{U}{2}(n_{x\uparrow} + n_{x\downarrow} - 1)^2, \tag{8.3}$$

and the quantum interaction is $(T_{\boldsymbol{A}})$; $\boldsymbol{A} = (< x, y >, \sigma)$, where $< x, y >$ is a pair of neighbouring sites, and $\sigma \in \{\uparrow, \downarrow\}$. If $\boldsymbol{A} = (< x, y >, \sigma)$, then

$$T_{\boldsymbol{A}} = t_\sigma c^\dagger_{x\sigma} c_{y\sigma}. \tag{8.4}$$

1.1. Duhamel expansion of the partition function. With the use of Duhamel formula (see Chapter 7) we can get

$$\begin{aligned} Z_\Lambda &= \mathrm{Tr}\ \mathrm{e}^{-\beta H} = \mathrm{Tr}\ \mathrm{e}^{-\beta V - \beta T} \\ &= \mathrm{Tr} \sum_{m=0}^{\infty} \int_{0<\tau_1<\ldots<\tau_m<\beta} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_m\, \mathrm{e}^{-\tau_1 V}\,(-T)\,\mathrm{e}^{-(\tau_2-\tau_1)V}\,(-T)\ldots(-T)\,\mathrm{e}^{-(\beta-\tau_m)V}\,. \end{aligned} \tag{8.5}$$

Expanding the unit operator $\mathbb{1} = \sum_n |n\rangle\langle n|$ at the right of each operator V, we obtain

$$\begin{aligned} Z_\Lambda = \sum_{m \geqslant 0} \sum_{n^1,\ldots,n^m} \sum_{\substack{\boldsymbol{A}_1,\ldots,\boldsymbol{A}_m \\ \boldsymbol{A}_i = (<x_i,y_i>,\sigma_i)}} \int_{0<\tau_1<\ldots<\tau_m<\beta} \\ \mathrm{e}^{-\tau_1\Phi(n^1)}\,\langle n^1|\,T_{\boldsymbol{A}_1}\,|n^2\rangle\,\mathrm{e}^{-(\tau_2-\tau_1)\Phi(n^2)}\ \ldots\,\langle n^m|\,T_{\boldsymbol{A}_m}\,|n^1\rangle\,\mathrm{e}^{-(\beta-\tau_m)\Phi(n^1)}\,. \end{aligned} \tag{8.6}$$

We have the following geometrical interpretation, see Fig. 8.1.

We consider the space-time $\Lambda \times [0, \beta]$. We sum over an integer m, over $\boldsymbol{A}_1, \ldots, \boldsymbol{A}_m$, on m successive configurations, and we integrate over m successive times $\tau_1, \ldots, \tau_m$. The partition function is now a (continuous) sum over all the *quantum configurations*; it is specified by a set of transitions $(\boldsymbol{A}_1, \tau_1), \ldots, (\boldsymbol{A}_m, \tau_m)$, and by a *space-time configurations* $\boldsymbol{n}$: $[0, \beta] \to \{0, \uparrow, \downarrow, 2\}^\Lambda$, which is constant except at times $\tau_1, \ldots, \tau_m$. The second line of (8.6) gives the weight of a space-time configuration.

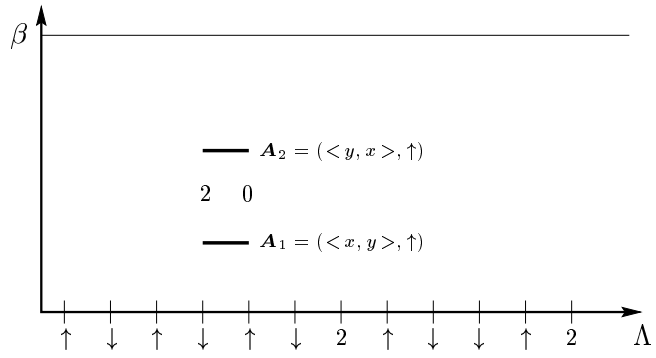


FIGURE 8.1

It is useful to consider this partition function as the one of a *classical* model (in one more dimension), and to use classical intuition. Namely, at low temperature and with non zero hopping, we expect that the thermodynamical states will be those that allow for a lot of quantum fluctuations. This is similar to the cases studied by Bricmont and Slawny [BS 1989], where low temperature states of classical systems can be chosen by thermal fluctuations. The nature of quantum fluctuations is however very different, and we took advantage of the study by Messager and Miracle-Solé of the Falicov-Kimball model [MM 1996].

1.2. Identification of small and big "quantum contours". See Fig. 8.2. We say that a space-time site $(x, \tau) \in \Lambda \times [0, \beta]$ is *excited* if the space-time configuration takes value 0 or 2 on (x, τ), i.e. $[\boldsymbol{n}(\tau)]_x \in \{0, 2\}$.

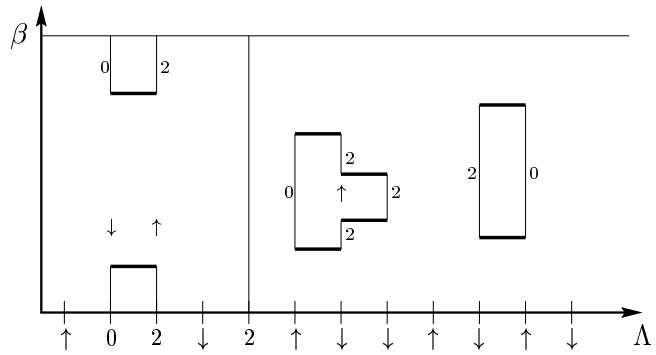


FIGURE 8.2. Four space-time contours. The first three are big while the last one is a small quantum contour.

Quantum contours are formed by connected sets of excitations and transitions. They are *small* if there are only two transitions of $\uparrow$ spins, otherwise they are big. Let γ denote a big quantum contour, and ξ denote a small one. We have the following decomposition of the partition function

$$Z_\Lambda = \int \mathrm{d}\boldsymbol{n}\varepsilon(\Gamma(\boldsymbol{n})) \prod_{\gamma\in\Gamma(\boldsymbol{n})} z(\gamma) \int_{\Xi\sim\boldsymbol{n}} \mathrm{d}\Xi \prod_{\xi\in\Xi} z(\xi). \tag{8.7}$$

The first integral is over space-time configurations $\boldsymbol{n}$ such that all their contours are big; we denote the set of contours by $\Gamma(\boldsymbol{n})$. The set of small contours Ξ is such that there exists a configuration $\boldsymbol{n}'$, which coincides with $\boldsymbol{n}$ outside of the supports of small contours.

The sign $\varepsilon(\Gamma(\boldsymbol{n})) = \pm 1$ is associated with the permutation of the electrons due to $\Gamma(\boldsymbol{n})$ (it is present because we have fermions). The weights are given by

$$z(\gamma) = \Big(\prod_{\boldsymbol{A}=(<x,y>,\sigma)\in\gamma} t_\sigma \Big)\, \mathrm{e}^{-\frac{U}{2}\ell_0(\gamma)}\,. \tag{8.8}$$

Here $\ell_0(\gamma)$ is the vertical length of γ. The same equation holds for $z(\xi)$; but since ξ has a simpler structure, so does its weight, which can be written as

$$z(\xi) = t_\uparrow^2\, \mathrm{e}^{-\frac{U}{2}\ell_0(\xi)}\,. \tag{8.9}$$

Remark that the constraints over big quantum contours are non-local; indeed, we can have a situation as displayed in Fig. 8.3. The two contours have disjoint supports, and because of the periodicity in the time direction, it is impossible to have one contour without the other.

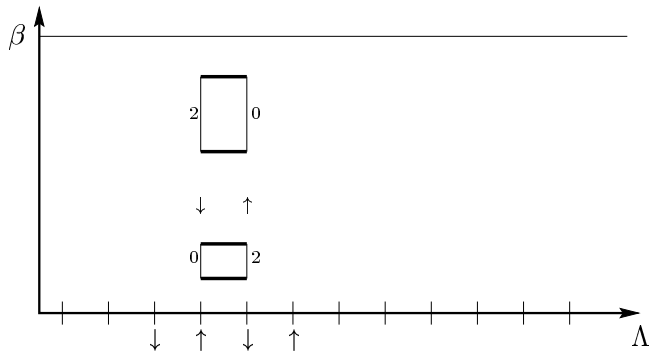


FIGURE 8.3

On the contrary, the constraints on the small quantum contours, for a given $\boldsymbol{n}$, are local (namely, only non-intersection), and hence we can apply cluster expansion techniques. However, we proceed here with this expansion more naively and non rigorously, since it is simpler.

1.3. Expansion of the small quantum contours. Since $z(\xi)$ is a small quantity, the small contours are rare and the condition of non-intersection is irrelevant; therefore we can approximate[1]

$$\begin{aligned}\log\Big[\int_{\Xi\sim\boldsymbol{n}} \mathrm{d}\Xi \prod_{\xi\in\Xi} z(\xi)\Big] &\simeq \int_{\xi\sim\boldsymbol{n}} \mathrm{d}\xi z(\xi) \\ &= \sum_{<x,y>} \int_0^\beta \mathrm{d}\tau \int_{\substack{\xi\sim\boldsymbol{n},\mathrm{Supp}\,\xi\ni(x,\tau)\\ \boldsymbol{A}=(<x,y>,\uparrow)\in\xi}} \mathrm{d}\xi \frac{2z(\xi)}{\ell_0(\xi)}.\end{aligned} \tag{8.10}$$

The small quantum contours cannot intersect the big ones. But releasing this constraint only means a small change on the contributions of the big quantum contours, and since the latter will be shown as being unimportant, we can do this approximation.[2] Hence

[1] This step can be achieved rigorously using cluster expansions. Extra terms appear and they are not local; but their contribution decays exponentially fast with their size.

[2] This may also be set rigorous by considering "decorations" of the big quantum contours.

we write,

$$\sum_{<x,y>} \int_0^\beta \mathrm{d}\tau \int_{\substack{\xi \sim \boldsymbol{n}, \mathrm{Supp}\,\xi \ni (x,\tau) \\ \boldsymbol{A}=(<x,y>,\uparrow)\in\xi}} \mathrm{d}\xi \frac{2z(\xi)}{\ell_0(\xi)} \simeq \sum_{<x,y>} \int_0^\beta \mathrm{d}\tau \int_{\substack{\xi \sim \boldsymbol{n}_{<x,y>}(\tau) \\ \mathrm{Supp}\,\xi \ni (x,\tau) \\ \boldsymbol{A}=(<x,y>,\uparrow)\in\xi}} \mathrm{d}\xi \frac{2z(\xi)}{\ell_0(\xi)}. \tag{8.11}$$

We define now the *effective potential* $\Psi_{\{x,y\}}(n_{\{x,y\}})$

$$\Psi_{\{x,y\}}(n_{\{x,y\}}) \doteq -\int_{\substack{\xi \sim n_{\{x,y\}} \\ \mathrm{Supp}\,\xi \ni (x,\tau) \\ A=(<x,y>,\uparrow)\in\xi}} \mathrm{d}\xi \frac{2z(\xi)}{\ell_0(\xi)}. \tag{8.12}$$

Let us compute it explicitely (see Fig. 8.4).

- If $n_{\{x,y\}} \in \{(\uparrow,\downarrow),(\downarrow,\uparrow)\}$: we have

$$\begin{aligned}
\Psi_{\{x,y\}}(n_{\{x,y\}}) &= -t_\uparrow^2 \int_0^\infty \mathrm{d}\tau_1 \int_{\tau_1}^\infty \mathrm{d}\tau_2 \frac{\mathrm{e}^{-\tau_2 U}}{\tau_2} \\
&= -t_\uparrow^2 \int_0^\infty \mathrm{d}\tau_2 \int_0^\infty \mathrm{d}\tau_1 \frac{\mathrm{e}^{-\tau_2 U}}{\tau_2} \mathbb{I}\left[\tau_2 > \tau_1\right] \\
&= -t_\uparrow^2 \int_0^\infty \mathrm{d}\tau_2\, \mathrm{e}^{-\tau_2 U} \\
&= -\frac{t_\uparrow^2}{U}.
\end{aligned}$$

- If $n_{\{x,y\}} \notin \{(\uparrow,\downarrow),(\downarrow,\uparrow)\}$, it is zero.

We see that the effective potential favours pairs of opposite spins, hence we expect to have chessboard-like structure.

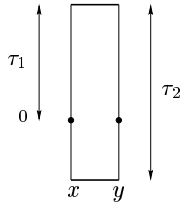


FIGURE 8.4

1.4. Definition of a classical contour model. Let us come back to the partition function. With the expansion of small quantum contours, and with our approximations, Equation (8.7) becomes

$$Z_\Lambda \simeq \int \mathrm{d}\boldsymbol{n}\varepsilon(\Gamma(\boldsymbol{n})) \prod_{\gamma\in\Gamma(\boldsymbol{n})} z(\gamma) \exp\Big[-\sum_{<x,y>} \int_0^\beta \mathrm{d}\tau \Psi_{\{x,y\}}(\boldsymbol{n}_{\{x,y\}}(\tau))\Big], \tag{8.13}$$

with the weights of the quantum contours given by (8.8). We redefine now the big quantum contours, by considering the pairs $(\uparrow,\uparrow)$ and $(\downarrow,\downarrow)$ as excited, see Fig. 8.5. Now, an admissible set of contours Γ specifies the whole quantum configuration $\boldsymbol{n}$.[3]

[3] The contour model that we define here is different from the setting introduced in Chapter 6. However, we only need in this heuristical discussion a model where it is plausible to apply the Peierls argument.

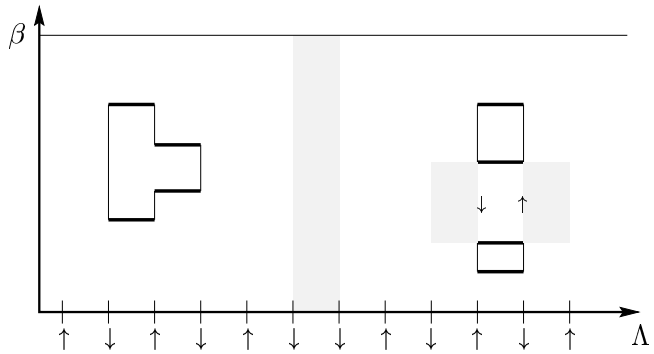


FIGURE 8.5. Three contours; their supports are formed excited sites with 0 or 2 particles, or by excited pairs with same spins.

Then we obtain

$$Z_\Lambda = \mathrm{e}^{-\beta|\Lambda|t_\uparrow^2/U} \int \mathrm{d}\Gamma \prod_{\gamma\in\Gamma} \mathfrak{z}(\gamma) \tag{8.14}$$

with the new weight given by

$$\mathfrak{z}(\gamma) = (\prod_{\boldsymbol{A}=(<x,y>,\sigma)\in\gamma} t_\sigma)\varepsilon(\gamma)\,\mathrm{e}^{-\frac{U}{2}\ell_0(\gamma)-\frac{t_\uparrow^2}{U}\ell(\gamma)}\,. \tag{8.15}$$

The length $\ell(\gamma)$ is the vertical length of the part of $\mathrm{Supp}\gamma$ that is formed by pairs $(\uparrow,\uparrow)$ or $(\downarrow,\downarrow)$. $\varepsilon(\gamma)=\pm1$ is a sign due to the fermionic character of the particles. Actually, it is not easy to show that the initial $\varepsilon(\Gamma)$ factorizes with respect to the contours; it is done in Section 4.2 of [DFF 1996].

1.5. Peierls argument. The weight of the contours decays exponentially quickly with respect to their lengths, so we are in the situation where the Peierls argument applies [Pei 1936, Dob 1965, Gri 1964]. Heuristically, contours are rare, and therefore the "typical space-time configuration" is a constant chessboard. Therefore the expectation value of any local operator is, up to small corrections, the matrix element of this operator with respect to the chessboard state.

2. General system

This section is a rewriting of the previous one; however, we consider now a more general class of models (satisfying the assumptions of Section 4, Chapter 3), and the approximations above are turned into a rigorous treatment.

2.1. Contour representation. As discussed in Chapter 7, we can suppose that our Hamiltonian is translation invariant.

We expand $\mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}$ with the Duhamel formula, see Chapter 7. As before, we get

$$\mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}} = \sum_{m\geqslant 0}\sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m\\ \bar{A}_i\subset\Lambda}} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1\dots\mathrm{d}\tau_m$$
$$\mathrm{e}^{-\tau_1 V_\Lambda^{\mathrm{per}}} T_{\boldsymbol{A}_1}\,\mathrm{e}^{-(\tau_2-\tau_1)V^{\mathrm{per}}} T_{\boldsymbol{A}_2}\dots T_{\boldsymbol{A}_m}\,\mathrm{e}^{-(\beta-\tau_m)V^{\mathrm{per}}}\,. \tag{8.16}$$

Inserting the expansion of unity $\mathbb{1}_{\mathcal{H}_\Lambda} = \sum_{n_\Lambda} |n_\Lambda\rangle\langle n_\Lambda|$ to the right of operators $T_{\boldsymbol{A}_j}$, we obtain

$$Z_\Lambda^{\mathrm{per}} = \sum_{m \geqslant 0} \sum_{n_\Lambda^1,\dots,n_\Lambda^m} \sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m \\ \bar{A}_i \subset \Lambda}} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_m$$

$$\mathrm{e}^{-\tau_1 V_\Lambda^{\mathrm{per}}(n_\Lambda^1)} \langle n_\Lambda^1 | T_{\boldsymbol{A}_1} | n_\Lambda^2 \rangle \, \mathrm{e}^{-(\tau_2-\tau_1)V_\Lambda^{\mathrm{per}}(n_\Lambda^2)} \dots \langle n_\Lambda^m | T_{\boldsymbol{A}_m} | n_\Lambda^1 \rangle \, \mathrm{e}^{-(\beta-\tau_m)V_\Lambda^{\mathrm{per}}(n_\Lambda^1)} . \quad (8.17)$$

Recall that we interpret this object as a classical partition function on the $(\nu+1)$-dimensional space $\Lambda \times [0,\beta]_{\mathrm{per}}$. Namely, calling the additional dimension "time direction", the partition function Z_Λ^{per} is a (continuous) sum over all space-time configurations $\boldsymbol{n}_\Lambda = \boldsymbol{n}_\Lambda(\tau)$, $\tau \in [0,\beta]$, and all possible transitions at times corresponding to discontinuities of $\boldsymbol{n}_\Lambda(\tau)$. Notice that $\boldsymbol{n}_\Lambda(\tau)$ is periodic in the time direction. Thus, actually, we obtain a classical partition function on the $(\nu+1)$-dimensional torus $\mathbb{T}_\Lambda = \Lambda \times [0,\beta]_{\mathrm{per}}$ with a circle $[0,\beta]_{\mathrm{per}}$ in time direction (for simplicity we omit in $\mathbb{T}_\Lambda$ a reference to β). Introducing the *quantum configuration* $\boldsymbol{\omega}_{\mathbb{T}_\Lambda}$ consisting of the space-time configuration $\boldsymbol{n}_\Lambda(\tau)$ and the transitions $(\boldsymbol{A}_i, \tau_i)$ at corresponding times, we can rewrite (8.17) in a compact form

$$Z_\Lambda^{\mathrm{per}} = \int \mathrm{d}\boldsymbol{\omega}_{\mathbb{T}_\Lambda} \rho^{\mathrm{per}}(\boldsymbol{\omega}_{\mathbb{T}_\Lambda}) \quad (8.18)$$

with $\rho^{\mathrm{per}}(\boldsymbol{\omega}_{\mathbb{T}_\Lambda})$ standing for the second line of (8.17).

Now, we are going to specify excitations within a space-time configuration $\boldsymbol{n}$ and identify classes of small excitations — *the loops*[4] — and large ones — *the quantum contours*.

A configuration $n \in \boldsymbol{\Omega}$ is said to be in the state $g \in G$ at site x whenever $n_{U(x)} = g_{U(x)}$ (notice that, in general, g is not unique). If there is no such $g \in G$, the configuration n is said to be *classically excited* at x. We use $E(n)$ to denote the set of all classically excited sites of $n \in \Omega^{\mathbb{Z}^\nu}$. For any $\Lambda \subset \mathbb{Z}^\nu$, let us consider the set $\mathcal{W}_\Lambda^{\mathrm{per}}$ of quantum configurations on the torus $\mathbb{T}_\Lambda$. Whenever $\boldsymbol{\omega} \in \mathcal{W}_\Lambda^d$, its *boundary* $\boldsymbol{B}^{(0)}(\boldsymbol{\omega}) \subset \mathbb{T}_\Lambda$ is defined as the union

$$\boldsymbol{B}^{(0)}(\boldsymbol{\omega}) = (\cup_{\tau\in[0,\beta]}(E(\boldsymbol{n}(\tau)) \times \tau)) \cup (\cup_{i=1}^m (\bar{A}_i \times \tau_i)). \quad (8.19)$$

The sets $\bar{A}_i \times \tau_i \subset \mathbb{T}_\Lambda$ represent the effect of the operator $\boldsymbol{T}$ and for this reason are called *quantum transitions*. It is worth to notice that the set $\boldsymbol{B}^{(0)}(\boldsymbol{\omega})$ is closed.

Next step is to identify the smallest quantum excitations — those consisting of a sequence of transitions from the list $\mathcal{S}$. First, let us use $\mathcal{B}^{(0)}(\boldsymbol{\omega})$ to denote the set of connected components of $\boldsymbol{B}^{(0)}(\boldsymbol{\omega})$ (so that $\boldsymbol{B}^{(0)}(\boldsymbol{\omega}) = \cup_{B\in\mathcal{B}^{(0)}(\boldsymbol{\omega})} B$). To any $B \in \mathcal{B}^{(0)}(\boldsymbol{\omega})$ that is not wrapped around the cylinder (i.e. for which there exists a time $\tau_B \in [0,\beta]_{\mathrm{per}}$ with $B \cap (\mathbb{Z}^\nu \times \tau_B) = \varnothing$) we assign its sequence of transitions, $S(B,\boldsymbol{\omega})$, ordered according to their times (starting from τ_B to β and proceeding from 0 to τ_B) as well as the smallest box $\tilde{B}$ containing B. Here, a box is any subset of $\mathbb{T}_{\mathbb{Z}^\nu}$ of the form $A \times [\tau_1,\tau_2]$ with connected $A \subset \mathbb{Z}^\nu$ and $[\tau_1,\tau_2] \subset [0,\beta]_{\mathrm{per}}$ (if $\tau_1 > \tau_2$, we interpret the segment $[\tau_1,\tau_2]$ as that interval in $[0,\beta]_{\mathrm{per}}$ (with endpoints τ_1 and τ_2) that contains the point $0 \equiv \beta$).

We would like to declare the excitations with $S(B,\boldsymbol{\omega}) \in \mathcal{S}$ to be small. However, we need to be sure that there are no other excitations in their close neighbourhood. If this were the case, we would "glue" the neighbouring excitations together. This motivates the following iterative procedure.

[4]Even though the present framework is more general, the name comes from thinking about simplest excitations in Hubbard type models. Namely, a jump of an electron to a neighbouring site and returning afterwards to its original position.

Given $\boldsymbol{\omega}$, let us first consider the set $\mathcal{B}_0^{(0)}(\boldsymbol{\omega})$ of those components $B \in \mathcal{B}^{(0)}(\boldsymbol{\omega})$ that are not wrapped around the cylinder and for which $S(B,\boldsymbol{\omega}) \in \bar{\mathcal{S}}$, where $\bar{\mathcal{S}}$ is the set of all subsequences of sequences from $\mathcal{S}$. Next, we define the first extension of the boundary,

$$\boldsymbol{B}^{(1)}(\boldsymbol{\omega}) = (\cup_{B\in\mathcal{B}^{(0)}(\boldsymbol{\omega})\setminus\mathcal{B}_0^{(0)}(\boldsymbol{\omega})} B) \cup (\cup_{B\in\mathcal{B}_0^{(0)}(\boldsymbol{\omega})} \tilde{B}).$$

Using $\mathcal{B}^{(1)}(\boldsymbol{\omega})$ to denote the set of connected components of $\boldsymbol{B}^{(1)}(\boldsymbol{\omega})$ and $\mathcal{B}_0^{(1)}(\boldsymbol{\omega}) \subset \mathcal{B}^{(1)}(\boldsymbol{\omega})$ the set of those components B in $\mathcal{B}^{(1)}(\boldsymbol{\omega})$ that are not wrapped around the cylinder and for which[5] $S(B,\boldsymbol{\omega}) \in \bar{\mathcal{S}}$, we define

$$\boldsymbol{B}^{(2)}(\boldsymbol{\omega}) = (\cup_{B\in\mathcal{B}^{(1)}(\boldsymbol{\omega})\setminus\mathcal{B}_0^{(1)}(\boldsymbol{\omega})} B) \cup (\cup_{B\in\mathcal{B}_0^{(1)}(\boldsymbol{\omega})} \tilde{B}).$$

Iterating this procedure, it is clear that after a finite number of steps we obtain the final extension of the boundary,

$$\boldsymbol{B}(\boldsymbol{\omega}) = (\cup_{B\in\mathcal{B}^{(k)}(\boldsymbol{\omega})\setminus\mathcal{B}_0^{(k)}(\boldsymbol{\omega})} B) \cup (\cup_{B\in\mathcal{B}_0^{(k)}(\boldsymbol{\omega})} B).$$

Here, every $B \in \mathcal{B}_0^{(k)}(\boldsymbol{\omega})$ is a box of the form $A \times [\tau_1,\tau_2]$ (that is not wrapped around the cylinder) and $S(B,\boldsymbol{\omega}) \in \bar{\mathcal{S}}$. Let us denote $\mathcal{B}(\boldsymbol{\omega}) \equiv \mathcal{B}_0^{(k)}(\boldsymbol{\omega})$ and consider the set $\mathcal{B}_0(\boldsymbol{\omega}) \subset \mathcal{B}(\boldsymbol{\omega})$ of all those sets $B \in \mathcal{B}_0^{(k)}(\boldsymbol{\omega})$ for which actually $S(B,\boldsymbol{\omega}) \in \mathcal{S}$ and, moreover, $n_A(\tau_1 - 0) = n_A(\tau_2 + 0)$. Finally, let $\mathcal{B}_{\rm l}(\boldsymbol{\omega}) = \mathcal{B}(\boldsymbol{\omega}) \setminus \mathcal{B}_0(\boldsymbol{\omega})$ — "l" for "large": it represents the set of all excitations of $\boldsymbol{\omega}$ that are not loops. Taking, for any closed $B \subset \mathbb{T}_\Lambda$, the restriction $\boldsymbol{n}_B$ of a space-time configuration $\boldsymbol{n}$ to be defined by $(\boldsymbol{n}_B)_x(\tau) = \boldsymbol{n}_x(\tau)$ for any $x\times\tau \in B$, we introduce the useful notion of the restriction $\boldsymbol{\omega}_B$ of a quantum configuration $\boldsymbol{\omega}$ to B as to consist of $\boldsymbol{n}_B$ and those quantum transitions from $\boldsymbol{\omega}$ that are contained in B, $A\times\tau \subset B$ (we suppose here that $\boldsymbol{\omega}$ and B are such that no transition intersects both B and its complement; we do not define $\boldsymbol{\omega}_B$ in this case).

Now the loops and and the quantum contours can be defined. First, the *loops* of a quantum configuration $\boldsymbol{\omega}$ are the triplets $\xi \equiv (B, \boldsymbol{\omega}_B, g_A^\xi)$; $B \equiv A\times[\tau_1,\tau_2] \in \mathcal{B}_0(\boldsymbol{\omega})$ is the *support* of the loop ξ and $g_A^\xi = n_A(\tau_1 - 0) = n_A(\tau_2 + 0)$, a restriction of a configuration $g \in G$. (While the configuration g is not unique, its restriction to A is determined by the loop ξ in a unique way.) We say that ξ is *immersed* in g. Given a quantum configuration $\boldsymbol{\omega}$, we obtain a new configuration $\check{\boldsymbol{\omega}}$ by erasing all loops $(B, \boldsymbol{\omega}_B, g_A^\xi)$, i.e. for each ξ we remove all the transitions in its support B and change the space-time configuration on B into $g \in G$ into which ξ is immersed. Let us remark that $\mathcal{B}(\check{\boldsymbol{\omega}}) = \mathcal{B}_{\rm l}(\boldsymbol{\omega})$. Notice that, since we started our construction from (8.19), we have automatically $\operatorname{diam} A \geqslant 2R_0$ for a support $A\times[\tau_1,\tau_2]$ of any loop ξ.

Quantum contours of a configuration $\boldsymbol{\omega}$ will be constructed by extending pairs $(B,\boldsymbol{\omega}_B)$ with $B \in \mathcal{B}_{\rm l}(\boldsymbol{\omega})$ by including also the regions of nondominating states from G. Namely, summing over loops we will see that "loop free energy" favours the regions with dominating configurations from $D \subset G$. However, to recognize the influence of loops, we have to look on regions of size comparable to the size of loops. This motivates the following definitions with $U'(x) = \{y \in \mathbb{Z}^\nu, |x-y| < R\}$ being an extension of original neighbourhood $U(x)$. Thus, we enlarge the set $E(n)$ of classically excited sites to $\tilde{E}(n)$, with

$$\tilde{E}(n) = \{x \in \mathbb{Z}^\nu : n_{U'(x)} \neq g_{U'(x)} \text{ for any } g \in G\}$$

[5] A set $B \in \mathcal{B}_0^{(1)}(\boldsymbol{\omega})$ may actually contain several original components from $\mathcal{B}_0^{(0)}(\boldsymbol{\omega})$. We take for $S(B,\boldsymbol{\omega})$ the sequence of all transitions in all those components.

and we introduce the set $F(n)$ of *softly excited sites* by

$$F(n) = \{x \in \mathbb{Z}^\nu \setminus \tilde{E}(n) : n_{U'(x)} \neq d_{U'(x)} \text{ for any } d \in D\}.$$

Then, for a quantum configuration such that $\boldsymbol{\omega} = \check{\boldsymbol{\omega}}$, we define the new extended boundary

$$\boldsymbol{B}_{\rm e}(\check{\boldsymbol{\omega}}) = \bigcup_{\tau\in[0,\beta]_{\rm per}} \Big(\big[\tilde{E}(\boldsymbol{n}(\tau)) \cup F(\boldsymbol{n}(\tau))\big] \times \tau \Big) \bigcup \bigcup_{i=1}^{m} \Big(\big[\bigcup_{x\in A_i} U'(x) \big] \times \tau_i \Big),$$

and if $\boldsymbol{\omega} \neq \check{\boldsymbol{\omega}}$, we set $\boldsymbol{B}_{\rm e}(\boldsymbol{\omega}) = \boldsymbol{B}_{\rm e}(\check{\boldsymbol{\omega}})$. Notice that $\boldsymbol{B}(\check{\boldsymbol{\omega}}) \subset \boldsymbol{B}_{\rm e}(\boldsymbol{\omega})$, since the first set is the union of classical excitations, quantum transitions and boxes; obviously the classical excitations and the quantum transitions also belong to $\boldsymbol{B}_{\rm e}(\boldsymbol{\omega})$, and the boxes being such that their diameter is smaller than $2R$ and they contain $U(x)$-excited sites at each time, they are $U'(x)$-excited. Decomposing $\boldsymbol{B}_{\rm e}(\boldsymbol{\omega})$ into connected components, we get our quantum contours, namely $\gamma = (B, \boldsymbol{\omega}_B)$. Notice that the configuration $\boldsymbol{\omega}_B$ contains actually also the information determining which dominant ground state lies outside B. We call the set B the *support* of γ, $B = \mathrm{Supp}\,\gamma$, and introduce also its "truly excited part", the *core*, $\mathrm{core}\,\gamma \subset \mathrm{Supp}\,\gamma$, by taking

$$\mathrm{core}\,\gamma = \mathrm{Supp}\,\gamma \bigcap \Big(\cup_{\tau\in[0,\beta]_{\rm per}} \big(\tilde{E}(\boldsymbol{n}(\tau)) \times \tau\big) \cup \bigcup_{i=1}^{m} \Big(\big[\bigcup_{x\in A_i} U'(x) \big] \times \tau_i \Big) \Big).$$

Finally, notice that if the contour is not wrapped around the torus in its spatial direction, there exists a space-time configuration $\boldsymbol{\omega}^\gamma$ and we have $B = \boldsymbol{B}_{\rm e}(\boldsymbol{\omega}^\gamma)$.

A set of quantum contours $\Gamma = \{\gamma_1, \ldots, \gamma_k\}$ is called admissible if there exists a quantum configuration $\boldsymbol{\omega}^\Gamma \in \mathcal{W}_\Lambda^{\rm per}$ which has Γ as set of quantum contours. Clearly, if it exists, it is unique under assumption that it contains no loops ($\boldsymbol{\omega}^\Gamma = \check{\boldsymbol{\omega}}^\Gamma$).[6] We use $\mathcal{G}_\Lambda^{\rm per}$ to denote the set of all collections Γ of admissible quantum contours.

Given $\Gamma \in \mathcal{G}_\Lambda^{\rm per}$, a set of loops $\Xi = \{\xi_1, \ldots, \xi_\ell\}$ is said admissible and compatible with Γ if there exists $\boldsymbol{\omega}^{\Gamma\cup\Xi}$ which has Ξ as set of loops and Γ as set of quantum contours (it is also unique whenever it exists). More explicitly,

- two loops $\xi = (B, \boldsymbol{\omega}_B, g_A^\xi)$ and $\xi' = (B', \boldsymbol{\omega}'_{B'}, g_{A'}^{\xi'})$ are compatible iff $B \cup B'$ is not connected;
- using $\mathrm{core}\,\Gamma = \cup_{\gamma\in\Gamma} \mathrm{core}\,\gamma$, a loop $\xi = (B, \boldsymbol{\omega}_B, g_A^\xi)$, with $B = A \times [\tau_1, \tau_2]$, is compatible with Γ iff

$$B \cup \mathrm{core}\,\Gamma \text{ is not connected,} \tag{8.20}$$

$$g_A^\xi = \boldsymbol{n}_A^\Gamma(\tau) \quad \forall \tau \in [\tau_1, \tau_2]; \tag{8.21}$$

- a collection of loops $\Xi = \{\xi_1, \ldots, \xi_\ell\}$ is admissible and compatible with Γ iff any two loops from Ξ are compatible and each loop from Ξ is compatible with Γ.

We use $\mathcal{G}_\Lambda^{\rm loop}(\Gamma)$ to denote the set of all admissible collections Ξ that are compatible with Γ.

The conditions of admissibility and compatibility above can be, for any given set of transitions $\{\boldsymbol{A}_1, \ldots, \boldsymbol{A}_m\}$, formulated as a finite number of restrictions on corresponding transition times $\{\tau_1, \ldots, \tau_m\}$. Given the restrictions on admissibility of $\Gamma \in \mathcal{G}_\Lambda^{\rm per}$, the restrictions on Ξ to belong to $\mathcal{G}_\Lambda^{\rm loop}(\Gamma)$ factorize. As a result, the partition function $Z_\Lambda^{\rm per}$ in (8.18) can be rewritten in terms of integrations over $\mathcal{G}_\Lambda^{\rm per}$ and $\mathcal{G}_\Lambda^{\rm loop}(\Gamma)$ [the summation

[6] In fact, it is unique on the projection of $\mathrm{Supp}\,\Gamma$ on $\mathbb{Z}^\nu$; but from now on, we suppose that Γ also contains information on which configuration of G lives on $\Lambda \setminus \mathrm{Supp}\,\Gamma$ (when G is finite, this remark is not relevant).

over Γ and Ξ accompanied with the integration, *a priori* over the interval $[0,\beta]$, over times τ_i of corresponding transitions, subjected to above formulated restrictions, c.f. (8.17)]. Furthermore the contribution of $\Gamma\cup\Xi$ factorizes as a contribution of Γ times a product of terms for $\xi\in\Xi$ [BKU 1996, DFF 1996][7], we get

$$\begin{aligned} Z_\Lambda^{\mathrm{per}} &= \int_{\mathcal{G}_\Lambda^{\mathrm{per}}} \mathrm{d}\Gamma \int_{\mathcal{G}_\Lambda^{\mathrm{loop}}(\Gamma)} \mathrm{d}\Xi\ \rho^{\mathrm{per}}(\boldsymbol{\omega}^{\Gamma\cup\Xi}) \\ &= \int_{\mathcal{G}_\Lambda^{\mathrm{per}}} \mathrm{d}\Gamma \rho^{\mathrm{per}}(\boldsymbol{\omega}^{\Gamma}) \int_{\mathcal{G}_\Lambda^{\mathrm{loop}}(\Gamma)} \mathrm{d}\Xi \prod_{\xi\in\Xi} z(\xi). \end{aligned} \tag{8.22}$$

Here, using $\{(\boldsymbol{A}_i,\tau_i), i=1,\dots,m\}$ to denote the quantum transitions of $\Gamma\cup\Xi$, we put

$$\rho^{\mathrm{per}}(\boldsymbol{\omega}^{\Gamma\cup\Xi}) = \prod_{i=1}^{m} \langle \boldsymbol{n}_{A_i}^{\Gamma\cup\Xi}(\tau_i-0)|\, T_{\boldsymbol{A}_i}\, |\boldsymbol{n}_{A_i}^{\Gamma\cup\Xi}(\tau_i+0)\rangle \exp\Big\{-\int_{\mathbb{T}_\Lambda} \mathrm{d}(x,\tau)\Phi_x(\boldsymbol{n}_{U(x)}^{\Gamma\cup\Xi}(\tau))\Big\}, \tag{8.23}$$

where $\int_B \mathrm{d}(x,\tau)$ is the shorthand for $\int_0^\beta \mathrm{d}\tau \sum_{x:x\times\tau\in B}$ (used here for $B=\mathbb{T}_\Lambda$). Similarly for $\rho^{\mathrm{per}}(\boldsymbol{\omega}^\Gamma)$. Further, the weight of a loop $\xi=(B^\xi,\boldsymbol{\omega}_{B^\xi},g_A^\xi)$ with the set of quantum transitions $\{(\boldsymbol{A}_i,\tau_i), i=1,\dots,\ell\}$ and $\boldsymbol{n}^\xi$ the space-time configuration corresponding to $\boldsymbol{\omega}_{B^\xi}$, is

$$\begin{aligned} z(\xi) = \exp\Big\{-\int_{B^\xi} \mathrm{d}(x,\tau)[\Phi_x(\boldsymbol{n}_{U(x)}^\xi(\tau)) - \Phi_x(g_{U(x)}^\xi)]\Big\} \langle g_{A_1}^\xi|\, T_{\boldsymbol{A}_1}\, |\boldsymbol{n}_{A_1}^\xi(\tau_1+0)\rangle \times \\ \times \langle \boldsymbol{n}_{A_2}^\xi(\tau_2-0)|\, T_{\boldsymbol{A}_2}\, |\boldsymbol{n}_{A_2}^\xi(\tau_2+0)\rangle \dots \langle \boldsymbol{n}_{A_\ell}^\xi(\tau_\ell-0)|\, T_{\boldsymbol{A}_\ell}\, |g_{A_\ell}^\xi\rangle. \end{aligned} \tag{8.24}$$

Given $\Gamma\in\mathcal{G}_\Lambda^{\mathrm{per}}$, the second integral in (8.22) is over the collections of the loops that interact only through a condition of non-intersection. This is the usual framework for applying the cluster expansion of polymers.

Recall the definition (5.18) of the truncated function; here $\operatorname{Supp}\xi\equiv B^\xi$.

We use $\mathcal{L}_\Lambda$ and $\mathcal{C}_\Lambda$ to denote the set of all loops and clusters, respectively, and use $\int_{\mathcal{C}_\Lambda}\mathrm{d}\boldsymbol{C}$ as a shorthand for $\sum_{n\geqslant 1}\int_{\mathcal{L}_\Lambda}\mathrm{d}\xi_1\cdots\int_{\mathcal{L}_\Lambda}\mathrm{d}\xi_n$, in obvious meaning. Whenever $\Gamma\in\mathcal{G}_\Lambda^{\mathrm{per}}$ is fixed, we use $\mathcal{L}_\Lambda(\Gamma)$ to denote the set of all loops compatible with Γ and write $\boldsymbol{C}\in\mathcal{C}_\Lambda(\Gamma)$ whenever the cluster $\boldsymbol{C}$ contains only loops from $\mathcal{L}_\Lambda(\Gamma)$. Again, $\int_{\mathcal{C}_\Lambda(\Gamma)}\mathrm{d}\boldsymbol{C}$ is a shorthand for $\sum_{n\geqslant 1}\int_{\mathcal{L}_\Lambda(\Gamma)}\mathrm{d}\xi_1\cdots\int_{\mathcal{L}_\Lambda(\Gamma)}\mathrm{d}\xi_n$. Finally, we also need similar integrals conditioned by the time of the first transition encountered in the loop ξ or the cluster $\boldsymbol{C}$. Namely, using C to denote the support of $\boldsymbol{C}$, i.e. the union of the supports of the loops of $\boldsymbol{C}$, and $I_C=\{\tau_1(\boldsymbol{C}),\tau_2(\boldsymbol{C})\}$ to denote its vertical projection[8], $I_C=\{\tau\in[0,\beta]_{\mathrm{per}}: \mathbb{Z}^\nu\times\tau\cap C\neq\varnothing\}$, we use $\mathcal{C}_\Lambda^{(x,\tau)}$ for the set of all clusters $\boldsymbol{C}\in\mathcal{C}_\Lambda$ with the first transition time $\tau_1(\boldsymbol{C})=\tau$, for which their first loop ξ_1 with support $B_1=A_1\times[\tau_1(\boldsymbol{C}),\tau_2]$, contains the site x, $A_1\ni x$. Then $\int_{\mathcal{L}_\Lambda^{(x,\tau)}}\mathrm{d}\xi$ and $\int_{\mathcal{C}_\Lambda^{(x,\tau)}}\mathrm{d}\boldsymbol{C}$ are shorthands for the corresponding integrals with first transition time fixed — formally one replaces $\int\mathrm{d}\xi_1$ by $\int\mathbb{I}\,[A_1\ni x]\delta(\tau_1(\xi_1)-\tau)\mathrm{d}\xi_1$. With this notation we can formulate the cluster expansion lemma.

[7] The factorization is clear for spin or boson systems; for fermions it is delicate because of the anticommutation relations between creation and annihilation operators, but factorization holds. See the discussion in Chapter 7, and the proof in [DFF 1996], Section 4.2.

[8] Again, if $\tau_1>\tau_2$, the segment $[\tau_1,\tau_2]\subset[0,\beta]_{\mathrm{per}}$ contains the point $0\equiv\beta$.

LEMMA 8.1. **Cluster expansion.**

For any $c \in \mathbb{R}$, $\alpha_1 < (2R_0)^{-\nu}$, $\alpha_2 < R^{-2\nu}\Delta_0$ and $\delta > 0$, there exists $\varepsilon_0 > 0$ such that whenever $\|T\| \leqslant \varepsilon_0$ and $\Gamma \in \mathcal{G}_\Lambda^{\mathrm{per}}$, we have the loop cluster expansion,

$$\int_{\mathcal{G}_\Lambda^{\mathrm{loop}}(\Gamma)} \mathrm{d}\Xi \prod z(\xi) = \exp\Big\{ \int_{\mathcal{C}_\Lambda(\Gamma)} \mathrm{d}\boldsymbol{C} \Phi^{\mathrm{T}}(\boldsymbol{C}) \Big\}. \tag{8.25}$$

Moreover, the weights of the clusters are exponentially decaying (uniformly in Λ and β):

$$\int_{\mathcal{C}_\Lambda} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\big[C \ni (x,\tau)\big] |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi \in \boldsymbol{C}} \mathrm{e}^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \leqslant \delta \tag{8.26}$$

and

$$\int_{\mathcal{C}_\Lambda^{(x,\tau)}} \mathrm{d}\boldsymbol{C} |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi \in \boldsymbol{C}} \mathrm{e}^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \leqslant \delta \tag{8.27}$$

for every $(x,\tau) \in \mathbb{T}_\Lambda$.

PROOF. It is very similar to the proof of Proposition 5.3. Assuming that inequality (8.27) holds true, we have a finite bound

$$\sum_{n \geqslant 1} \frac{1}{n!} \int_{\mathcal{L}_\Lambda(\Gamma)^n} \mathrm{d}\xi_1 \dots \mathrm{d}\xi_n |\varphi^{\mathrm{T}}(\mathcal{G}(\xi_1, \dots, \xi_n))| \prod_{i=1}^n |z(\xi_i)| \leqslant \delta\beta|\Lambda|. \tag{8.28}$$

Lemma 8.1 then follows from Proposition 5.4. Let us turn to the proof of the two inequalities. Let

$$f(\xi) = |z(\xi)|\, \mathrm{e}^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|}.$$

Skipping the condition that ξ_j is compatible with Γ, we define

$$I_n = n\Big[\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_1\, \mathbb{I}\big[B_1 \ni (x,\tau)\big] + \int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi_1 \Big] \int_{\mathcal{L}_\Lambda^{n-1}} \mathrm{d}\xi_2 \dots \mathrm{d}\xi_n |\varphi^{\mathrm{T}}(\xi_1, \dots, \xi_n)| \prod_{i=1}^n f(\xi_i) \tag{8.29}$$

(it does not depend on $(x,\tau) \in \mathbb{T}_\Lambda$). The lemma will be completed once we shall have established that $I_n \leqslant n!(\frac{1}{2}\delta)^n$ (assuming that $\delta \leqslant 1$; otherwise, we show that $I_n \leqslant n!/2^n$). From Lemma 5.5, we get

$$|\varphi^{\mathrm{T}}(\xi_1, \dots, \xi_n)| \leqslant \sum_{\mathcal{T} \text{ tree on } n \text{ vertices}} \prod_{e(i,j) \in \mathcal{T}} \mathbb{I}\big[B_i \Cap B_j\big]. \tag{8.30}$$

Denoting $i_1, \dots, i_n$ the incidence numbers of vertices $1, \dots, n$, we first proceed with the integration on the loops $j \neq 1$ for which $i_j = 1$; in the tree $\mathcal{T}$, such j shares an edge only with one vertex i. The incompatibility between ξ_i and ξ_j, with $\xi = (B_i, \boldsymbol{\omega}_{B_i}^{(i)}, g_{A_i}^{\xi_i})$, $B_i = A_i \times [\tau_1^{(i)}, \tau_2^{(i)}]$, and similarly for ξ_j, means that either $B_j \cup [A_i \times \tau_1^{(i)}]$ is connected, or $[A_j \times \tau_1^{(j)}] \cup B_i$ is connected. Hence, the bound for the integral over the ξ_j that are

incompatible with ξ_i is

$$\begin{aligned}\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_j \, \mathbb{I}\left[B_j \cap B_i \text{ connected}\right] f(\xi_j) \\ \leqslant\ 2\nu|A_i| \int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_j \, \mathbb{I}\left[B_j \ni (x,\tau)\right] f(\xi_j) + 2\nu|B_i| \int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi_j f(\xi_j) \\ \leqslant\ 2\nu\Big(|A_i| + \alpha|B_i|\Big)\left(\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_j \, \mathbb{I}\left[B_j \ni (x,\tau)\right] f(\xi_j) + \frac{1}{\alpha}\int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi_j f(\xi_j)\right). \quad (8.31)\end{aligned}$$

(The constant α has been introduced in order to match with the conditions of the next lemma). Then

$$I_n \ \leqslant\ n(2\nu)^{n-1} \sum_{\mathcal{T} \text{ tree of } n \text{ vertices}} \Big[\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_1 \, \mathbb{I}\left[B_1 \ni (x,\tau)\right] + \int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi_1\Big] f(\xi_1)\Big(|A_1|+\alpha|B_1|\Big)^{i_1}$$
$$\prod_{j=2}^{n}\Big[\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi_j \, \mathbb{I}\left[B_j \ni (x,\tau)\right] f(\xi_j)\Big(|A_j|+\alpha|B_j|\Big)^{i_j-1} + \frac{1}{\alpha}\int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi_j f(\xi_j)\Big(|A_j|+\alpha|B_j|\Big)^{i_j-1}\Big]. \quad (8.32)$$

Now summing over all trees, knowing that the number of trees with n vertices and incidence numbers $i_1, \dots, i_n$ is equal to

$$\frac{(n-2)!}{(i_1-1)!\dots(i_n-1)!} \ \leqslant\ \frac{(n-1)!}{i_1!(i_2-1)!\dots(i_n-1)!},$$

we find a bound

$$I_n \ \leqslant\ n!(2\nu)^{n-1}(1+\alpha)\left[\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi \, \mathbb{I}\left[B \ni (x,\tau)\right] f(\xi)\, \mathrm{e}^{|A|+\alpha|B|} + \frac{1}{\alpha}\int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi f(\xi)\, \mathrm{e}^{|A|+\alpha|B|}\right]^n. \quad (8.33)$$

We conclude by using the following lemma which implies that the quantity between the brackets is small.

Remark: we used here translation invariance of the Hamiltonian, since we assumed that the objects do not depend on $(x,\tau) \in \mathbb{T}_{\mathbb{Z}^\nu}$. However, in view of the proof that states are thermodynamically stable, we must allow perturbations which are not necessarily translation invariant. This objection can be answered easily by choosing for $f(\xi)$ a bound that is uniform in the location of ξ.

□

Lemma 8.2.

Let $\alpha_1 < (2R_0)^{-\nu}$ and $\alpha_2 < R^{-2\nu}\Delta_0$. For any $c \in \mathbb{R}$ and $\delta > 0$, there exists $\varepsilon_0 > 0$ such that whenever $\|T\| \leqslant \varepsilon_0$ the following inequality holds true,

$$\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi \, \mathbb{I}\left[B \ni (x,\tau)\right] |z(\xi)|\, \mathrm{e}^{(c-\alpha_1 \log\|T\|)|A|+\alpha_2|B|} + \int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi |z(\xi)|\, \mathrm{e}^{(c-\alpha_1 \log\|T\|)|A|+\alpha_2|B|} \ \leqslant\ \delta,$$

where (x,τ) is any space-time site of $\mathbb{T}_\Lambda$.

Proof. Let us first consider the integral over ξ such that its box contains a given space-time site. We denote by ℓ_1 the number of quantum transitions of ξ at times bigger than τ, and ℓ_2 the number of the other quantum transitions. The integral over ξ can be done by summing over $(\ell_1+\ell_2)$ quantum transitions $\boldsymbol{A}_1^1, \dots, \boldsymbol{A}_{\ell_1}^1, \boldsymbol{A}_1^2, \dots, \boldsymbol{A}_{\ell_2}^2$, by summing over $(\ell_1+\ell_2)$ configurations $n_{A_j^i}^{i,j}$, and by integrating over times $\tau_1^1 < \dots < \tau_{\ell_1}^1$, $\tau_1^2 < \dots <$

$\tau^2_{\ell_2}$. Let us do the change of variables $\tilde\tau^1_1 = \tau^1_1 - \tau$, $\tilde\tau^1_2 = \tau^1_2 - \tau^1_1$, ..., $\tilde\tau^1_{\ell_1} = \tau^1_{\ell_1} - \tau^1_{\ell_1-1}$, and $\tilde\tau^2_1 = \tau - \tau^2_1$, ..., $\tilde\tau^2_{\ell_2} = \tau^2_{\ell_2-1} - \tau^2_{\ell_2}$. Then we can write the following upper bound

$$\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi\, \mathbb{I}\left[B \ni (x,\tau)\right] |z(\xi)|\, \mathrm{e}^{(c-\alpha_1 \log\|T\|)|A|+\alpha_2|B|}$$

$$\leqslant \sum_{\ell_1,\ell_2 \geqslant 1} \sum_{\substack{\boldsymbol{A}^1_1,\dots\boldsymbol{A}^2_{\ell_2} \\ \cup_{i,j}\bar A^i_j = A \ni x \\ A \text{ connected}}} \sum_{n^{1,1}_{A^1_1},\dots,n^{2,\ell_2}_{A^2_{\ell_2}} \notin G_A} \int_0^\infty \mathrm{d}\tilde\tau^1_1 \dots \mathrm{d}\tilde\tau^2_{\ell_2} \prod_{i=1,2}\prod_{j=1}^{\ell_i} |\langle n^{i,j}_A|\, T_{\boldsymbol{A}^i_j}\, |n^{i,j+1}_A\rangle|$$

$$\mathrm{e}^{(c-\alpha_1\log\|T\|)|\bar A^i_j|}\ \mathrm{e}^{-\tilde\tau^i_j \sum_{x\subset A}[\Phi_x(n^{i,j}_{U(x)}) - \Phi_x(g_{U(x)})]}\ \mathrm{e}^{\tilde\tau^i_j R^\nu \alpha_2} \qquad (8.34)$$

where $g_A \in G_A$ is the configuration in which the loop ξ is immersed (if the construction does not lead to a possible loop, we find a bound by picking any $g_A \in G_A$). Remark that we neglected a constraint on the sum over configurations, namely $n^{1,1}_A = n^{2,1}_A$. It is useful to note that the sums over ℓ_1, ℓ_2 and over the quantum transitions are finite, otherwise they cannot constitute a loop.

Using the definition (2.18) of the norm of a quantum interaction, we have

$$\sum_{\boldsymbol{A}: A=B} |\langle n'_B|\, T_{\boldsymbol{A}}\, |n_B\rangle| \ \leqslant\ \|T\|^{|B|}.$$

Furthermore

$$\sum_{x\subset A}[\Phi_x(n^{i,j}_{U(x)}) - \Phi_x(g_{U(x)})] \ \geqslant\ R^{-\nu}\Delta_0$$

as claimed in Property (3.4). Hence we have, since the number of configurations on A is bounded with $S^{|A|}$,

$$\int_{\mathcal{L}_\Lambda} \mathrm{d}\xi\, \mathbb{I}\left[B \ni (x,\tau)\right] |z(\xi)|\, \mathrm{e}^{(c-\alpha_1 \log\|T\|)|A|+\alpha_2|B|}$$

$$\leqslant \sum_{\ell_1,\ell_2 \geqslant 1} \sum_{\substack{A^1_1,\dots A^2_{\ell_2} \\ \cup_{i,j}\bar A^i_j = A \ni x \\ A \text{ connected}}} \prod_{i=1,2}\prod_{j=1}^{\ell_i} \frac{\left[\|T\|^{1-\alpha_1(2R_0)^\nu} S\, \mathrm{e}^{c(2R_0)^\nu}\right]^{|A^i_j|}}{R^{-\nu}\Delta_0 - R^\nu\alpha_2}. \qquad (8.35)$$

This is a small quantity since the sums are finite, by taking $\|T\|$ small enough. Now we turn to the second term, namely

$$\int_{\mathcal{L}^{(x,\tau)}_\Lambda} \mathrm{d}\xi |z(\xi)|\, \mathrm{e}^{(c-\alpha_1 \log\|T\|)|A|+\alpha_2|B|}\,.$$

The proof is similar; we first sum over the number of transitions ℓ, then over ℓ transitions $\boldsymbol{A}_1, \dots \boldsymbol{A}_\ell$ with $A = \cup_i \bar A_i \ni x$, A connected. Then we choose $\ell - 1$ intermediate configurations. Finally, we integrate over $\ell - 1$ time intervals. The resulting equation looks very close to (8.34) and is small for the same reasons.

□

Now, we single out the class of *small clusters*. Namely, a cluster is small if the sequence of its quantum transitions belongs to the list $\mathcal{S}$. To be more precise, we have to specify the order of transitions: considering a cluster $\boldsymbol{C} \equiv (\xi_1, \dots, \xi_k)$ and using $S(\xi^{(\ell)})$, $\ell = 1, \dots, k$, to denote the sequence of quantum transitions of the loop $\xi^{(\ell)} = (B^{(\ell)}, \boldsymbol{\omega}_{B^{(\ell)}}, g^{\xi^{(\ell)}}_A)$,

$S(\xi^{(\ell)}) \equiv S(B^{(\ell)}, \boldsymbol{\omega}_{B^{(\ell)}})$, we take the sequence $S(\boldsymbol{C})$ obtained by combining the sequences $S(\xi^{(1)}), \dots, S(\xi^{(k)})$ in this order. A cluster $\boldsymbol{C}$ is said to be *small* if $S(\boldsymbol{C}) \in \mathcal{S}$, it is *large* otherwise. We use $\mathcal{C}_\Lambda^{\text{small}}$ to denote the set of all small clusters on the torus $\mathbb{T}_\Lambda$.

The local contribution to the energy at time τ, when the system is in a state $\boldsymbol{n}_{U(x)}(\tau)$, is $\Phi_x(\boldsymbol{n}_{U(x)}(\tau))$. Similarly, we will introduce the local contribution of loops (and small clusters of loops) in the expansion of the partition function — the effective potential $\Psi_A^\beta(\boldsymbol{n}_A(\tau))$. The latter is a local quantity in the sense that it depends on $\boldsymbol{n}$ only on the set A at time τ. An explicit expression of $\Psi_A^\beta(g_A)$ with $g \in G$ is, in terms of small clusters,

$$\Psi_A^\beta(g_A) \doteq -\int_{\mathcal{C}_\Lambda^{\text{small}}} \mathrm{d}\boldsymbol{C} \frac{\Phi^{\mathrm{T}}(\boldsymbol{C})}{|I_C|} \mathbb{I}\left[\boldsymbol{C} \sim g_A, A_C = A, I_C \ni 0\right]. \tag{8.36}$$

Here, again, C is the support of $\boldsymbol{C}$, A_C its horizontal projection onto $\mathbb{Z}^\nu$, $A_C = \{x \in \mathbb{Z}^\nu; x \times [0,\beta]_{\text{per}} \cap C \neq \varnothing\}$, and I_C its vertical projection, $|A_C|$ and $|I_C|$ their corresponding areas, and the condition $\boldsymbol{C} \sim g_A$ means that each loop of $\boldsymbol{C}$ is immersed in the ground state g. Notice that the "horizontal extension" of any small cluster is at most R: if $\boldsymbol{C}$ is a small cluster, $\operatorname{diam}(A_C) \leqslant R$. The definitions of Section 4.2, Chapter 3, are now clear, once we identify the effective potential Ψ defined in (3.5) as the limit $\beta \to \infty$ of (8.36). Namely,

$$\Psi = \lim_{\beta\to\infty} \Psi^\beta.$$

Our assumptions in Section 4.4, Chapter 3, concern the limit $\beta \to \infty$ of the effective potential, but at non zero temperature we have to work with Ψ^β. To trace down the difference, we introduce $\psi^\beta = \Psi^\beta - \Psi$. Notice that (8.36) implies $\Psi_A^\beta(n_A) = 0$ whenever $n_A \notin G_A$ or $\operatorname{diam} A < 2R_0$.

Recalling that if $C \subset \mathbb{T}_\Lambda$, $\tilde{C}$ is the smallest box containing C, we introduce, for any cluster $\boldsymbol{C} \in \mathcal{C}_\Lambda^{\text{small}}$, the function

$$\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma) = \frac{\Phi^{\mathrm{T}}(\boldsymbol{C})}{|I_C|} \int_{I_C} \mathrm{d}\tau \Big(\mathbb{I}\left[\boldsymbol{C} \sim \Gamma\right] - \mathbb{I}\left[\boldsymbol{n}_{A_C}^\Gamma(\tau) \in G_{A_C}, \boldsymbol{C} \sim \boldsymbol{n}_{A_C}^\Gamma(\tau)\right] \Big). \tag{8.37}$$

Here, the first indicator function in the parenthesis singles out the clusters such that each loop is compatible with Γ, while the second indicator concerns the clusters for which $\boldsymbol{n}_{A_C}^\Gamma(\tau) \in G_{A_C}$ and each of their loop is immersed in the configuration $\boldsymbol{n}_A^\Gamma(\tau)$ (extended as a constant to all the time interval I_C). Observing that $\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma) = 0$ whenever $\tilde{C} \cap \operatorname{core}\Gamma = \textit{emptyset}$, we split the integral over small clusters into its bulk part expressed in terms of the effective potential and boundary terms "decorating" the quantum contours from Γ.

LEMMA 8.3.
For any fixed $\Gamma \in \mathcal{G}_\Lambda$, one has

$$\int_{\mathcal{C}_\Lambda^{\text{small}}(\Gamma)} \mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C}) = -\int_{\mathbb{T}_\Lambda} \mathrm{d}(A,\tau)\Psi_A(\boldsymbol{n}_A^\Gamma(\tau)) - \int_{\mathbb{T}_\Lambda} \mathrm{d}(A,\tau)\psi_A^\beta(\boldsymbol{n}_A^\Gamma(\tau)) + \int_{\mathcal{C}_\Lambda^{\text{small}}} \mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma).$$

The term $\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma)$ vanishes whenever $\tilde{C} \cap \operatorname{core}\Gamma = \varnothing$.

PROOF. To get the equality of integrals, it is enough to rewrite

$$\int_{\mathcal{C}_\Lambda^{\text{small}}(\Gamma)} \mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C}) = \int_{\mathcal{C}_\Lambda^{\text{small}}} \mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C}) \mathbb{I}\left[\boldsymbol{C} \sim \Gamma\right] \tag{8.38}$$

and

$$-\int_{\mathbb{T}_\Lambda} \mathrm{d}(A,\tau)\Psi_A^\beta(\boldsymbol{n}_A^\Gamma(\tau)) = \int_{\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\frac{\Phi^{\mathrm{T}}(\boldsymbol{C})}{|I_C|}\int_{I_C}\mathrm{d}\tau\,\mathbb{I}\left[\boldsymbol{n}_{A_C}^\Gamma(\tau)\in G_{A_C}, \boldsymbol{C}\sim\boldsymbol{n}_{A_C}^\Gamma(\tau)\right]. \tag{8.39}$$

Moreover, whenever $\tilde{C}\cap\operatorname{core}\Gamma=\varnothing$, the configuration $\boldsymbol{n}_{A_C}^\Gamma(\tau)$ belongs to G_{A_C}, and it is constant, for all $\tau\in I_C$. Under these circumstances, the condition $\boldsymbol{C}\sim\Gamma$ is equivalent to $\boldsymbol{C}\sim\boldsymbol{n}_{A_C}^\Gamma(\tau)$ and the right hand side of (8.37) vanishes.

□

Whenever $\Gamma\in\mathcal{G}_\Lambda$ is fixed, let $W_d(\Gamma)\subset\mathbb{T}_\Lambda$ be the set of space-time sites in the state d, i.e.

$$W_d(\Gamma)=\{(x,\tau)\in\mathbb{T}_\Lambda : \boldsymbol{n}_{U'(x)}^\Gamma(\tau)=d_{U'(x)}\}.$$

Notice that

$$\mathbb{T}_\Lambda=\operatorname{Supp}\Gamma\cup\bigcup_{d\in D}W_d(\Gamma);\quad W_d(\Gamma)\cap W_{d'}(\Gamma)=\varnothing \text{ if } d\neq d',$$

and the set $\operatorname{Supp}\Gamma\cap W_d(\Gamma)$ is of measure zero (with respect to the measure $\mathrm{d}(x,\tau)$ on $\mathbb{T}_\Lambda$). Let us recall that the equivalent potential Υ satisfies the equality $\sum_{x\in\Lambda}\Upsilon_x(n_{U(x)})=\sum_{A\subset\Lambda}(\Phi_A(n_A)+\Psi_A(n_A))+\mathrm{const}|\Lambda|$ for any configuration n on the torus Λ; actually, we can take const $=0$, since Υ and $\Upsilon'=\Upsilon+\mathrm{const}$ are also physically equivalent, and Υ' satisfies the same assumptions as Υ.

Lemma 8.4.
The partition function (8.22) *can be rewritten as*

$$Z_\Lambda^{\mathrm{per}}=\int_{\mathcal{G}_\Lambda^{\mathrm{per}}}\mathrm{d}\Gamma\prod_{d\in D}\mathrm{e}^{-|W_d(\Gamma)|e(d)}\prod_{\gamma\in\Gamma}z(\gamma)\,\mathrm{e}^{\mathcal{R}(\Gamma)}.$$

Here the weight $z(\gamma)$ *of a quantum contour* $\gamma=(B,\boldsymbol{\omega}_B)$ *with the sequence of transitions* $(\boldsymbol{A}_1,\dots,\boldsymbol{A}_m)$ *at times* $(\tau_1,\dots,\tau_m)$ *is*

$$z(\gamma)=\prod_{i=1}^m\langle\boldsymbol{n}_{A_i}^\gamma(\tau_i-0)|\,T_{\boldsymbol{A}_i}\,|\boldsymbol{n}_{A_i}^\gamma(\tau_i+0)\rangle\exp\Big\{-\int_B\mathrm{d}(x,\tau)\Upsilon_x(\boldsymbol{n}_{U'(x)}^\gamma(\tau))\Big\}. \tag{8.40}$$

The rest $\mathcal{R}(\Gamma)$ *is given by*

$$\mathcal{R}(\Gamma)=\int_{\mathcal{C}_\Lambda(\Gamma)\setminus\mathcal{C}_\Lambda^{\mathrm{small}}(\Gamma)}\mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C})-\int_{\mathbb{T}_\Lambda}\mathrm{d}(A,\tau)\psi_A^\beta(\boldsymbol{n}_A^\Gamma(\tau))+\int_{\mathcal{C}_\Lambda^{\mathrm{small}}}\mathrm{d}\boldsymbol{C}\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma). \tag{8.41}$$

Proof. Using the Lemmas 8.1 and 8.3 to substitute in (8.22) the contribution of loops by the action of the effective potential, we get

$$Z_\Lambda^{\mathrm{per}}=\int_{\mathcal{G}_\Lambda^{\mathrm{per}}}\mathrm{d}\Gamma\Big\{\prod_{i=1}^m\langle n_{A_i}^\Gamma(\tau_i-0)|\,T_{\boldsymbol{A}_i}\,|n_{A_i}^\Gamma(\tau_i+0)\rangle\Big\}\exp\Big\{-\int_{\mathbb{T}_\Lambda}\mathrm{d}(A,\tau)(\Phi_A(\boldsymbol{n}_A^\Gamma(\tau))+\Psi_A(\boldsymbol{n}_A^\Gamma(\tau)))\Big\}\,\mathrm{e}^{\mathcal{R}(\Gamma)}. \tag{8.42}$$

Replacing $\Phi + \Psi$ by the physically equivalent potential Υ, we obtain

$$Z_\Lambda^{\rm per} = \int_{\mathcal{G}_\Lambda^{\rm per}} {\rm d}\Gamma \Big\{ \prod_{i=1}^m \langle n_{A_i}^\Gamma(\tau_i - 0)| \, T_{\boldsymbol{A}_i} \, |n_{A_i}^\Gamma(\tau_i + 0)\rangle \Big\} \exp\Big\{ - \int_{{\rm Supp}\,\Gamma} {\rm d}(x,\tau) \Upsilon_x(\boldsymbol{n}^\gamma_{U'(x)}(\tau)) \Big\} \prod_{d\in D} {\rm e}^{-e(d)|W_d(\Gamma)|} \, {\rm e}^{\mathcal{R}(\Gamma)} \, . \quad (8.43)$$

We get our lemma by observing that the product over quantum transitions and the first exponential factorize with respect to the quantum contours, as it was the case for the loops (for fermions the sign arising because of anticommutation relations also factorize; we again refer to [DFF 1996] for the proof).

□

Our goal is to obtain a classical lattice system in $\nu + 1$ dimensions. Thus we introduce a discretization of the continuous time direction, by choosing suitable parameters $\tilde\beta > 0$ and $N \in \mathbb{N}$ with $\beta = N\frac{\tilde\beta}{\Delta}$.[9] Setting $\mathbb{L}_\Lambda$ to be the $(\nu+1)$-dimensional discrete torus $\mathbb{L}_\Lambda = \Lambda \times \{1, \dots, N\}^{\rm per}$ — let us recall that Λ has periodic boundary conditions in all spatial directions — and using $C(x,t) \subset \mathbb{T}_{\mathbb{Z}^\nu}$ to denote, for any $(x,t) \in \mathbb{L}_\Lambda$, the segment $x \times (\frac{\tilde\beta}{\Delta}(t-1), \frac{\tilde\beta}{\Delta}t]$, we have $\mathbb{T}_\Lambda = \cup_{(x,t)\in\mathbb{L}_\Lambda} C(x,t)$.

For any $M \subset \mathbb{L}_\Lambda$, we set $C(M)$ to be the union $C(M) = \cup_{(x,t)\in M} C(x,t) \subset \mathbb{T}_\Lambda$. Conversely, if $B \subset \mathbb{T}_\Lambda$, we take $M(B) \subset \mathbb{L}_\Lambda$ to be the smallest set such that $C(M(B)) \supset B$. Given a connected[10] set $M \subset \mathbb{L}_\Lambda$ and a collection of quantum contours $\Gamma \in \mathcal{G}_\Lambda^{\rm per}$, we define

$$\varphi(M;\Gamma) = \int_{\mathcal{C}_\Lambda(\Gamma)\setminus\mathcal{C}_\Lambda^{\rm small}(\Gamma)} {\rm d}\boldsymbol{C} \, \mathbb{I}\big[M(C) = M\big] \Phi^{\rm T}(\boldsymbol{C}) + \\ + \int_{\mathcal{C}_\Lambda^{\rm small}} {\rm d}\boldsymbol{C} \, \mathbb{I}\big[M(C) = M, C \not\subset C({\rm Supp}\,\Gamma)\big] \Phi^{\rm T}(\boldsymbol{C};\Gamma) - \int_{M(A\times\tau)=M} {\rm d}(A,\tau) \psi_A^\beta(\boldsymbol{n}_A^\Gamma(\tau)) \quad (8.44)$$

and

$$\tilde{\mathcal{R}}(\Gamma) = \int_{\mathcal{C}_\Lambda^{\rm small}} {\rm d}\boldsymbol{C} \, \mathbb{I}\big[C \subset C({\rm Supp}\,\Gamma)\big] \Phi^{\rm T}(\boldsymbol{C};\Gamma). \quad (8.45)$$

We have separated the contributions of the small clusters inside $C({\rm Supp}\,\Gamma) \equiv C(M({\rm Supp}\,\Gamma))$, because they are not necessarily a small quantity, and it is impossible to expand them. On the contrary, $\varphi(M;\Gamma)$ is small, and hence it is natural to write

$${\rm e}^{\mathcal{R}(\Gamma)} = {\rm e}^{\tilde{\mathcal{R}}(\Gamma)} \sum_{\mathcal{M}} \prod_{M\in\mathcal{M}} \Big({\rm e}^{\varphi(M;\Gamma)} - 1 \Big), \quad (8.46)$$

with the sum running over all collections $\mathcal{M}$ of connected subsets of $\mathbb{L}_\Lambda$.

Let ${\rm Supp}\,\mathcal{M} = \cup_{M\in\mathcal{M}} M$. Given a set of quantum contours $\Gamma \in \mathcal{G}_\Lambda^{\rm per}$ and a collection $\mathcal{M}$, we introduce contours on $\mathbb{L}_\Lambda$ by decomposing the set $M({\rm Supp}\,\Gamma) \cup {\rm Supp}\,\mathcal{M}$ into connected components [notice that if $(x,t) \notin M({\rm Supp}\,\Gamma) \cup {\rm Supp}\,\mathcal{M}$, then $C(x,t) \subset \cup_{d\in D} W_d(\Gamma)$]. Namely, a *contour* Y is a pair $({\rm Supp}\,Y, \alpha_Y)$ where ${\rm Supp}\,Y \subset \mathbb{L}_\Lambda$ is a (non-empty) connected subset of $\mathbb{L}_\Lambda$, and α_Y is a labeling of connected components F of $\partial C({\rm Supp}\,Y)$, $\alpha_Y(F) = 1, \dots, r$. We write $|Y|$ for the length (area) of the contour Y,

[9] Remark the difference from Chapter 7; here the vertical length of a segment is $\tilde\beta/\Delta$ and it depends on $\|T\|$, since so does the quantum Peierls constant Δ.

[10] Connectedness in $\mathbb{L}_\Lambda$ is meant in standard way via nearest neighbours.

i.e. the number of sites in $\mathrm{Supp}\, Y$. A set of contours $\mathcal{Y} = \{Y_1, \dots, Y_k\}$ is *admissible* if the contours are mutually disjoint and if the labeling is constant on the boundary of each connected component of $\mathbb{T}_\Lambda \setminus \cup_{Y\in\mathcal{Y}} C(\mathrm{Supp}\, Y)$. Finally, given an admissible set of contours $\mathcal{Y}$, we define $\mathcal{G}_d(\mathcal{Y})$ to be the union of all connected components M of $\mathbb{L}_\Lambda \setminus \cup_{Y\in\mathcal{Y}} \mathrm{Supp}\, Y$ such that $C(M)$ has label d on its boundary.

Consider now any quantum configuration $\boldsymbol{\omega} \in \mathcal{W}_\Lambda^{\mathrm{per}}$ yielding, together with a collection $\mathcal{M}$, a fixed set of contours $\mathcal{Y}$. Summing over all such configurations $\boldsymbol{\omega}$ and collections $\mathcal{M}$, we get the weight to be attributed to the set $\mathcal{Y}$. Let $\Gamma^{\boldsymbol{\omega}}$ be the collection of quantum contours corresponding to $\boldsymbol{\omega}$, $\cup_{Y\in\mathcal{Y}} \mathrm{Supp}\, Y = M(\mathrm{Supp}\, \Gamma^{\boldsymbol{\omega}}) \cup \mathrm{Supp}\, \mathcal{M}$. Given that the configurations $\boldsymbol{\omega}$ are necessarily constant with no transition on $\mathbb{T}_\Lambda \setminus C(\cup_{Y\in\mathcal{Y}} \mathrm{Supp}\, Y)$, we easily see that the weight factor splits into product of weight factors of single contours $Y \in \mathcal{Y}$. Namely, for the weight $\mathfrak{z}$ of a contour Y we get the expression

$$\mathfrak{z}(Y) = \int_{\mathcal{G}_\Lambda^{\mathrm{per}}(Y)} \mathrm{d}\Gamma \prod_{\gamma\in\Gamma} z(\gamma) \prod_{d\in D} \mathrm{e}^{-e(d)|W_d(\Gamma)\cap C(\mathrm{Supp}\, Y)|}\, \mathrm{e}^{\tilde{\mathcal{R}}(\Gamma)} \sum_{\mathcal{M}} \mathbb{I}\left[M(\mathrm{Supp}\, \Gamma) \cup \mathrm{Supp}\, \mathcal{M} = \mathrm{Supp}\, Y\right] \prod_{M\in\mathcal{M}} \Big(\mathrm{e}^{\varphi(M;\Gamma)} - 1\Big), \quad (8.47)$$

where $\mathcal{G}_\Lambda^{\mathrm{per}}(Y)$ is the set of collections Γ of quantum contours compatible with Y, $\Gamma \in \mathcal{G}_\Lambda^{\mathrm{per}}(Y)$ if $\mathrm{Supp}\, \Gamma \subset \mathrm{Supp}\, Y$ and the labels on the boundary of $\mathrm{Supp}\, \Gamma$ match with labels of Y. Thus, we can finally rewrite the partition function in a form that agrees with the standard Pirogov-Sinai setting, namely

$$Z_\Lambda^{\mathrm{per}} = \sum_{\mathcal{Y}} \prod_{d\in D} \mathrm{e}^{-\frac{\tilde{\beta}}{\Delta} e(d) |\mathcal{G}_d(\mathcal{Y})|} \prod_{Y\in\mathcal{Y}} \mathfrak{z}(Y), \quad (8.48)$$

with the sum being over all admissible sets of contours on $\mathbb{L}_\Lambda$.

In the next section we will evaluate the decay rate of contours weights in a preparation to apply the Pirogov-Sinai theory to prove Theorems 3.5, 3.6 and 3.7.

2.2. Exponential decay of the weight of the contours. In this section we show that the weight $\mathfrak{z}$ has exponential decay with respect to the length of the contours. We begin by a lemma proving that the contribution of $\mathcal{M}$ is small, that we shall use in Lemma 8.6 below for the bound of $\mathfrak{z}$.

Lemma 8.5.

Under the Assumptions 1–4, for any $c < \infty$ there exist constants β_0, $\tilde{\beta}_0 < \infty$, and $\varepsilon_0 > 0$ such that for any $\beta \geqslant \beta_0$, $\tilde{\beta}_0 \leqslant \tilde{\beta} < 2\tilde{\beta}_0$, and $\|T\| \leqslant \varepsilon_0$, one has

$$\sum_{M\ni(x,t)} \left|\, \mathrm{e}^{\varphi(M;\Gamma)} - 1\right| \mathrm{e}^{c|M|} \leqslant 1$$

for any contour Y and any set of quantum contours $\Gamma \in \mathcal{G}_\Lambda^{\mathrm{per}}(Y)$.

Proof. We show that

$$\sum_{M\ni(x,t)} \left|\varphi(M;\Gamma)\right| \mathrm{e}^{c|M|} \leqslant 1.$$

This implies that $|\varphi(M;\Gamma)| \leqslant 1$ and consequently Lemma 8.5 holds — with a slightly smaller constant c.

Let us consider separately, in (8.44), the three terms on the right hand side: *(a)* the integral over big clusters, *(b)* the integral over small clusters, and *(c)* the expression involving ψ^β.

(a) Big clusters. Our aim is to estimate

$$J = \sum_{M \ni (x,t)} \mathrm{e}^{c|M|} \int_{\mathcal{C}_\Lambda(\Gamma)\setminus\mathcal{C}_\Lambda^{\mathrm{small}}(\Gamma)} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[M(C) = M\right] \left|\Phi^{\mathrm{T}}(\boldsymbol{C})\right|.$$

Since $M(C) = M$ and $M \ni (x,t)$, the segment $C(x,t)$ either intersects a quantum transition of $\boldsymbol{C}$, or it is contained in a box B belonging to a loop of $\boldsymbol{C}$ (both possibilities may occur at the same time). In the first case we start the integral over clusters by choosing the time for the first quantum transition, which yields a factor $\tilde\beta/\Delta$. In the second case we simply integrate over all loops containing the given site. In the same time, given a cluster $\boldsymbol{C} = (\xi_1, \dots, \xi_n)$, $\xi_i = (B_i, \boldsymbol{\omega}_{B_i}^{(i)}, g_{A_i}^{\xi_i})$ and $B_i = A_i \times [\tau_1^{(i)}, \tau_2^{(i)}]$, the condition $M(C) = M$ implies that

$$\sum_{i=1}^{n} \Big\{ |A_i| + \frac{\Delta}{\tilde\beta} |B_i| \Big\} \;\geqslant\; |M|. \tag{8.49}$$

Using it to bound $|M|$, we get the estimate

$$\begin{aligned} J \;\leqslant\; \frac{\tilde\beta}{\Delta} \int_{\mathcal{C}_\Lambda^{(x,\tau)}\setminus\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C} |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{c|A| + c\frac{\Delta}{\tilde\beta}|B|} \\ + \int_{\mathcal{C}_\Lambda\setminus\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[C \ni (x,\tau)\right] |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{c|A| + c\frac{\Delta}{\tilde\beta}|B|}. \end{aligned} \tag{8.50}$$

Taking, in Lemma 4.1, the constant c as above as well as $\alpha_1 = \frac{1}{2}(2R_0)^{-\nu}$, $\alpha_2 = c\Delta/\tilde\beta$, $\delta = 1$, and choosing the corresponding $\varepsilon_0(c, \alpha_1, \alpha_2, \delta)$, we can bound the second term of (8.50), for any $\|T\| \leqslant \varepsilon_0$, with the help of (8.26) once $\tilde\beta$ is chosen large enough to satisfy

$$\frac{\tilde\beta}{\Delta} > \frac{c}{\Delta_0} R^{2\nu}. \tag{8.51}$$

To estimate the first term of (8.50), we first consider the contribution of those clusters for which

$$\frac{\tilde\beta}{\Delta} \;\leqslant\; \prod_{\xi\in\boldsymbol{C}} \|T\|^{\frac{1}{2}(2R_0)^{-\nu}|A|}.$$

Applying it together with (8.51) we can directly use the bound (8.27).

Thus it remains to estimate the contribution of those terms for which

$$\frac{2}{(2R_0)^\nu} \sum_{\xi\in\boldsymbol{C}} |A| < \frac{\log(\Delta/\tilde\beta)}{\log\|T\|}. \tag{8.52}$$

Let us first fix $\tilde\beta$ and $\varepsilon_0 \;\leqslant\; \varepsilon_0(c, \alpha_1, \alpha_2, \delta)$ with the constants c, α_1, α_2, and δ as above, so that

$$\frac{\tilde\beta}{\varepsilon_0} > \frac{c}{\Delta_0} R^{2\nu} \tag{8.53}$$

and, in the same time,

$$\tilde\beta \;\leqslant\; \varepsilon_0^{k - 2k'(2R_0)^{-\nu}} \tag{8.54}$$

for a suitable large k' (we also assume that $\varepsilon_0 \leqslant 1$). Here k is the constant that appears in Assumption 2, $\Delta(\|T\|) \geqslant \|T\|^k$. Observing further that $\Delta(\|T\|)$ can be taken to increase with $\|T\|$ (one can always consider a weaker lower bound Δ when taking smaller $\|T\|$), we conclude that (8.51), as well as the condition

$$\tfrac{1}{2}(2R_0)^\nu \frac{\log(\Delta/\tilde\beta)}{\log\|T\|} \leqslant k',$$

are satisfied for every $\|T\| \leqslant \varepsilon_0$. Thus, it suffices to find an upper bound to

$$J' = \frac{\tilde\beta}{\Delta} \int_{\mathcal{C}_\Lambda^{(x,\tau)} \setminus \mathcal{C}_\Lambda^{\text{small}}} \mathrm{d}\boldsymbol{C} |\Phi^{\mathrm{T}}(\boldsymbol{C})| \, \mathbb{I}\big[\sum_{\xi\in\boldsymbol{C}} |A| < k'\big]. \tag{8.55}$$

The main problem in estimating this term stems from the factor $1/\Delta$ that may be large if $\|T\|$ is small. Thus, to have a bound valid for all small $\|T\|$, some terms, coming from the integral, that would suppress this factor must be displayed.

The condition $\sum_{\xi\in\boldsymbol{C}} |A| < k'$ will be used several times by applying its obvious consequences: (i) the number of loops in $\boldsymbol{C}$ is smaller than k', (ii) the number of transitions for each loop is smaller than k', (iii) each transition $\boldsymbol{A}$ is such that $|A| < k'$, and (iv) the distance between each transition and x is smaller than k'.

Furthermore, we use Assumption 3 to bound the contribution of the transitions of $\boldsymbol{C}$; recalling the definition (8.24) of the weight of ξ, we have, for any large $\boldsymbol{C}$,

$$\begin{aligned}\prod_{\xi\in\boldsymbol{C}} |z(\xi)| &\leqslant b_1(\|T\|)\Delta \prod_{\xi\in\boldsymbol{C}} \exp\Big\{-\int_B \mathrm{d}(x,\tau)[\Phi_x(n^\xi_{U(x)}(\tau)) - \Phi_x(g^\xi_{U(x)}(\tau))]\Big\} \\ &\leqslant b_1(\|T\|)\Delta \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{-R^{-2\nu}\Delta_0|B|}. \end{aligned} \tag{8.56}$$

In the last inequality we used Assumption 1 in the form of the bound (3.4) as well as the lower bound $|\tau_2 - \tau_1| = \frac{|B|}{|A|} \geqslant \frac{|B|}{R^\nu}$ for the support $B = A \times [\tau_1, \tau_2]$ of the loop ξ.

For any $\xi \in \boldsymbol{C} = (\xi_1, \dots \xi_n)$, let τ be the time at which the first transition in C occurs (we assume that it happens for the "first" loop ξ_1) and τ^ξ be such that $\tau + \tau^\xi$ is the time at which the first transition in ξ occurs ($\tau^{\xi_1} = 0$). Referring to the condition (i) on the number of loops in $\boldsymbol{C}$, we get the inequality

$$\sum_{\xi\neq\xi_1} |\tau^\xi| \leqslant k' \sum_\xi |B|,$$

and thus also

$$1 \leqslant \prod_\xi \mathrm{e}^{-\frac{\Delta_0}{2k'R^{2\nu}}|\tau^\xi|} \prod_\xi \mathrm{e}^{\frac{1}{2}R^{-2\nu}\Delta_0|B|}.$$

Integrating now over the time of the first transition for each $\xi \in \boldsymbol{C}$, $\xi \neq \xi_1$, and taking into account that $|\varphi^{\mathrm{T}}(\xi_1, \dots, \xi_n)| \leqslant n^{n-2}$, we get

$$J' \leqslant \tilde\beta b_1(\|T\|) \sum_{n=1}^{k'} \frac{n^{n-2}}{(n-1)!} \Big(\frac{2k'R^{2\nu}}{\Delta_0}\Big)^{n-1} \Big\{\int_{\mathcal{L}_\Lambda^{(x,\tau)}} \mathrm{d}\xi \, \mathrm{e}^{-\frac{1}{2}R^{-2\nu}\Delta_0|B|} \, \mathbb{I}\left[\xi : k'\right]\Big\}^n. \tag{8.57}$$

Here the constraint $\mathbb{I}\left[\xi_i : k'\right]$ means that the loop ξ_i satisfies the conditions (ii)–(iv) above. We have then a finite number of finite terms, the contribution of which is bounded by a fixed number $K < \infty$ (depending on ε_0, $\tilde\beta$, and k'). Thus $J' \leqslant \tilde\beta b_1(\|T\|)K$ which can be made small by taking $\|T\|$ sufficiently small.

(b) Small clusters. Let us first notice that $|\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma)| \leqslant |\Phi^{\mathrm{T}}(\boldsymbol{C})|$, and since $M(C) = M$, inequality (8.49) is valid. Moreover C must contain at least one of the two boundary points $(y, t\frac{\tilde\beta}{\Delta} \pm \frac{\tilde\beta}{2\Delta})$ of some cell $C(y,t)$ for which $\mathrm{dist}(x,y) \leqslant R$. Indeed, given that $\boldsymbol{C}$ is small and in the same time $\tilde C \cap \operatorname{core}\Gamma \neq \varnothing$ (c.f. Lemma 8.3), this is the only way to satisfy also $C \not\subset C(\operatorname{Supp}\Gamma)$ [c.f. (8.44)]. Thus it suffices to use again (8.26) and (8.51) to estimate

$$(2R)^\nu \int_{\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[C \ni (x,\tau)\right] |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{c|A| + c\frac{\Delta}{\beta}|B|}\,.$$

(c) Bound for ψ^β. Finally, we estimate the expression involving ψ^β. We first observe that

$$\mathrm{e}^{\alpha\beta}\,|\psi^\beta_A(g_A)| \leqslant 1 \tag{8.58}$$

for any $A \subset \mathbb{Z}^\nu$ and with $\alpha = \frac12 R^{-2\nu}\Delta_0$, Indeed,

$$\begin{aligned}
&\mathrm{e}^{\alpha\beta}\,|\psi^\beta_A(g_A)| = \mathrm{e}^{\alpha\beta}\,|\Psi^\beta_A(g_A) - \Psi_A(g_A)| = \\
&= \mathrm{e}^{\alpha\beta}\Big| - \int_{\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[\boldsymbol{C} \sim g_A, A_C = A, I_C \ni 0, C \subset \Lambda\times[0,\beta]_{\mathrm{per}}, |I_C| = \beta\right] \frac{\Phi^{\mathrm{T}}(\boldsymbol{C})}{|I_C|} + \\
&\quad + \int_{\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[\boldsymbol{C} \sim g_A, A_C = A, I_C \ni 0, C \subset \Lambda\times[-\infty,\infty], |I_C| \geqslant \beta\right] \frac{\Phi^{\mathrm{T}}(\boldsymbol{C})}{|I_C|}\Big|.
\end{aligned} \tag{8.59}$$

The first integral above corresponds to clusters wrapped around the torus in vertical direction, while the second one assumes integration over all clusters in $\Lambda\times[-\infty,\infty]$. For any $\boldsymbol{C}$ above, $|I_C| \geqslant \beta$ and thus

$$\mathrm{e}^{\alpha\beta} \leqslant \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{\alpha|B|}\,.$$

Observing now that every cluster in both integrals necessarily contains in its support at least one of the points $(x,0)$, $x\in A$, and using the fact that $\operatorname{diam} A \leqslant 2R$, we can bound the first integral by

$$\frac{(2R)^\nu}{\beta} \int_{\mathcal{C}_\Lambda^{\mathrm{small}}} \mathrm{d}\boldsymbol{C}\, \mathbb{I}\left[C \ni (x,0)\right] |\Phi^{\mathrm{T}}(\boldsymbol{C})| \prod_{\xi\in\boldsymbol{C}} \mathrm{e}^{\alpha|B|}\,,$$

which can be directly evaluated by (8.26). The same bound can be actually used also for the second integral, once we realize that the estimate (8.26) is uniform in β.

Using now the fact that $\psi^\beta_A = 0$ if $\operatorname{diam} A \geqslant 2R$, the condition $M(A\times\{\tau\}) = M$ implies that M has less than $(2R)^\nu$ sites, hence $\mathrm{e}^{c|M|} \leqslant \mathrm{e}^{c(2R)^\nu}$. Furthermore, referring to (8.58), we have

$$\int_{\mathbb{T}_\Lambda} \mathrm{d}(A,\tau)|\psi^\beta_A(\cdot)|\, \mathbb{I}\left[M(A\times\{\tau\}) = M\right] \mathrm{e}^{c|M|} \leqslant \frac{\tilde\beta}{\Delta}\, \mathrm{e}^{-\frac12 R^{-2\nu}\Delta_0\beta + c(2R)^\nu}\,, \tag{8.60}$$

which can be made small for β sufficiently large and concludes thus the proof of the lemma. □

Using Lemma 8.5 and introducing $e_0 = \min_{d\in D} e(d)$, we can estimate the weight $\mathfrak{z}$ of the contours in the discrete space of cells.

LEMMA 8.6.

Under the Assumptions 1–4, for any $c < \infty$, there exist $\beta_0, \tilde\beta_0 < \infty$ and $\varepsilon_0 > 0$ such that for any $\beta \geqslant \beta_0$, $\tilde\beta_0 \leqslant \tilde\beta < 2\tilde\beta_0$, and $\|T\| \leqslant \varepsilon_0$, one has

$$|\mathfrak{z}(Y)| \leqslant \mathrm{e}^{-\frac{\tilde\beta}{\Delta} e_0 |Y|} \mathrm{e}^{-c|Y|}$$

for any contour Y.

PROOF. For a given Γ (such that $M(\operatorname{Supp}\Gamma) \subset \operatorname{Supp} Y$) with transitions $\{\boldsymbol{A}_1, \dots, \boldsymbol{A}_m\}$ at times $\{\tau_1, \dots, \tau_m\}$, we define $A(\Gamma) = \cup_{i=1}^m \cup_{x \in A_i} [U'(x) \times \tau_i]$, $\mathcal{A} = M(A(\Gamma))$, and $\mathcal{E} \subset \operatorname{Supp} Y \setminus \mathcal{A}$ to be the set of sites (x,t) such that $\boldsymbol{n}^\Gamma_{U'(x)}(\tau) \notin D_{U'(x)}$ for some $(x,\tau) \in C(x,t)$. The latter can be split into two disjoint subsets, $\mathcal{E} = \mathcal{E}^{\mathrm{core}} \cup \mathcal{E}^{\mathrm{soft}}$, with $(x,t) \in \mathcal{E}^{\mathrm{core}}$ whenever $\boldsymbol{n}^\Gamma_{U'(x)}(\tau) \notin G_{U'(x)}$ for some $(x,\tau) \in C(x,t)$. The condition $M(\operatorname{Supp}\Gamma) \cup \operatorname{Supp}\mathcal{M} = \operatorname{Supp} Y$ in (8.47) implies the inequality

$$\mathrm{e}^{c|Y|} \leqslant \mathrm{e}^{c(2R)^\nu |A(\Gamma)|} \mathrm{e}^{c|\mathcal{E}|} \prod_{M \in \mathcal{M}} \mathrm{e}^{c|M|}.$$

From definitions (8.47) of $\mathfrak{z}(Y)$ and (8.40) of $z(\gamma)$, and using Assumption 2, we have

$$\begin{aligned}
\mathrm{e}^{c|Y|} |\mathfrak{z}(Y)| \leqslant \sum_{\mathcal{A} \subset \operatorname{Supp} Y} \mathrm{e}^{-\frac{\tilde\beta}{\Delta} e_0 |\operatorname{Supp} Y \setminus \mathcal{A}|} \sum_{\mathcal{E} \subset \operatorname{Supp} Y \setminus \mathcal{A}} \sum_{\mathcal{E}^{\mathrm{core}} \subset \mathcal{E}} \mathrm{e}^{-(\tilde\beta - c)|\mathcal{E} \setminus \mathcal{E}^{\mathrm{core}}|} \\
\mathrm{e}^{-(\frac{\tilde\beta}{\Delta} \frac{\Delta_0}{2} (2R)^{-\nu} - c)|\mathcal{E}^{\mathrm{core}}|} \int_{\mathcal{G}^{\mathrm{per}}_\Lambda} \mathrm{d}\Gamma \, \mathbb{I}\left[M(A(\Gamma)) = \mathcal{A}, M(\operatorname{core}\Gamma) = \mathcal{E}^{\mathrm{core}} \right] \\
\prod_{i=1}^m \left| \langle \boldsymbol{n}^\Gamma_{A_i}(\tau_i - 0) | \, T_{\boldsymbol{A}_i} \, | \boldsymbol{n}^\Gamma_{A_i}(\tau_i + 0) \rangle \right| \mathrm{e}^{c(2R)^\nu |A_i|} \exp\Big\{ - \int_{C(\mathcal{A})} \mathrm{d}(x,\tau) \Upsilon_x(\boldsymbol{n}^\Gamma_{U'(x)}(\tau)) \Big\} \\
\mathrm{e}^{|\tilde{\mathcal{R}}(\Gamma)|} \sum_{\mathcal{M}, \operatorname{Supp}\mathcal{M} \subset \operatorname{Supp} Y} \prod_{M \in \mathcal{M}} \left| \mathrm{e}^{\varphi(M;\Gamma)} - 1 \right| \mathrm{e}^{c|M|}. \qquad (8.61)
\end{aligned}$$

All elements in $\mathcal{M}$ are different, because it is so in the expansion (8.46). Therefore we have

$$\begin{aligned}
\sum_{\mathcal{M}, \operatorname{Supp}\mathcal{M} \subset \operatorname{Supp} Y} \prod_{M \in \mathcal{M}} \left| \mathrm{e}^{\varphi(M;\Gamma)} - 1 \right| \mathrm{e}^{c|M|} &\leqslant \sum_{n \geqslant 0} \frac{1}{n!} \Big[\sum_{M \subset \operatorname{Supp} Y} \left| \mathrm{e}^{\varphi(M;\Gamma)} - 1 \right| \mathrm{e}^{c|M|} \Big]^n \\
&\leqslant \sum_{n \geqslant 0} \frac{1}{n!} \Big[|Y| \sum_{M \ni (x,t)} \left| \mathrm{e}^{\varphi(M;\Gamma)} - 1 \right| \mathrm{e}^{c|M|} \Big]^n \qquad (8.62)
\end{aligned}$$

and using Lemma 8.5 this may be bounded by $\mathrm{e}^{|Y|}$.

In (8.45) clusters are small, and they must contain a space-time site (x,τ) such that there exists x' with $(x',\tau) \in \operatorname{core}\Gamma$ and $\operatorname{dist}(x,x') < R$. So we have the bound

$$|\tilde{\mathcal{R}}(\Gamma)| \leqslant (2R)^\nu |\operatorname{core}\Gamma| \int_{\mathcal{C}^{\mathrm{small}}_\Lambda} \mathrm{d}\boldsymbol{C} \, \mathbb{I}\left[C \ni (x,\tau) \right] \left| \Phi^{\mathrm{T}}(\boldsymbol{C}) \right|,$$

since $|\Phi^{\mathrm{T}}(\boldsymbol{C};\Gamma)| \leqslant |\Phi^{\mathrm{T}}(\boldsymbol{C})|$. Taking now, in Lemma 8.1, the constants $c = \alpha_1 = \alpha_2 = 0$ and $\delta = \frac{\Delta_0}{4(2R)^{2\nu}}$, and choosing the corresponding ε_0, we apply (8.26) to get, for any $\|T\| \leqslant \varepsilon_0$, the bound

$$|\tilde{\mathcal{R}}(\Gamma)| \leqslant \frac{\Delta_0}{4} (2R)^{-\nu} |\operatorname{core}\Gamma| \leqslant \frac{\tilde\beta}{\Delta} \frac{\Delta_0}{4} (2R)^{-\nu} |\mathcal{E}^{\mathrm{core}}| + \frac{\Delta_0}{4} (2R)^{-\nu} |\operatorname{core}\Gamma \cap C(\mathcal{A})|.$$

Assuming $\tilde\beta \geqslant c$ and $\frac{\tilde\beta}{\Delta}\frac{\Delta_0}{4} \geqslant (2R)^\nu c$ [c.f. (8.51)], we bound

$$\mathrm{e}^{-(\tilde\beta - c)|\mathcal{E}\setminus\mathcal{E}^{\mathrm{core}}|}\ \mathrm{e}^{-(\frac{\tilde\beta}{\Delta}\frac{\Delta_0}{4}(2R)^{-\nu}-c)|\mathcal{E}^{\mathrm{core}}|} \leqslant 1.$$

Inserting these estimates into (8.61), we get

$$\begin{aligned}\mathrm{e}^{c|Y|}\,|\mathfrak{z}(Y)| \leqslant\ & \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e_0|Y|}\,\mathrm{e}^{|Y|}\sum_{\mathcal{A}\subset\mathrm{Supp}\,Y} 3^{|\mathrm{Supp}\,Y\setminus\mathcal{A}|}\int_{\mathcal{G}_\Lambda^{\mathrm{per}}}\mathrm{d}\Gamma\,\mathbb{I}\left[M(A(\Gamma))=\mathcal{A}\right]\\ &\prod_{i=1}^m\left|\langle \boldsymbol{n}^\Gamma_{A_i}(\tau_i-0)|\,T_{\boldsymbol{A}_i}\,|\boldsymbol{n}^\Gamma_{A_i}(\tau_i+0)\rangle\right|\mathrm{e}^{c(2R)^\nu|A_i|}\\ &\exp\Big\{-\int_{C(\mathcal{A})}\mathrm{d}(x,\tau)[\Upsilon_x(\boldsymbol{n}^\Gamma_{U'(x)}(\tau))-e_0-\frac{\Delta_0}{4}(2R)^{-\nu}\,\mathbb{I}\left[(x,\tau)\in\mathrm{core}\,\Gamma\right]]\Big\}. \quad (8.63)\end{aligned}$$

To estimate the above expression, we will split the "transition part" of the considered quantum contours into connected components, to be called *fragments*, and deal with them separately. Even though the weight of a quantum contour cannot be partitioned into the corresponding fragments,[11] we will get an upper bound combined from fragment bounds. Consider thus the set

$$\hat A(\Gamma) = \mathrm{core}\,\Gamma\cap C(A(\Gamma))$$

and the fragments $\zeta_i = (B_i, \boldsymbol{\omega}_{B_i})$ on the components B_i of $\hat A(\Gamma)$, $\hat A(\Gamma) = \cup_{i=1}^n B_i$, $\boldsymbol{\omega}_{B_i}$ is the restriction of $\boldsymbol{\omega}^\Gamma$ onto B_i.

From Assumption 2, we have

$$\int_{C(\mathcal{A})}\mathrm{d}(x,\tau)\Big[\Upsilon_x(\boldsymbol{n}^\Gamma_{U'(x)}(\tau))-e_0-\frac{\Delta_0}{4}(2R)^{-\nu}\,\mathbb{I}\left[(x,\tau)\in\mathrm{core}\,\Gamma\right]\Big] \geqslant \tfrac14(2R)^{-\nu}\Delta_0\sum_{i=1}^n|B_i|.$$

Let us introduce a bound for the contribution of a fragment ζ with transitions $\boldsymbol{A}_j, j=1,\dots,k$,

$$\hat z(\zeta) = \mathrm{e}^{-\frac14(2R)^{-\nu}\Delta_0|B|}\prod_{j=1}^k\left|\langle \boldsymbol{n}^\zeta_{A_j}(\tau_1-0)|\,T_{\boldsymbol{A}_j}\,|\boldsymbol{n}^\zeta_{A_j}(\tau_1+0)\rangle\right|\mathrm{e}^{c(2R)^\nu|A_j|}.$$

Then, integrating over the set $\mathcal{F}_{C(\mathcal{A})}$ of all fragments in $C(\mathcal{A})$, we get

$$\mathrm{e}^{c|Y|}\,|\mathfrak{z}(Y)| \leqslant\ \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e_0|Y|}\,\mathrm{e}^{|Y|}\sum_{\mathcal{A}\subset\mathrm{Supp}\,Y}3^{|\mathrm{Supp}\,Y\setminus\mathcal{A}|}\sum_{n\geqslant 0}\frac{1}{n!}\Big(\int_{\mathcal{F}_{C(\mathcal{A})}}\mathrm{d}\zeta\,\hat z(\zeta)\Big)^n. \quad (8.64)$$

Anticipating the bound $\int_{\mathcal{F}_{C(\mathcal{A})}}\mathrm{d}\zeta\,\hat z(\zeta) \leqslant |\mathcal{A}|$, we immediately get the claim,

$$\mathrm{e}^{c|Y|}\,|\mathfrak{z}(Y)| \leqslant\ \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e_0|Y|}\,\mathrm{e}^{3|Y|},$$

with a slight change of constant $c\to c-3$.

A bound on the integral of fragments. Let us first consider *short* fragments $\zeta=(B,\boldsymbol{\omega}_B)$ satisfying the condition

$$\frac12\sum_{j=1}^k|A_j| \leqslant \frac{\log(\Delta/\tilde\beta)}{\log\|T\|}. \quad (8.65)$$

[11] In fact, it partitions in the case of spins or bosons. Only the sign coming with fermions brings problem.

The integral over the time of occurrence of the first transition yields the factor $\tilde{\beta}/\Delta$. Notice that ζ is not a loop. This follows from the construction of quantum contours and the fact that B is a connected component of $\hat{A}(\Gamma)$, where every transition is taken together with its R-neighbourhood. Thus, either its sequence of transitions does not belong to $\mathcal{S}$, or the starting configuration does not coincide with the ending configuration. In the first case we use Assumption 3, in the second case Assumption 4, and since (8.65) means that the sum over transitions is bounded, we can write

$$\int_{\mathcal{F}^{\mathrm{short}}_{C(\mathcal{A})}} \mathrm{d}\zeta\, \hat{z}(\zeta) \;\leqslant\; \tfrac{1}{2}|\mathcal{A}|. \tag{8.66}$$

Finally, we estimate the integral over ζ's that are not short. We have

$$\int_{\mathcal{F}_{C(\mathcal{A})}\setminus\mathcal{F}^{\mathrm{short}}_{C(\mathcal{A})}} \mathrm{d}\zeta\, \hat{z}(\zeta) \;\leqslant\; |\mathcal{A}|\frac{\tilde{\beta}}{\Delta}\int_{\mathcal{F}^{(x,\tau)}_{C(\mathcal{A})}\setminus\mathcal{F}^{\mathrm{short}}_{C(\mathcal{A})}} \mathrm{d}\zeta\, \hat{z}(\zeta). \tag{8.67}$$

Here $\mathcal{F}^{(x,\tau)}_{C(\mathcal{A})}$ is the set of all fragments ζ whose first quantum transition (A_1,τ_1) is such that $x\in A_1$ and $\tau=\tau_1$. Whenever ζ is not short, we have

$$1 \;\leqslant\; \frac{\Delta}{\tilde{\beta}}\prod_{j=1}^{k}\|T\|^{-\frac{1}{2}|A_j|}.$$

Thus, defining

$$\hat{z}'(\zeta) = \mathrm{e}^{-\frac{1}{4}(2R)^{-\nu}\Delta_0|B|}\prod_{j=1}^{k}\Big[\|T\|^{\frac{1}{2}}\,\mathrm{e}^{c(2R)^{\nu}+1}\Big]^{|A_j|}, \tag{8.68}$$

we find the bound

$$|\mathcal{A}|\int_{\mathcal{F}(x,\tau)}\mathrm{d}\zeta\,\hat{z}'(\zeta).$$

Here, slightly overestimating, we take for $\mathcal{F}(x,\tau)$ the set of all fragments containing a quantum transition (A,τ) with $x\in A$.

The support B of a fragment $\zeta=(B,\boldsymbol{\omega}_B)\in\mathcal{F}(x,\tau)$, is a finite union of vertical segments (i.e. sets of the form $\{y\}\times[\tau_1,\tau_2]\subset\mathbb{T}_\Lambda$) and k horizontal quantum transitions $A_1,\dots,A_k$.

We finish the proof by showing by induction the bound

$$\int_{\mathcal{F}(x,\tau;k)}\mathrm{d}\zeta\,\hat{z}'(\zeta) \;\leqslant\; 1 \tag{8.69}$$

with $\mathcal{F}(x,\tau;k)$ denoting the set of fragments from $\mathcal{F}(x,\tau)$ with at most k quantum transitions.

Consider thus a fragment ζ with k horizontal quantum transitions connected by vertical segments. Let (A,τ) be the transition containing the point (x,τ) and let $(A_1,\tau+\tau_1),\dots,(A_\ell,\tau+\tau_\ell)$ be the transitions that are connected by (one or several) vertical segments of the respective lengths $|\tau_1|,\dots,|\tau_\ell|$ with the transition (A,τ). If we remove all those segments, the fragment ζ will split into the "naked" transition (A,τ) and additional $\bar{\ell}\leq\ell$ fragments $\zeta_1,\dots,\zeta_{\bar{\ell}}$, such that each fragment ζ_j, $j=1,\dots,\bar{\ell}$, belongs to $\mathcal{F}(y_j,\tau+\tau_j;k-1)$ with $y_j\in A$. Taking into account that the number of configurations (determining the possible vertical segments attached to A) above and below A is bounded

by $S^{2|A|}$ and that the number of possibilities to choose the points y_j is bounded by $|A|^{\bar\ell}$, we get

$$\begin{aligned}\int_{\mathcal{F}(x,\tau;k)} \mathrm{d}\zeta\, \hat z'(\zeta) \;&\leqslant\; \sum_{A,\mathrm{dist}(A,x)<R} \big[\|T\|^{\frac12}\, \mathrm{e}^{c(2R)^{\nu}+1}\, S^2\big]^{|A|} \sum_{\bar\ell=1}^{\infty} \frac{|A|^{\bar\ell}}{\bar\ell!} \int \mathrm{d}\tau_1 \cdots \int \mathrm{d}\tau_{\bar\ell} \\ &\qquad \mathrm{e}^{-\frac12 (2R)^{-\nu}\Delta_0(\tau_1+\cdots+\tau_{\bar\ell})} \prod_{j=1}^{\bar\ell} \int_{\mathcal{F}(y_j,\tau+\tau_j;k-1)} \mathrm{d}\zeta\, \hat z'(\zeta_j) \\ &\leqslant \sum_{A,\mathrm{dist}(A,x)<R} \big[\|T\|^{\frac12} S^2\, \mathrm{e}^{c(2R)^{\nu}+2}\,\big]^{|A|}\, \mathrm{e}^{2(2R)^{\nu}/\Delta_0} \\ &\leqslant\; 1 \end{aligned} \tag{8.70}$$

once $\|T\|$ is sufficiently small. □

In the application of Pirogov-Sinai theory we shall also need a bound on derivatives of the weight of contours.

Lemma 8.7.

Under the Assumptions 1–5, for any $c<\infty$, there exist constants $\alpha, \beta_0, \tilde\beta_0 < \infty$ and $\varepsilon_0 > 0$ such that if $\beta \geqslant \beta_0$, $\tilde\beta_0 \leqslant \tilde\beta < 2\tilde\beta_0$, and $\|T\| + \sum_{i=1}^{r-1} \|\frac{\partial}{\partial\mu_i} T\| \leqslant \varepsilon_0$, one has

$$\big|\frac{\partial}{\partial\mu_i}\mathfrak{z}(Y)\big| \;\leqslant\; \alpha\tilde\beta|Y|\, \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e_0^{\mu}|Y|}\, \mathrm{e}^{-c|Y|}$$

for any contour Y.

Proof. From the definition (8.47) of $\mathfrak{z}$, one has

$$\begin{aligned}\big|\frac{\partial}{\partial\mu_i}\mathfrak{z}(Y)\big| \;\leqslant\; |\mathfrak{z}(Y)|\Big\{\sum_{\gamma\in\Gamma}\big|\frac{\partial}{\partial\mu_i} z(\Gamma)\big| + \sum_{d\in D}\big|W_d\cap C(\mathrm{Supp}\, Y)\big|\big|\frac{\partial}{\partial\mu_i} e^{\mu}(d)\big| + \big|\frac{\partial}{\partial\mu_i}\tilde{\mathcal{R}}(\Gamma)\big|\Big\} \\ + \int_{\mathcal{G}_{\Lambda}^{\mathrm{per}}(Y)} \mathrm{d}\Gamma \prod_{\gamma\in\Gamma}|z(\gamma)| \prod_{d\in D} \mathrm{e}^{-e^{\mu}(d)|W_d\cap C(\mathrm{Supp}\, Y)|}\, \mathrm{e}^{|\tilde{\mathcal{R}}(\Gamma)|}\end{aligned}$$

$$\sum_{\mathcal{M}} \mathbb{I}\left[\mathcal{M}(\mathrm{Supp}\,\Gamma)\cup\mathrm{Supp}\,\mathcal{M} = \mathrm{Supp}\, Y\right] \sum_{M\in\mathcal{M}} \Big|\, \mathrm{e}^{\varphi(M;\Gamma)}\, \frac{\partial}{\partial\mu_i}\varphi(M;\Gamma)\Big| \prod_{M'\in\mathcal{M}, M'\neq M} \big|\, \mathrm{e}^{\varphi(M';\Gamma)} - 1\big|. \tag{8.71}$$

The bound for $|\frac{\partial}{\partial\mu_i} z(\Gamma)|$ is standard, see [BKU 1996], and $|\frac{\partial}{\partial\mu_i} e^{\mu}(d)|$ is assumed to be bounded in Assumption 5. For the other terms we have to control clusters of loops. Since we have exponential decay for $z(\xi)$ with any strength (by taking β large and $\|T\|$ small), we have the same for $\frac{\partial}{\partial\mu_i} z(\xi)$ (by taking β larger and $\|T\|$ smaller). The integrals over $\boldsymbol{C}$ can be estimated as before, the only effect of the derivative being an extra factor n (when the clusters have n loops). □

2.3. Expectation values of local observables and construction of pure states. So far we have obtained an expression (8.48) for the partition function $Z_{\Lambda}^{\mathrm{per}}$ of the quantum model on torus Λ in terms of that of a classical lattice contour model with the weights of the contours showing an exponential decay with respect to their length. Using the same weights $\mathfrak{z}(Y)$, we can also introduce the partition functions $Z_{\Lambda(L)}^{d}$ with the torus Λ replaced by a hypercube $\Lambda(L)$ and with fixed boundary conditions d. Namely, we take simply the

sum only over those collections $\mathcal{Y}$ of contours whose external contours are labeled by d and are not close to the boundary.[12] Notice, however, that here we are defining $Z^d_{\Lambda(L)}$ directly in terms of the classical contour model, without ensuring existence of corresponding partition function directly for the original model. We will use these partition functions only as a tool for proving our Theorems that are stated directly in terms of quantum models.

To be more precise, we can extend the definition even more and consider, instead of the torus Λ, any finite set $V \subset \mathbb{L} = \mathbb{Z}^\nu \times \{1, \dots, N\}^{\rm per}$. There is a class of contours that can be viewed as having their support contained in $V \subset \mathbb{L}$. For any such contour Y we introduce its interior $\operatorname{Int} Y$ as the union of all finite components of $\mathbb{L} \setminus \operatorname{Supp} Y$ and $\operatorname{Int}_d Y$ as the union of all components of $\operatorname{Int} Y$ whose boundary is labeled by d. Recalling that we assumed $\nu \geqslant 2$, we note that the set $\mathbb{L} \setminus (\operatorname{Supp} Y \cup \operatorname{Int} Y)$ is a connected set, implying that the label $\alpha_Y(\cdot)$ is constant on the boundary of the set $V(Y) = \operatorname{Supp} Y \cup \operatorname{Int} Y$. We say that Y is a d-contour, if $\alpha_Y = d$ on this boundary. Two contours Y and Y' are called *mutually external* if $V(Y) \cap V(Y') = \varnothing$. Given an admissible set $\mathcal{Y}$ of contours, we say that $Y \in \mathcal{Y}$ is an *external contour* in $\mathcal{Y}$, if $\operatorname{Supp} Y \cap V(Y') = \varnothing$ for all $Y' \in \mathcal{Y}$, $Y' \neq Y$. The sets $\mathcal{Y}$ contributing to Z^d_V are such that all their external contours are d-contours and $\operatorname{dist}(Y, \partial V) > 1$ for every $Y \in \mathcal{Y}$.

In this way we find ourselves exactly in the setting of standard Pirogov-Sinai theory, see Chapter 6. In particular, for sufficiently large β and sufficiently small $\|T\| + \sum_{i=1}^{r-1} \|\frac{\partial}{\partial \mu_i} T\|$, there exist functions $f^{\beta,\mu}(d)$, metastable free energies, such that the condition $\operatorname{Re} f^{\beta,\mu}(d) = f_0$, with $f_0 \equiv f_0^{\beta,\mu}$ defined by $f_0 = \min_{d' \in D} \operatorname{Re} f^{\beta,\mu}(d')$, characterizes the existence of a pure stable phase d. Namely, as will be shown next, a pure stable phase $\langle \cdot \rangle^d_\beta$ exists and is close to the pure ground state $|d\rangle$.

There is one subtlety in the definition of $f^{\beta,\mu}(d)$. Namely, after choosing a suitable $\tilde\beta_0$, given β, there exist several pairs $(\tilde\beta, N)$ such that $\tilde\beta \in (\tilde\beta_0, 2\tilde\beta_0)$ and $N\tilde\beta = \beta$. To be specific, we may agree to choose among them that one with maximal N. The function $f^{\beta,\mu}(d)$ is then uniquely defined for each $\beta > \beta_0$. Notice, however, that while increasing β, we pass, at the particular value $\beta_N = N\tilde\beta_0$, from discretization of temporal size N to $N+1$. As a result, the function $f^{\beta,\mu}(d)$ might be discontinuous at β_N with $\beta = \infty$ being an accumulation point of such discontinuities. Nevertheless, these discontinuities are harmless. They can appear only when $\operatorname{Re} f^{\beta,\mu}(d) > f_0$ and do not change anything in the following argument.

Before we come to the construction of pure stable phases, notice that the first claim of Theorem 3.6 (equality of f_0 with the limiting free energy) is now a direct consequence of the bound

$$\left| Z^{\rm per}_\Lambda - |Q|\, \mathrm{e}^{-\tilde\beta f_0 N L^\nu} \right| \leqslant \mathrm{e}^{-\tilde\beta f_0 N L^\nu}\, O(\mathrm{e}^{-\mathrm{const}\, L}) \tag{8.72}$$

[c.f. [BKU 1996], (7.14)]. Here $Q = \{d; \operatorname{Re} f^{\beta,\mu}(d) = f_0\}$.

The expectation value of a local observable K is defined as

$$\langle T \rangle^{\rm per}_\Lambda = \frac{\operatorname{Tr} K\, \mathrm{e}^{-\beta H^{\rm per}_\Lambda}}{\operatorname{Tr}\, \mathrm{e}^{-\beta H^{\rm per}_\Lambda}}. \tag{8.73}$$

So far we have obtained a contour expression for $Z^{\rm per}_\Lambda = \operatorname{Tr}\, \mathrm{e}^{-\beta H^{\rm per}_\Lambda}$. We retrace here the same steps for $Z^{\rm per}_\Lambda(K) \doteq \operatorname{Tr} K\, \mathrm{e}^{-\beta H^{\rm per}_\Lambda}$. Duhamel expansion (8.16) for $Z^{\rm per}_\Lambda(K)$ leads

[12] In the terminology of Pirogov-Sinai theory we rather mean *diluted partition functions* — see the more precise definition below.

to an equation analogous to (8.17),

$$Z_\Lambda^{\rm per}(K) = \sum_{m\geqslant 0}\sum_{n_\Lambda^0,\dots,n_\Lambda^m}\sum_{\substack{\boldsymbol{A}_1,\dots,\boldsymbol{A}_m\\ \bar{A}_i\subset\Lambda}}\int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1\dots\mathrm{d}\tau_m \langle n_\Lambda^0|\,K\,|n_\Lambda^1\rangle$$
$$\mathrm{e}^{-\tau_1 V_\Lambda^{\rm per}(n_\Lambda^1)}\,\langle n_\Lambda^1|\,T_{\boldsymbol{A}_1}\,|n_\Lambda^2\rangle\,\mathrm{e}^{-(\tau_2-\tau_1)V_\Lambda^{\rm per}(n_\Lambda^2)}\,\dots\,\langle n_\Lambda^m|\,T_{\boldsymbol{A}_m}\,|n_\Lambda^0\rangle\,\mathrm{e}^{-(\beta-\tau_m)V_\Lambda^{\rm per}(n_\Lambda^0)}\,. \quad (8.74)$$

Configurations n_Λ^0 and n_Λ^1 match on $\Lambda\setminus\operatorname{Supp}K$ ($\operatorname{Supp}K\subset\Lambda$ is a finite set due to the locality of K), but may differ on $\operatorname{Supp}K$ if K is an operator with non zero off-diagonal terms. Let $\mathcal{W}_\Lambda^{\rm per}(K)$ be the set of quantum configurations with $\boldsymbol{n}_\Lambda(\tau)$ that is constant except possibly at $\cup_{i=1}^m(A_i\times\tau_i)\cup(\operatorname{Supp}K\times 0)$. Then

$$Z_\Lambda^{\rm per}(K) = \int_{\mathcal{W}_\Lambda^{\rm per}(K)} \mathrm{d}\boldsymbol{\omega}_{\mathbb{T}_\Lambda}\langle n_\Lambda^0|\,K\,|n_\Lambda^1\rangle\rho^{\rm per}(\boldsymbol{\omega}_{\mathbb{T}_\Lambda}). \quad (8.75)$$

We identify loops with the same iteration scheme as before, starting with the set $\boldsymbol{B}^{(0)}(\boldsymbol{\omega})\cup(\operatorname{Supp}K\times 0)$ instead of $\boldsymbol{B}^{(0)}(\boldsymbol{\omega})$ only. This leads to the set $\boldsymbol{B}^K(\boldsymbol{\omega})$. Removing the loops, we define $\boldsymbol{B}_{\rm e}^K(\boldsymbol{\omega})$, whose connected components form quantum contours. There is one special quantum contour, namely that which contains $\operatorname{Supp}K\times 0$. Let us denote it by γ^K and define its weight [see (8.40)]

$$z^K(\gamma^K) = \langle \boldsymbol{n}^{\gamma^K}_{\operatorname{Supp}K}(-0)|\,K\,|\boldsymbol{n}^{\gamma^K}_{\operatorname{Supp}K}(+0)\rangle\prod_{i=1}^m\langle \boldsymbol{n}^{\gamma^K}_{A_i}(\tau_i-0)|\,T_{\boldsymbol{A}_i}\,|\boldsymbol{n}^{\gamma^K}_{A_i}(\tau_i+0)\rangle$$
$$\exp\Big\{-\int_B \mathrm{d}(x,\tau)\Upsilon_x(\boldsymbol{n}^{\gamma^K}_{U'(x)}(\tau))\Big\}. \quad (8.76)$$

Let $\Gamma^K=\{\gamma^K,\gamma_1,\dots,\gamma_k\}$ be an admissible set of quantum contours, defining a quantum configuration $\boldsymbol{\omega}^{\Gamma^K}\in\mathcal{W}_\Lambda^{\rm per}(K)$. Then we have an expression similar to that of Lemma 8.4,

$$Z_\Lambda^{\rm per}(K) = \int_{\mathcal{G}_\Lambda^{\rm per}(K)}\mathrm{d}\Gamma^K\prod_{d\in D}\mathrm{e}^{-|W_d(\Gamma^K)|e(d)}\,z^K(\gamma^K)\prod_{\gamma\in\Gamma^K\setminus\{\gamma^K\}}z(\gamma)\,\mathrm{e}^{\mathcal{R}(\Gamma^K)}\,, \quad (8.77)$$

with $\mathcal{R}(\Gamma^K)$ as in (8.41) with Γ replaced by Γ^K.

Next step is to discretize the lattice, to expand $\mathrm{e}^{\mathcal{R}(\Gamma^K)}$, and if Y^K is the contour that contains $\operatorname{Supp}K\times 0\subset\mathbb{L}_\Lambda$, to define $\mathfrak{z}^K(Y^K)$ [see (8.47)]:

$$\mathfrak{z}^K(Y^K) = \int_{\mathcal{G}_\Lambda^{\rm per}(Y^K)}\mathrm{d}\Gamma^K z^K(\gamma^K)\prod_{\gamma\in\Gamma^K\setminus\{\gamma^K\}}z(\gamma)\prod_{d\in D}\mathrm{e}^{-e(d)|W_d(\Gamma^K)\cap C(\operatorname{Supp}Y^K)|}\,\mathrm{e}^{\tilde{\mathcal{R}}(\Gamma^K)}$$
$$\sum_{\mathcal{M}}\mathbb{I}\left[M(\operatorname{Supp}\Gamma^K\cup\operatorname{Supp}\mathcal{M}=\operatorname{Supp}Y^K\right]\prod_{M\in\mathcal{M}}\big(\mathrm{e}^{\varphi(M;\Gamma^K)}-1\big). \quad (8.78)$$

We also need a bound for $\mathfrak{z}^K(Y^K)$. It is clear that the situation is the same as for Lemmas 8.5 and 8.6, except for a factor $\langle \boldsymbol{n}^{\gamma^K}_{\operatorname{Supp}K}(-0)|\,K\,|\boldsymbol{n}^{\gamma^K}_{\operatorname{Supp}K}(+0)\rangle$ that is bounded by $\|K\|$. We can thus summarize:

Lemma 8.8.

Under the Assumptions 1–4, for any $c < \infty$, there exist $\beta_0, \tilde\beta_0 < \infty$, and $\varepsilon_0 > 0$ such that if $\beta \geqslant \beta_0$, $\tilde\beta_0 \leqslant \tilde\beta < 2\tilde\beta_0$ and $\|T\| \leqslant \varepsilon_0$, we have

$$Z_\Lambda^{\mathrm{per}}(K) = \sum_{\mathcal{Y}^K=\{Y^K,Y_1,\dots,Y_k\}} \prod_{d\in D} \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e(d)|\mathcal{G}_d(\mathcal{Y}^K)|}\, \mathfrak{z}^K(Y^K) \prod_{Y\in\mathcal{Y}^K\setminus\{Y^K\}} \mathfrak{z}(Y), \tag{8.79}$$

for every local observable K, with

$$|\mathfrak{z}^K(Y^K)| \leqslant \|K\|\, \mathrm{e}^{c|\operatorname{Supp} K|}\, \mathrm{e}^{-\frac{\tilde\beta}{\Delta}e_0|Y^K|}\, \mathrm{e}^{-c|Y^K|}$$

for any contour Y^K.

In a similar manner as at the beginning of this section, we can introduce $Z_V^d(K)$ for any $V \subset \mathbb{L}$ by restricting ourselves in the sum (8.79) to the collections $\mathcal{Y}^K$ whose all external contours are d-contours and $\operatorname{dist}(Y, \partial V) > 1$ for every $Y \in \mathcal{Y}^K$. Thus we can *define* the expectation value

$$\langle K\rangle_V^d = \frac{Z_V^d(K)}{Z_V^d} \tag{8.80}$$

for any $V \subset \mathbb{L}$ and, in particular, the expectation $\langle K\rangle_{\Lambda(L)}^d$ for a hypercube $\Lambda(L)$.

This is exactly the setting discussed in detail in [BKU 1996]. We can use directly the corresponding results (c.f. [BKU 1996], Lemma 6.1) to prove first that the limiting state $\langle\cdot\rangle_\beta^d$ exists. Further, retracing the proof of Theorem 2.2 in [BKU 1996] we prove that the limit

$$\langle K\rangle_\beta^{\mathrm{per}} = \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{\operatorname{Tr} K\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}}{\operatorname{Tr}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}} \tag{8.81}$$

exists for every local K (proving thus Theorem 3.5). Moreover,

$$\langle K\rangle_\beta^{\mathrm{per}} = \frac{1}{Q}\sum_{d\in Q}\langle K\rangle_\beta^d, \tag{8.82}$$

where, again, Q denotes the set of stable phases, $Q = \{d; \operatorname{Re} f^{\beta,\mu}(d) = f_0\}$. Thus we proved the claim d) of Theorem 3.6.

Also the assertion c) follows in standard manner from contour representation employing directly the exponential decay of contour activities and corresponding cluster expansion [c.f. [BKU 1996], (2.27)].

Before passing to the proof of b), we shall verify that $\langle\cdot\rangle_\beta^d$ is actually a pure stable state according to our definition, i.e. a limit of thermodynamically stable states.[13] To this end, let us first discuss how metastable free energies $f^{\beta,\mu}(d)$ change with μ. The standard construction yields $f^{\beta,\mu}(d)$ in the form of a sum $e^\mu(d) + s^{\beta,\mu}(d)$, where $s^{\beta,\mu}(d)$ is the free energy of "truncated" contour model $K'_d(Y)$ [see [BKU 1996], (5.13) and (5.6)] constructed from labeled contour model (8.48), which is under control by cluster expansions. As a result, we have bounds of the form $O\big(\mathrm{e}^{-\beta} + \|T\| + \sum_{i=1}^{r-1}\big\|\frac{\partial T}{\partial\mu_i}\big\|\big)$ on $|s^{\beta,\mu}(d)|$ as well as on the derivatives with respect to μ. Hence, in view of Assumption (5), the leading behaviour is yielded by $e^\mu(d)$.

[13] Recall that, up to now, the state $\langle\cdot\rangle_\beta^d$ is defined only in terms of the contour representation [see (8.80), (8.79), and (8.48)], and the only proven connection with a state of original quantum model is the equality (8.82).

Starting thus from a given potential Φ^μ with $Q^\mu = \{d \in D; \operatorname{Re} f^{\beta,\mu}(d) = f_0^\mu\}$, one can easily add to Φ^μ a suitable "external field" that favours a chosen $d \in Q^\mu$. For example, one can take

$$\Phi_A^{\mu,\alpha}(n) = \Phi_A^\mu(n) + \alpha\delta_A^d(n)$$

with δ_A^d defined by taking $\delta_A^d(n) = 0$ for $n_A = d_A$ and $\delta_A^d(n) = 1$ otherwise.[14] Now, since $\frac{\partial e^{\mu,\alpha}(d)}{\partial\alpha}$ is bounded from below by a positive constant (while $\frac{\partial e^{\mu,\alpha}(d')}{\partial\alpha} = 0$ for $d' \neq d$), for any $\alpha > 0$ the only stable phase is d, $\operatorname{Re} f^{\beta,\mu,\alpha}(d) = f_0^{\beta,\mu,\alpha} \equiv \min_{d' \in D} \operatorname{Re} f^{\beta,\mu,\alpha}(d')$, and, in the same time, $\operatorname{Re} f^{\beta,\mu,\alpha}(d') > f_0^{\beta,\mu,\alpha}$ for $d' \neq d$. Thus, $Q^{\mu,\alpha} = \{d\}$ and $\langle\cdot\rangle_{\beta,\mu,\alpha}^d = \langle\cdot\rangle_{\beta,\mu,\alpha}^{\mathrm{per}}$. This state is thermodynamically stable — when adding any small perturbation, metastable free energies will change only a little and that one corresponding to the state d will still be the only one attaining the minimum. The fact that in the limit of vanishing perturbation we recover $\langle\cdot\rangle_{\beta,\mu,\alpha}^d$, as well as the fact that

$$\lim_{\alpha\to 0+} \langle\cdot\rangle_{\beta,\mu,\alpha}^{\mathrm{per}} \equiv \lim_{\alpha\to 0+} \langle\cdot\rangle_{\beta,\mu,\alpha}^d = \langle\cdot\rangle_{\beta,\mu}^d,$$

follows by inspecting the contour representations of the corresponding expectations and observing that it can be expressed in terms of converging cluster expansions whose terms depend smoothly on α as well as on the additional perturbation.

To prove, finally, the claim b) of Theorem 3.6, it suffices to show that it is valid for $\langle\cdot\rangle_{\beta,\mu,\alpha}^{\mathrm{per}} = \langle\cdot\rangle_{\beta,\mu,\alpha}^d$ for every $\alpha > 0$. Abbreviating $\langle\cdot\rangle_{\beta,\mu,\alpha}^{\mathrm{per}} = \langle\cdot\rangle^{\mathrm{per}}$ and $H_\Lambda^{\mu,\alpha,\mathrm{per}} = H_\Lambda^{\mathrm{per}}$, we first notice that the expectation value of the projector onto the configuration d on $\operatorname{Supp} K$, $P^d_{\operatorname{Supp} K} \doteq |d_{\operatorname{Supp} K}\rangle\langle d_{\operatorname{Supp} K}|$, is close to 1, since its complement $\langle(\mathbb{1} - P^d_{\operatorname{Supp} K})\rangle^{\mathrm{per}} = \langle(\mathbb{1} - P^d_{\operatorname{Supp} K})\rangle^d$ is related to the presence of a contour intersecting or surrounding $\operatorname{Supp} K$ (loops intersecting $\operatorname{Supp} K \times \{0\}$ are considered here as part of quantum contours), whose weight is small. More precisely, for any $\delta > 0$ we have

$$\langle(\mathbb{1} - P^d_{\operatorname{Supp} K})\rangle^{\mathrm{per}} \leqslant \delta|\operatorname{Supp} K|,$$

whenever $\|T\|$ is small enough and β large enough. Furthermore,

$$\begin{aligned}\langle K\rangle_\Lambda^{\mathrm{per}} = \frac{1}{Z_\Lambda^{\mathrm{per}}}\Big[&\operatorname{Tr}\big(P^d_{\operatorname{Supp} K} K P^d_{\operatorname{Supp} K}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big) + \\ &+ \operatorname{Tr}\big((\mathbb{1} - P^d_{\operatorname{Supp} K}) K P^d_{\operatorname{Supp} K}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big) + \operatorname{Tr}\big(K(\mathbb{1} - P^d_{\operatorname{Supp} K})\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big)\Big] \quad (8.83)\end{aligned}$$

and

$$\begin{aligned}\operatorname{Tr}\big(P^d_{\operatorname{Supp} K} K P^d_{\operatorname{Supp} K}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big) &= \langle d_\Lambda|\, K\, |d_\Lambda\rangle \operatorname{Tr}\big(P^d_{\operatorname{Supp} K}\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big) \\ &= \langle d_\Lambda|\, K\, |d_\Lambda\rangle\big[\operatorname{Tr}\big(\mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big) - \operatorname{Tr}\big((\mathbb{1} - P^d_{\operatorname{Supp} K})\, \mathrm{e}^{-\beta H_\Lambda^{\mathrm{per}}}\big)\big], \quad (8.84)\end{aligned}$$

so that we have

$$\begin{aligned}&\big|\langle K\rangle_\Lambda^{\mathrm{per}} - \langle d_\Lambda|\, K\, |d_\Lambda\rangle\big| \leqslant \\ &\leqslant \big|\langle d_\Lambda|\, K\, |d_\Lambda\rangle\big|\langle(\mathbb{1} - P^d_{\operatorname{Supp} K})\rangle_\Lambda^{\mathrm{per}} + \big|\langle(\mathbb{1} - P^d_{\operatorname{Supp} K}) K P^d_{\operatorname{Supp} K}\rangle_\Lambda^{\mathrm{per}}\big| + \big|\langle K(\mathbb{1} - P^d_{\operatorname{Supp} K})\rangle_\Lambda^{\mathrm{per}}\big|. \quad (8.85)\end{aligned}$$

[14] Actually, we can restrict δ_A^d only to a particular type of sets A — for example all hypercubes of side R.

The mapping $(K, K') \mapsto \langle K^\dagger K' \rangle_\Lambda^{\rm per}$, with any two local operators K, K', is a scalar product; therefore the Schwarz inequality yields

$$\begin{aligned} \big|\langle K\rangle_\Lambda^{\rm per} - \langle d_\Lambda|\, K\,|d_\Lambda\rangle\big| \;&\leqslant\; \big|\langle d_\Lambda|\, K\,|d_\Lambda\rangle\big| \langle (\mathbb{1} - P^d_{\mathrm{Supp}\, K})\rangle_\Lambda^{\rm per} \\ &\quad + \Big(\langle (\mathbb{1} - P^d_{\mathrm{Supp}\, K})\rangle_\Lambda^{\rm per}\Big)^{\frac12} \Big(\big[\langle P^d_{\mathrm{Supp}\, K} K^\dagger K P^d_{\mathrm{Supp}\, K}\rangle_\Lambda^{\rm per}\big]^{\frac12} + \big[\langle K^\dagger K\rangle_\Lambda^{\rm per}\big]^{\frac12}\Big) \\ &\leqslant\; \|K\| \Big[\langle (\mathbb{1} - P^d_{\mathrm{Supp}\, K})\rangle_\Lambda^{\rm per} + 2\big(\langle (\mathbb{1} - P^d_{\mathrm{Supp}\, K})\rangle_\Lambda^{\rm per}\big)^{1/2}\Big] \;\leqslant\; \|K\|\, |\,\mathrm{Supp}\, K|(\delta + 2\delta^{\frac12}). \end{aligned} \tag{8.86}$$

The proof of the remaining Theorem 3.7 is a standard application of the implicit function theorem. Thus, for example, the point $\bar\mu_0$ of maximal coexistence, $\mathrm{Re}\, f^{\beta,\bar\mu_0}(d) = \mathrm{Re}\, f^{\beta,\bar\mu_0}(d')$ for every pair $d, d' \in D$, can be viewed as the solution of the vector equation $f(\bar\mu_0) = 0$, with $f(\mu) = (\mathrm{Re}\, f^{\beta,\mu}(d_i) - \mathrm{Re}\, f^{\beta,\mu}(d_r))_{i=1}^{r-1}$. Now, $f = e + s$, $e(\mu) = (e^\mu(d_i) - e^\mu(d_r))_{i=1}^{r-1}$, $s(\mu) = (\mathrm{Re}\, s^{\beta,\mu}(d_i) - \mathrm{Re}\, s^{\beta,\mu}(d_r))_{i=1}^{r-1}$, with $\|s\|$ as well as $\big\|\frac{\partial s}{\partial \mu}\big\|$ bounded by a small constant once $\|T\| + \sum_{i=1}^{r-1} \big\|\frac{\partial T}{\partial \mu_i}\big\|$ is sufficiently small β is sufficiently large. The existence of a unique solution $\bar\mu_0 \in \mathcal{U}$ then follows once we notice the existence of the solution $\mu_0 \in \mathcal{U}$ of the equation $e(\mu_0) = 0$ (equivalent with $e^{\mu_0}(d) = e^{\mu_0}(d')$, $d, d' \in D$) and the fact that the mapping

$$\mathcal{T} : \mu \to A^{-1}\big(\frac{\partial e}{\partial \mu}\big|_{\mu=\mu_0}(\mu - \mu_0) - f(\mu)\big)$$

with A^{-1} the matrix inverse to $\big(\frac{\partial e}{\partial \mu}\big)$, is a contraction. To this end it is enough just to recall Assumption 5 and the bounds on $s^{\beta,\mu}(d)$, $d \in D$, and its derivatives.

CHAPTER 9

Concluding remarks

At the end of his talk in a conference in Marseille (July 1998), Roman Kotecký described the last step of our method that shows the stabilization effect of quantum perturbations (the effective interactions, Chapter 8) as to "harvest phase diagrams". The expression is pleasant, and I will often refer to it in this conclusion.

To harvest represents quite a lot of work, but a walk along fields of mature cereals costs little pain, and brings nice illustration of harvesting tools. So let us have a look.

Attractive spin-1 Hubbard model. Here quantum particles are fermions or hard-core bosons, and can be in three different states. With well chosen chemical potential, the classical ground states have 0 or 3 particles at each site, and there is a gap for all excitations.

An effective interaction of strength t^2/U should stabilize chessboard phases. There is no quantum instability, because the passage from a classical ground state to another one requires the move of 3 particles, hence a factor t^3/U^2.

This could be generalized to attractive spin-S Hubbard models. When $S = 2$, chessboard phases (0,5) are expected. Moreover, a phase with one particle on each site of a sublattice, and four particles on the sites of the other sublattice, should also be stabilized by the effective potential, for suitable chemical potential. For larger S, other similar phases could also appear.

Incompressibility and zero susceptibility in the asymmetric Hubbard model. These properties have been conjectured in Chapter 4, see (4.10) and (4.11). Adapting the ideas of [BKU 1997], the difference between the density in the Gibbs state and that of the classical ground state, should be related to the presence of a winding contour in the space-time picture. Since its length is of the order β, we should find a bound $\mathrm{e}^{-\beta}$. Compressibility coefficient and susceptibility should be zero in the ground state of the (quantum) model. The magnetization as a function of the magnetic field is depicted in Fig. 9.1 and 9.2; the density with respect to the chemical potential also has a plateau.

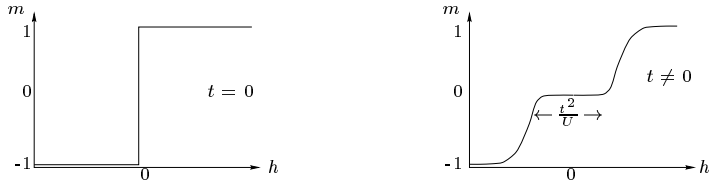


FIGURE 9.1. Magnetization as a function of the magnetic field, in the ground state of the asymmetric Hubbard model. Actually, it is reasonable to expect other plateaus of width t^4/U^3 and smaller, by analogy with the Falicov-Kimball model (see [GM 1996]); rather than a continuous curve, a devil's staircase structure could appear.

This should remain true in the standard Hubbard model, for the same reason. However, the way to prove it remains obscure to me.

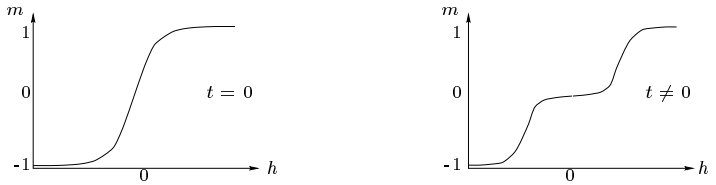


FIGURE 9.2. Magnetization as a function of the magnetic field in the asymmetric Hubbard model, at low temperature (other quasi-plateaus are also expected when $t \neq 0$).

Two-bands electronic system. We are interested in a physical system where the low temperature physical behaviour is governed by the electrons of two different bands interacting with Coulomb repulsion. The Hamiltonian is

$$H = t \sum_{<x,y>,\sigma} c^\dagger_{x,\sigma} c_{y,\sigma} + t' \sum_{<x,y>,\sigma} d^\dagger_{x,\sigma} d_{y,\sigma} + U \sum_x c^\dagger_{x,\uparrow} c_{x,\uparrow} c^\dagger_{x,\downarrow} c_{x,\downarrow} \\ - V \sum_{x,\sigma,\sigma'} c^\dagger_{x,\sigma} c_{x,\sigma} d^\dagger_{x,\sigma'} d_{x,\sigma'} - \mu \sum_{x,\sigma} c^\dagger_{x,\sigma} c_{x,\sigma} - \mu' \sum_{x,\sigma} d^\dagger_{x,\sigma} d_{x,\sigma}. \quad (9.1)$$

Operators $c^\dagger_{x,\sigma}, c_{x,\sigma}$ create, annihilate electrons of spin σ at site x, in the most external band. Similarly $d^\dagger_{x,\sigma}, d_{x,\sigma}$ create, annihilate holes in the interior band. This model represents a situation where some electrons of the full first band have been excited to the second band. U is the repulsive Coulomb energy of electrons of the external band, and V is the difference of Coulomb energy that an external electron feels when there is a hole on the same site.

We assume that only one hole may be present at a given site (i.e. hard-core repulsion between the holes) and since the distance between two external electrons, at a given site, is bigger than the distance between these electrons from the inner ones, we have $U < V$. We remark that when $t' = 0$, $U = 0$, the model reduces to the original Falicov-Kimball model, where both holes and electrons have spins.

When $2V - U = -2\mu - \mu'$, $-\mu \in (0, V - U)$ and $-\mu' > 0$ (it is possible to choose $\mu = \mu'$ if $2U < V$), the set G of low energy configurations contains all the configurations where the sites are either empty, or have a hole and two electrons of different spins.

Our results with the effective interaction almost apply and yield a nearest-neighbour interaction leading to a chessboard phase. Almost, because the set D of dominant states is infinite ($|D| = 2 \cdot 2^{\frac{1}{2}|\Lambda|}$ in a finite volume Λ); indeed, each hole has indifferently spin $\uparrow$ or $\downarrow$. Our method should nevertheless adapt to this situation.

Falicov-Kimball model with spin-$\frac{1}{2}$ electrons. This model was considered in [MN 1996] and is very similar to the previous one. The single site phase space is $\Omega = \{0, 1, \uparrow, \downarrow, 1\uparrow, 1\downarrow, \uparrow\downarrow, 3\}$, where "1" means the presence of an ion. The formal Hamiltonian is

$$H = -t' \sum_{<x,y>} a^\dagger_x a_y - t \sum_{\substack{<x,y> \\ \sigma \in \{\uparrow,\downarrow\}}} c^\dagger_{x\sigma} c_{y\sigma} + U \sum_x w_x (n_{x\uparrow} + n_{x\downarrow}) + V \sum_x n_{x\uparrow} n_{x\downarrow}$$

with $a^\dagger_x$, resp. $c^\dagger_{x\sigma}$, the creation operator for atoms, resp. electrons. Here $w_x = a^\dagger_x a_y$ and $n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}$. The range of parameters would be

$$t' \ll t \ll U, V.$$

If the chemical potentials are chosen such that the classical ground states have either one isolated ion, or two electrons at each site, the harvest should be easy. An effective interaction selecting the chessboard phases would appear.

More difficult is the situation where the classical ground states have exactly one particle at each site (the degeneracy is $3^{|\Lambda|}$). Suppose $U < V$. A nearest-neighbour effective interaction appears, that attributes energy $-t^2/U$ to pairs $(1,\uparrow)$ and $(1,\downarrow)$, $-t^2/V$ to pairs $(\uparrow,\downarrow)$, and zero otherwise. It does not remove totally the degeneracy, since the ground states are now all configurations where the ions occupy a sublattice, while the sites of the other sublattice have an electron with spin $\uparrow$ or $\downarrow$. The degeneracy is now $2 \cdot 2^{\frac{1}{2}|\Lambda|}$.

Fourth order terms in the effective interaction would remove this degeneracy, but there is "quantum instability": two electrons at distance 2 can permute at a cost t^4/U^3. What we expect however, is that for intermediate temperatures, such that

$$\beta\frac{t^2}{U} \gg 1 \qquad \text{and} \qquad \beta\frac{t^4}{U^3} \ll 1,$$

ions are ordered, while electrons are in a phase that is similar to a high temperature phase for one sublattice. The corresponding Gibbs state has period 2 (translation invariance is broken), but is still rotation invariant.

Lattice Helium model. The physical system that we consider here consists in a gas of Helium atoms in porous media. Helium has two isotopic forms: ^{3}He with two protons and one neutron, and ^{4}He with two protons and two neutrons. The first atom behaves as a fermion, while the second one is a boson. With $a_x^\dagger$ being the creation operator of an atom ^{4}He at site x, and $c_x^\dagger$ the counterpart for ^{3}He, and setting $w_x = a_x^\dagger a_x$ and $n_x = c_x^\dagger c_x$, the formal Hamiltonian takes the form

$$H = -t' \sum_{<x,y>} a_x^\dagger a_y - t \sum_{<x,y>} c_x^\dagger c_y + U \sum_x w_x n_x + V \sum_x (w_x)^2 - \mu' \sum_x w_x - \mu \sum_x n_x.$$

A funny observation is that we obtain known models by taking different limits of the Helium model.

- If $V \to \infty$ with μ' scaled so that μ'/V is an odd integer, there are n_0 or $n_0 + 1$ bosons at each site (n_0 depends on μ') and we obtain a model with fermions and hard-core bosons. If moreover $t' \to 0$, the model is the Falicov-Kimball one.
- Still with $V \to \infty$ and μ'/V an odd integer, but now with $t \to 0$, we obtain a Falicov-Kimball model where quantum particles are hard-core bosons.
- In the absence of interactions between bosons and fermions, that is, when $U \to 0$, this is the Bose-Hubbard model.

There is certainly a lot to harvest in this model, and in extensions of this model by introducing spins, longer-range hoppings or interactions, ...

Quantum Bricmont-Slawny theory. States chosen by thermal fluctuations are stable with respect to other thermal fluctuations [BS 1989], and they should be also stable when adding a very small quantum interaction T ($\|T\| \ll \mathrm{e}^{-\beta}$). It would be interesting to prove this, but it looks desperately difficult. If this would be possible, an application should be the 3D Bose-Hubbard model with nearest-neighbour and next-nearest-neighbour interactions, at quarter integer filling, where we expect that thermal fluctuations favour different phases than quantum fluctuations.

This walk through pleasant models where our theory applies sometimes totally, sometimes only as intuitive guide, should not bring a wrong impression about this work. Our aim was not to develop tools for getting results on special models, but rather to bring a modest contribution — indeed extremely modest, but maybe non-zero — to the question of phase transitions in quantum systems.

We have considered a rather large class of quantum lattice models; this made the theory technically heavy, but had an important advantage: this allowed to identify the mechanisms at work in these quantum systems, that are more than mathematical curiosities valid for peculiar models.

Let us summarize in two sentences the results described in this thesis.

- Small quantum fluctuations do not destroy the stability of phases of "nice" classical models.
- Quantum fluctuations create an effective interaction; in some cases, other effects are negligible and the quantum model behaves like a classical one.

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Article 16 1) de l'Ordonnance sur le doctorat, directives d'applications : "un curriculum vitæ doit figurer à la fin du travail de thèse".

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Voilà.

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