Lattice systems of particles

- Setting for fermions & bosons

- Bose-Einstein condensation
  (for non-interacting bosons)

- The Hubbard model
  (relation to Heisenberg antiferromagnet)

Fermionic & bosonic systems

In Physics, particles are either fermions (electrons, ...) or bosons (e.g. He^4).

- 1 particle on $\Lambda \in \mathbb{Z}^d$: $\mathcal{H}_{\Lambda,1} = \ell^2(\Lambda)$
- n distinguishable particles: $\mathcal{H}_{\Lambda,n} = \bigotimes_{i=1}^{n} \ell^2(\Lambda) \simeq \ell^2(\Lambda^n)$
- n bosons: $\mathcal{H}_{\Lambda,n}^{(+)} = P_+ \mathcal{H}_{\Lambda,n}$
- n fermions: $\mathcal{H}_{\Lambda,n}^{(-)} = P_- \mathcal{H}_{\Lambda,n}$

See the lecture notes for details.

Here: we build the setting with occupation numbers & creation, annihilation operators

Hilbert spaces

$$\mathcal{N}^{(+)}_{\Lambda,n} = \{ (n_x)_{x\in\Lambda} : n_x \in \mathbb{N}_0 , \sum_{x\in\Lambda} n_x = n \}$$

$$\mathcal{N}^{(-)}_{\Lambda,n} = \{ (n_x)_{x\in\Lambda} : n_x \in \{0,1\} , \sum_{x\in\Lambda} n_x = n \}$$

Then $\mathcal{H}^{(\pm)}_{\Lambda,n} = \ell^2(\mathcal{N}^{(\pm)}_{\Lambda,n})$

Fock spaces: for variable numbers of particles

$$\mathcal{F}^{(+)}_{\Lambda} = \bigoplus_{n=0}^{\infty} \mathcal{H}^{(+)}_{\Lambda,n} , \qquad \mathcal{F}^{(-)}_{\Lambda} = \bigoplus_{n=0}^{|\Lambda|} \mathcal{H}^{(-)}_{\Lambda,n}$$

$$\simeq \ell^2(\mathcal{N}^{(+)}_{\Lambda}) \qquad \simeq \ell^2(\mathcal{N}^{(-)}_{\Lambda})$$

Creation & annihilation operators

Bosons:

$$a_x : \mathcal{H}^{(+)}_{\Lambda,n} \to \mathcal{H}^{(+)}_{\Lambda,n-1}$$

$$a_x |\underline{n}\rangle = \begin{cases} \sqrt{n_x}\, |\underline{n} - \delta_x\rangle & \text{if } n_x \geq 1 \\ 0 & \text{if } n_x = 0 \end{cases}$$

$= (n_x)_{x\in\Lambda}$

(here: $\underline{n} = (n_x) \in \mathcal{N}^{(+)}_{\Lambda,n}$)

$$a_x^* : \mathcal{H}^{(+)}_{\Lambda,n} \to \mathcal{H}^{(+)}_{\Lambda,n+1}$$

$$a_x^* |\underline{n}\rangle = \sqrt{n_x+1}\, |\underline{n} + \delta_x\rangle$$

Note: $a_x^* a_x |n\rangle = n_x |n\rangle$

Fermions: Let $<$ be an order on Λ

$$c_x : \mathcal{H}^{(-)}_{\Lambda,n} \longrightarrow \mathcal{H}^{(-)}_{\Lambda,n-1}$$

$$c_x |\underline{n}\rangle = \begin{cases} (-1)^{\sum_{y<x} n_y} |\underline{n} - \delta_x\rangle & \text{if } n_x = 1 \\ 0 & \text{if } n_x = 0 \end{cases}$$

$$c_x^* : \mathcal{H}^{(-)}_{\Lambda,n} \longrightarrow \mathcal{H}^{(-)}_{\Lambda,n+1}$$

$$c_x^* |\underline{n}\rangle = \begin{cases} (-1)^{\sum_{y<x} n_y} |\underline{n} + \delta_x\rangle & \text{if } n_x = 0 \\ 0 & \text{if } n_x = 1 \end{cases}$$

Note: $c_x^* c_x |\underline{n}\rangle = n_x |\underline{n}\rangle$

Commutation relations

The bosonic operators satisfy the Canonical Commutation Relations (CCR):

$$[a_x, a_y] = 0, \quad [a_x^*, a_y^*] = 0, \quad [a_x, a_y^*] = \delta_{x,y}$$

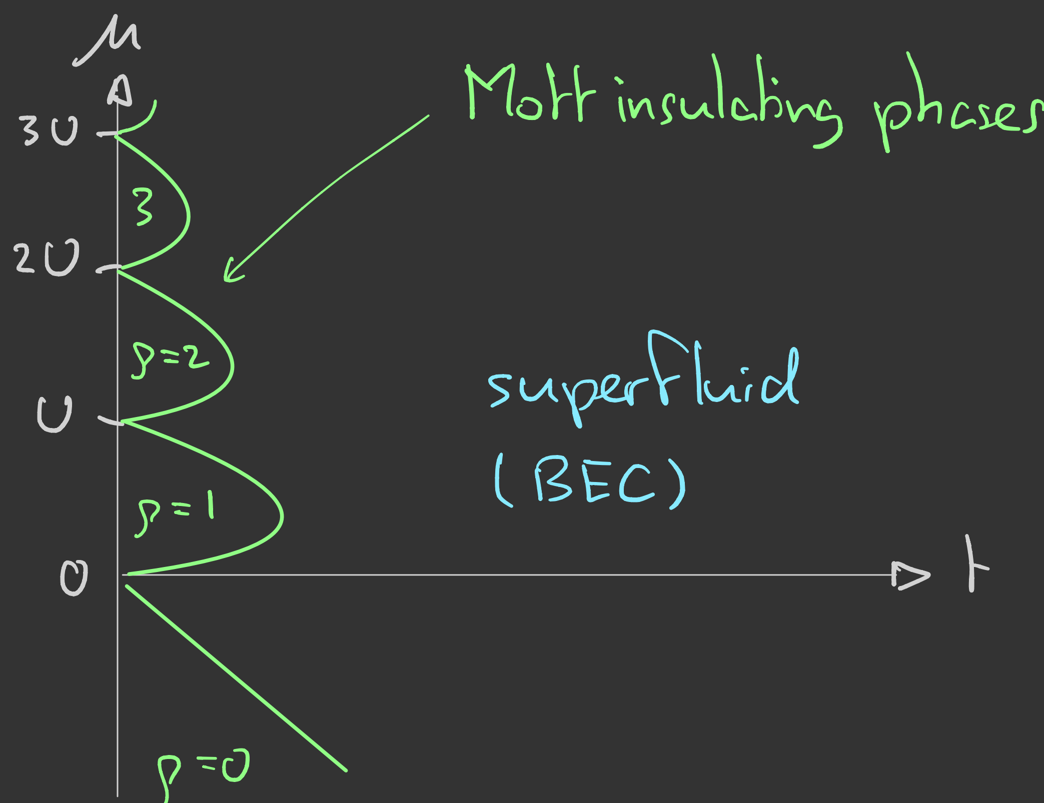
The fermionic operators satisfy the Canonical Anticommutation Relations (CAR):

$$\{c_x, c_y\} = 0, \quad \{c_x^*, c_y^*\} = 0, \quad \{c_x, c_y^*\} = \delta_{x,y}$$

The Bose-Hubbard model

On $\mathcal{H}^{(+)}_{\Lambda,n}$ or $\mathcal{F}^{(+)}_{\Lambda}$

$$H_{\Lambda,\mu} = -t \sum_{xy \in \mathcal{E}_\Lambda} \left(a_x^* a_y + a_y^* a_x\right) + \frac{1}{2} U \sum_{x\in\Lambda} \underbrace{n_x}_{= a_x^* a_x} (n_x - 1) - \mu \sum_x n_x$$



Remark: In the limit $U \to \infty$, we get hard-core bosons, equivalent to the quantum XY spin model

Bose-Einstein condensation

First description of a phase transition (Einstein '25)

We show two properties:

- The free energy is not analytic
- There is "off-diagonal long range order"

Free energy: $$f_\Lambda(\beta,\rho) = -\frac{1}{\beta|\Lambda|} \log \operatorname{Tr}_{\mathcal{H}^{(+)}_{\Lambda,\rho|\Lambda|}} e^{-\beta H_\Lambda}$$

$\lfloor \rho|\Lambda| \rfloor$

$$f(\beta,\rho) = \lim_{\Lambda \Uparrow \mathbb{Z}^d} f_\Lambda(\beta,\rho)$$

Here: $H_\Lambda = - \sum_{xy \in \mathcal{E}_\Lambda} (a_x^* a_y + a_y^* a_x)$

Pressure: $p_\Lambda(\beta,\mu) = \frac{1}{|\Lambda|} \log \sum_{n \geq 0} e^{\beta \mu n} \operatorname{Tr}_{\mathcal{H}^{(+)}_{\Lambda,n}} e^{-\beta H_\Lambda}$

$$p(\beta,\mu) = \lim_{\Lambda \Uparrow \mathbb{Z}^d} p_\Lambda(\beta,\mu)$$

Fact: (more soon!) The limits $\Lambda \Uparrow \mathbb{Z}^d$ exist.

Theorem

Pressure & free energy are related by Legendre transforms:

$$f(\beta,\rho) = \sup_\mu \left(\rho\mu - \frac{1}{\beta} p(\beta,\mu)\right)$$

$$p(\beta,\mu) = \sup_\rho \left(\beta\rho\mu - \beta f(\beta,\rho)\right)$$

Ideas behind the proof: Laplace principle.

Let us consider $p(\beta,\mu) = \sup_{\rho} \left(\beta\rho\mu - f(\beta,0) \right)$.

From the definition:

$$p_\Lambda(\beta,\mu) = \frac{1}{|\Lambda|} \log \underbrace{\sum_{n\geq 0}}_{} e^{\beta\mu n} \, e^{-\beta|\Lambda| f_\Lambda(\beta,\rho)}$$

$\frac{n}{|\Lambda|}$

$$\sum_{n\geq 0} g(n) = \sum_{n\geq 0} g(n) \int_0^\infty d\rho \; 1_{n = \lfloor |\Lambda|\rho \rfloor} \, |\Lambda| = |\Lambda| \int_0^\infty d\rho \; g(|\Lambda|\rho)$$

$$\lim_{\Lambda \Uparrow \mathbb{Z}^d} p_\Lambda(\beta,\mu) = \lim_{\Lambda \Uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \int_0^\infty d\rho \; e^{|\Lambda|(\beta\rho\mu - \beta f_\Lambda(\beta,\rho))}$$

$$\gtrsim \frac{1}{|\Lambda|} \log e^{|\Lambda| \sup(\beta\rho\mu - \beta f_\Lambda(\beta,\rho))}$$

For the upper bound, one needs to control $f(\beta,\rho)$ for large ρ.

Pressure of the ideal (non-interacting) Bose gas

Consider $H_\Lambda = - \sum_{xy \in \mathcal{E}_\Lambda} (a_x^* a_y + a_y^* a_x) + 2d \sum_x a_x^* a_x$

where $\Lambda = \{0, \dots, \ell - 1\}^d_{per}$ and $\mathcal{E}_\Lambda$: set of nearest-neighbours

Fourier transform of a_x, a_x^* :

$$\hat{a}_k = \frac{1}{\ell^{d/2}} \sum_{x \in \Lambda} e^{-ikx} a_x \quad , \quad k \in \Lambda^* = \left(\frac{2\pi}{\ell} \left\{ -\frac{\ell}{2} + 1, \dots, \frac{\ell}{2} \right\} \right)^d$$

$$\subset [-\pi, \pi]^d$$

$$\hat{a}_k^* = \frac{1}{\ell^{d/2}} \sum_{x \in \Lambda} e^{ikx} a_x^*$$

Then $$a_x = \frac{1}{\ell^{d/2}} \sum_{k \in \Lambda^*} e^{ikx} \hat{a}_k$$

$$a_x^* = \frac{1}{\ell^{d/2}} \sum_{k \in \Lambda^*} e^{-ikx} \hat{a}_k^*$$

This can be written as a unitary transformation $P_+ \ell^2(\Lambda^n) \to P_+ \ell^2(\Lambda^{*n})$

$\to$ $\hat{a}_k^* a_k$ has eigenvalues $0, 1, 2, \dots$

$$H_\Lambda = \sum_{k \in \Lambda^*} \varepsilon(k)\, \hat{a}_k^* \hat{a}_k$$

$$\varepsilon(k) = 2\sum_{i=1}^{d} (1 - \cos k_i)$$

$$\varepsilon_k \geq 0$$

$$\boxed{p_\Lambda(\beta,\mu) = \frac{1}{\ell^d} \log \sum_{(n_k)_{k\in\Lambda^*}} e^{-\beta \sum_k (\varepsilon(k)-\mu)\, n_k}}$$

$$k=0: \sum_{n_0 \geq 0} e^{\beta\mu n_0}$$

$$= \frac{1}{\ell^d} \log \prod_{k \in \Lambda^*} \left(\sum_{n_k \geq 0} e^{-\beta(\varepsilon(k)-\mu))\, n_k} \right)$$

$$= \frac{1}{\ell^d} \sum_{k\in\Lambda^*} \log \frac{1}{1 - e^{-\beta(\varepsilon(k)-\mu)}}$$

$$\xrightarrow{\ell \to \infty} \boxed{-\frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} dk \, \log\left(1 - e^{-\beta(\varepsilon(k)-\mu)}\right)}$$

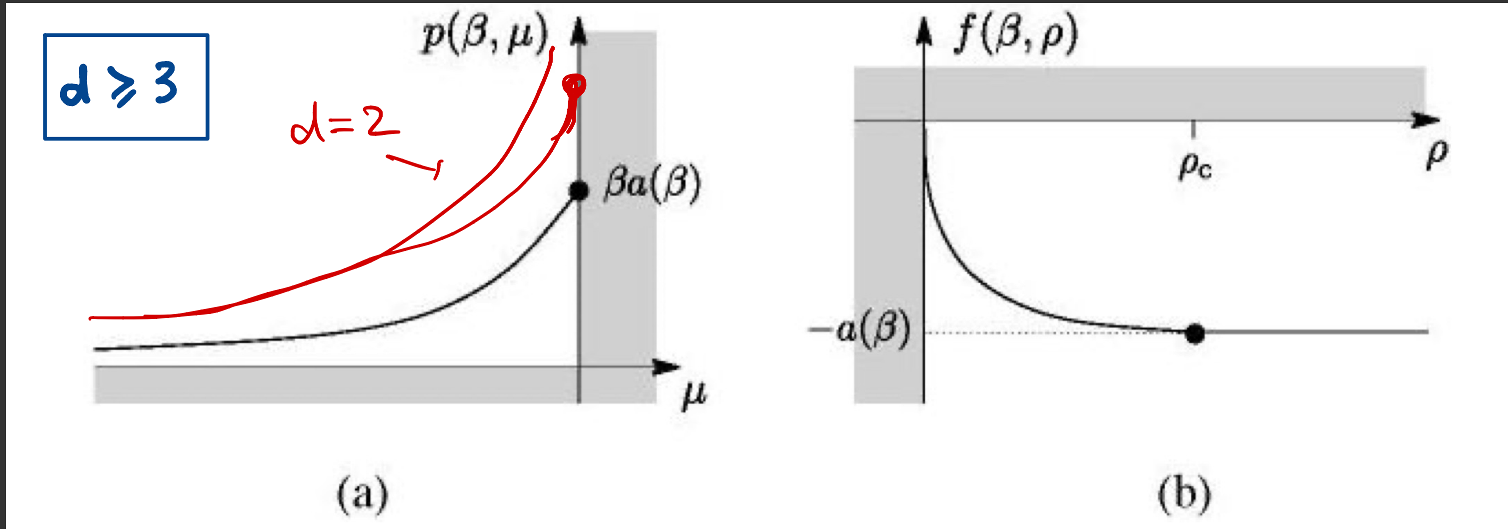


FIGURE 2.1. (a) The pressure of the ideal Bose gas; (b) its Legendre transform, the free energy.

The free energy is not always analytic!

The density $\rho(\beta,\mu)$ is

$$\rho(\beta,\mu) = \frac{1}{\beta}\frac{\partial}{\partial\mu} p(\beta,\mu) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} dk \, \frac{1}{e^{\beta(\varepsilon(k)-\mu)}-1} \qquad \sim \frac{1}{k^2}$$

Critical density: $\boxed{\rho_c(\beta) = \lim_{\mu\uparrow 0} \rho(\beta,\mu) = \frac{1}{(2\pi)^d}\int dk \, \frac{1}{e^{\beta\varepsilon(k)}-1}}$

Broken symmetry / long-range order

Recall that $H_\Lambda = -\sum_{xy \in \mathcal{E}_\Lambda} (a_x^* a_y + a_y^* a_x)$

Notice that $[H_\Lambda, \underbrace{N_\Lambda}_{=\sum_{x\in\Lambda} n_x}] = 0$.

This implies a continuous symmetry:

$$H_\Lambda = e^{i\theta N_\Lambda} H_\Lambda e^{-i\theta N_\Lambda}, \qquad \theta \in [0, 2\pi)$$

Relevant correlation function:

$$\langle a_x^* a_y \rangle_{\Lambda,\beta,n} = \frac{1}{Z_{\Lambda,\beta,n}} \overline{\mathrm{Tr}}_{\mathcal{H}^{(+)}_{\Lambda,n}} a_x^* a_y e^{-\beta H_\Lambda}$$

As $\Lambda \Uparrow \mathbb{Z}^d$ with $n = \rho|\Lambda|$, does $\langle a_x^* a_y \rangle$ decays to 0 as $|x-y| \to \infty$?

Existence of long-range order (ideal Bose gas)

Theorem 2.2.

$$\lim_{\ell\to\infty} \frac{1}{|\Lambda_\ell^{\mathrm{per}}|} \sum_{x\in\Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x\rangle_{\Lambda_\ell^{\mathrm{per}},\beta,\lfloor \rho \ell^d\rfloor} = \max(0,\rho-\rho_{\mathrm{c}})$$

where the critical density is equal to

$$\rho_{\mathrm{c}} = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} \frac{1}{\mathrm{e}^{\beta\varepsilon(k)}-1}\mathrm{d}k.$$

Consequence: $\langle a_0^* a_x\rangle \not\to 0$ as $|x|\to\infty$, when $\rho>\rho_c$.

$\sim \langle a_0^*\rangle\langle a_x\rangle = 0$

Proof: We again work with the Fourier transforms of creation & annihilation operators.

$$\frac{1}{\ell^d}\sum_{x\in\Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x\rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{\ell^d}\langle \hat a_0^* \hat a_0\rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,\rho}} \sum_{(n_k)_{k\in\Lambda_\ell^*}:\sum_k n_k = n} \frac{n_0}{\ell^k} \mathrm{e}^{-\beta\sum_k \varepsilon(k) n_k}.$$

d

$= \frac{1}{\sqrt{\ell^d}} \sum_x a_x^*$

$$\frac{1}{\ell^d}\sum_{x\in\Lambda_\ell^{\mathrm{per}}}\langle a_0^* a_x\rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{\ell^d}\mathbb{E}[n_0] = \frac{n}{\ell^d} - \frac{1}{\ell^d}\sum_{k\neq 0}\mathbb{E}[n_k]$$

$$E[N] = \sum_{n\geq 1} n\, P[N=n] = \sum_{n\geq 1} P[N=n]\sum_{i=1}^{n} 1 = \sum_{i\geq 1}\sum_{n\geq i} P[N=n] = \sum_{i\geq 1} P[N\geq i]$$

$$= \frac{n}{\ell^d} - \frac{1}{\ell^d}\sum_{k\neq 0}\sum_{i\geq 1}\mathbb{P}[n_k\geq i]$$

$$= \frac{n}{\ell^d} - \frac{1}{\ell^d}\sum_{k\neq 0}\frac{1}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n}}\sum_{i\geq 1}\sum_{(n_{k'}):\sum_{k'} n_{k'}=n, n_k\geq i} \mathrm{e}^{-\beta\sum_{k'}\varepsilon(k')n_{k'}}$$

$$= \frac{n}{\ell^d} - \frac{1}{\ell^d}\sum_{k\neq 0}\sum_{i\geq 1}\mathrm{e}^{-\beta\varepsilon(k)i}\frac{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n-i}}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n}} \quad \text{ratio} \leq 1$$

$$\geq \frac{n}{\ell^d} - \frac{1}{\ell^d}\sum_{k\neq 0}\frac{1}{\mathrm{e}^{\beta\varepsilon(k)}-1}. \quad \xrightarrow{\ell\to\infty} \rho-\rho_c$$

For the converse inequality:

$$\lim_{\ell\to\infty}\frac{1}{\beta\ell^d}\log\mathbb{P}[n_0\geq \ell^d\eta] = \lim_{\ell\to\infty}\frac{1}{\beta\ell^d}\log\frac{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n-\ell^d\eta}}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n}} = f(\beta,\rho)-f(\beta,\rho-\eta)$$

If $\eta > \max(0,\rho-\rho_c)$: $\quad \mathbb{P}[n_0 > \ell^d\eta] \leq e^{-\ell^d\delta}$, with $\delta>0$.

Then $\frac{1}{\ell^d}\mathbb{E}[n_0] \leq \max(0,\rho-\rho_c)$ $\quad\square$