Lattice fermion systems

+ states & Gibbs states (finite volume)

* Today's slides are already online.

* Tuesday 25 November: no lectures!

  Options: $\boxed{\text{1. One more lecture on 9 December.}}$ ✓

  2. Extend 2 lectures by 1 hour.

  3. Extend remaining lectures to 65 + 65 minutes (instead of 55+55)

  4. Do nothing.

Lattice fermions – Hubbard model

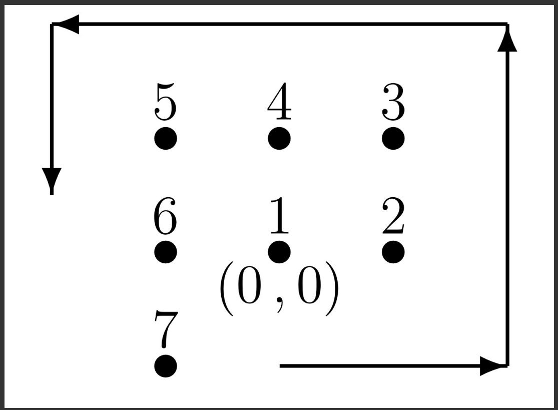
Electrons (fermions) carrying spins.

$\Lambda \Subset \mathbb{Z}^d$

Hilbert space: $\mathcal{H}_\Lambda = \ell^2(\{0,1\}^{\Lambda\times\{\uparrow,\downarrow\}}) \simeq \ell^2(\{0,\uparrow,\downarrow,2\}^{\Lambda})$.

$\dim \mathcal{H}_\Lambda = 4^{|\Lambda|}$

Order on $\mathbb{Z}^d$, such as the spiral order:



$\downarrow < \uparrow$

$\underset{\Lambda}{\overset{\cap}{x}}, \underset{\{\uparrow,\downarrow\}}{\overset{\cap}{\sigma}}$: $(x,\sigma) < (x',\sigma')$ if $x < x'$

or $x = x'$ and $\sigma = \downarrow,\ \sigma' = \uparrow$

Creation & annihilation operators

$$c^*_{x,\sigma}|\eta\rangle = (-1)^{\sum_{(y,\sigma')<(x,\sigma)}\eta_{y,\sigma'}}\begin{cases}|\eta+\delta_{x,\sigma}\rangle & \text{if } \eta_{x,\sigma}=0,\\ 0 & \text{otherwise.}\end{cases}$$

$$c_{x,\sigma}|\eta\rangle = (-1)^{\sum_{(y,\sigma')<(x,\sigma)}\eta_{y,\sigma'}}\begin{cases}|\eta-\delta_{x,\sigma}\rangle & \text{if } \eta_{x,\sigma}=1,\\ 0 & \text{otherwise.}\end{cases}$$

$\eta = (\eta_{x\sigma}) \in \{0,1\}^{\Lambda \times \{\uparrow,\downarrow\}}$

They satisfy the Canonical Anticommutation Relations (CAR):

$$\{c^*_{x,\sigma}, c^*_{y,\sigma'}\} = \{c_{x,\sigma}, c_{y,\sigma'}\} = 0,$$
$$\{c^*_{x,\sigma}, c_{y,\sigma'}\} = \delta_{x,y}\delta_{\sigma,\sigma'}\mathbb{1}.$$

$\{A,B\}$
$= AB + BA$

Particle number operator: $$n_{x,\sigma}|\eta\rangle = \eta_{x,\sigma}|\eta\rangle.$$

$n_{x\sigma} = c^*_{x\sigma}c_{x\sigma}$

Usefull expression for basis vectors: $$|\eta\rangle = c^*_{x_1,\sigma_1}c^*_{x_2,\sigma_2}\ldots c^*_{x_N,\sigma_N}|0\rangle.$$

(with $(x_1,\sigma_1) < \ldots < (x_N,\sigma_N)$)

$|0\rangle \neq 0$

Hubbard hamiltonian:

$$H_\Lambda = -t \sum_{xy \in \mathcal{E}(\Lambda)} \sum_{\sigma=\downarrow,\uparrow} \left(c^*_{x,\sigma} c_{y,\sigma} + c^*_{y,\sigma} c_{x,\sigma} \right) + U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} - \mu \sum_{x \in \Lambda} (n_{x,\uparrow} + n_{x,\downarrow}). \tag{2.64}$$

Phase diagram: complicated, it depends on the lattice, and may include phases displaying ferromagnetism, antiferromagnetism / Ferrimagnetism, superconductivity, ...

Here: We explain antiferromagnetism due to "Anderson superexchange".

Spin operators:

$$S_x^{(+)} = c^*_{x,\uparrow} c_{x,\downarrow}, \qquad S_x^{(-)} = c^*_{x,\downarrow} c_{x,\uparrow}, \qquad S_x^{(3)} = \frac{1}{2}(n_{x,\uparrow} - n_{x,\downarrow}).$$

Then $\boxed{S_x^{(1)} = \frac{1}{2}(S_x^{(+)} + S_x^{(-)})}$ and $\boxed{S_x^{(2)} = \cancel{\frac{1}{2}}(S_x^{(+)} - S_x^{(-)}).}$

$\frac{1}{2i}$

It follows from CAR that

$$[S_x^{(1)}, S_y^{(2)}] = \mathrm{i}\delta_{x,y} S_x^{(3)}, \qquad [S_x^{(2)}, S_y^{(3)}] = \mathrm{i}\delta_{x,y} S_x^{(1)}, \qquad [S_x^{(3)}, S_y^{(1)}] = \mathrm{i}\delta_{x,y} S_x^{(2)}.$$

Some important symmetries:

$n_x = n_{x\uparrow} + n_{x\downarrow}$

Proposition 2.5.

(a) *SU(2) symmetry:* $[H_\Lambda, \sum_{x\in\Lambda} S_x^{(i)}] = 0$ *for* $i = 1, 2, 3$.
(b) *Gauge invariance:* $[H_\Lambda, \sum_{x\in\Lambda} n_x] = 0$.

Consequences: $\langle S_x^{(i)} \rangle_{\Lambda,\beta} = 0$, $\langle c^*_{x,\sigma} \rangle_{\Lambda,\beta} = 0$, $\langle c^*_{x,\uparrow} c^*_{y,\downarrow} \rangle_{\Lambda,\beta} = 0$

Relation between Hubbard and Heisenberg antiferromagnet

We use Lie-Schwinger expansion.

The "adjoint operation":

$$\mathrm{ad}_A B = [A, B],$$
$$\mathrm{ad}_A^{-1} B = \sum_{\substack{a,a' \in \mathrm{Spec}(A) \\ a \neq a'}} P_a \frac{B}{a - a'} P_{a'}$$

Then $\mathrm{ad}_A \mathrm{ad}_A^{-1} B = \mathrm{ad}_A^{-1} \mathrm{ad}_A B = B^{\mathrm{od}}$, where $B^{\mathrm{od}} = \sum_{a \neq a'} P_a B P_{a'}$

Lemma 3.15 (Lie-Schwinger multicommutator expansion). *Let A and B be two operators on the same finite-dimensional Hilbert space. Then*

$$\mathrm{e}^{A} B \, \mathrm{e}^{-A} = \sum_{n \geq 0} \frac{1}{n!} \mathrm{ad}_A^n(B).$$

$[A, [A, \dots [A, B] \dots]$

Proof. We show that $\mathrm{e}^{sA} B \, \mathrm{e}^{-sA}$ and $\sum_n \frac{s^n}{n!} \mathrm{ad}_A^n(B)$ satisfy the same differential equation. First,

$$\frac{\mathrm{d}}{\mathrm{d}s} \mathrm{e}^{sA} B \, \mathrm{e}^{-sA} = \left[A, \, \mathrm{e}^{sA} B \, \mathrm{e}^{-sA}\right]. \tag{3.38}$$

Second,

$$\frac{\mathrm{d}}{\mathrm{d}s} \sum_{n \geq 0} \frac{s^n}{n!} \mathrm{ad}_A^n(B) = \sum_{n \geq 1} \frac{s^{n-1}}{(n-1)!} \mathrm{ad}_A\left(\mathrm{ad}_A^{n-1}(B)\right) = \left[A, \sum_{n \geq 0} \frac{s^n}{n!} \mathrm{ad}_A^n(B)\right]. \tag{3.39}$$

□

Back to the Hubbard model (at half-filling)

$H_\Lambda = H_\Lambda^{(0)} + t T_\Lambda$:

$$H_\Lambda^{(0)} = U \sum_{x\in\Lambda} (n_{x,\uparrow} - \tfrac{1}{2})(n_{x,\downarrow} - \tfrac{1}{2}),$$

$$T_\Lambda = \sum_{xy\in\mathcal{E}(\Lambda)} \sum_{\sigma=\uparrow,\downarrow} \left(c^*_{x,\sigma} c_{y,\sigma} + c^*_{y,\sigma} c_{x,\sigma}\right).$$

Let $S_\Lambda = -S_\Lambda^*$ and $U_\Lambda = e^{tS_\Lambda}$ (it is unitary).

From Lie-Schwinger:

$$U_\Lambda H_\Lambda U_\Lambda^{-1} = H_\Lambda^{(0)} + \underbrace{tT_\Lambda + t\,\mathrm{ad}_{S_\Lambda} H_\Lambda^{(0)}}_{\equiv 0 \text{ then } T_\Lambda = -\mathrm{ad}_{S_\Lambda} H_\Lambda^{(0)} = \mathrm{ad}_{H_\Lambda^{(0)}} S_\Lambda} + t^2 \mathrm{ad}_{S_\Lambda} T_\Lambda + \tfrac{1}{2} t^2 \mathrm{ad}^2_{S_\Lambda} H_\Lambda^{(0)} + O(t^3).$$

Then

$$S_\Lambda = \mathrm{ad}^{-1}_{H_\Lambda^{(0)}} T_\Lambda = \sum_{xy\in\mathcal{E}(\Lambda)} \mathrm{ad}^{-1}_{H_\Lambda^{(0)}} T_{xy} \equiv \sum_{xy\in\mathcal{E}(\Lambda)} S_{xy}.$$

Also: $\mathrm{ad}^2_{S_\Lambda} H^{(0)}_\Lambda = -\mathrm{ad}_{S_\Lambda} T_\Lambda.$

It follows that

$$U_\Lambda H_\Lambda U_\Lambda^{-1} = H^{(0)}_\Lambda + tT_\Lambda + t\mathrm{ad}_{S_\Lambda} H^{(0)}_\Lambda + t^2\mathrm{ad}_{S_\Lambda} T_\Lambda + \tfrac{1}{2}t^2\mathrm{ad}^2_{S_\Lambda} H^{(0)}_\Lambda + O(t^3).$$

becomes $U_\Lambda H_\Lambda U_\Lambda^{-1} = H^{(0)}_\Lambda + \tfrac{1}{2}t^2\mathrm{ad}_{S_\Lambda} T_\Lambda + O(t^3).$

One calculates matrix elements of $S_{x,y}$:

$$\langle 0,2|S_{xy}|\uparrow,\downarrow\rangle = \langle 2,0|S_{xy}|\uparrow,\downarrow\rangle = -\frac{1}{U} = -\langle\uparrow,\downarrow|S_{xy}|0,2\rangle = -\langle\uparrow,\downarrow|S_{xy}|2,0\rangle,$$
$$\langle 0,2|S_{xy}|\downarrow,\uparrow\rangle = \langle 2,0|S_{xy}|\downarrow,\uparrow\rangle = +\frac{1}{U} = -\langle\downarrow,\uparrow|S_{xy}|0,2\rangle = -\langle\downarrow,\uparrow|S_{xy}|2,0\rangle.$$

Let $P_\Lambda^{(1)}$ the projector onto the subspace with one particle per site:

$$\boxed{P_\Lambda^{(1)} = \otimes_{x\in\Lambda}\big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\big).}$$

The matrix elements restricted to the subspace are:

$$\langle\uparrow,\downarrow|S_{xy}T_{xy}|\uparrow,\downarrow\rangle = \langle\downarrow,\uparrow|S_{xy}T_{xy}|\downarrow,\uparrow\rangle = -\frac{2}{U},$$

$$\langle\uparrow,\downarrow|S_{xy}T_{xy}|\downarrow,\uparrow\rangle = \langle\downarrow,\uparrow|S_{xy}T_{xy}|\uparrow,\downarrow\rangle = +\frac{2}{U}.$$

Then

$$P_{xy}^{(1)}[S_{xy}, T_{xy}]P_\Lambda^{(1)} = \frac{8}{U}P_\Lambda^{(1)}\big(\vec{S}_x \cdot \vec{S}_y - \tfrac{1}{4}\big)P_\Lambda^{(1)}.$$

THEOREM 2.6.

$$P_\Lambda^{(1)}U_\Lambda H_\Lambda U_\Lambda^{-1}P_\Lambda^{(1)} = \frac{4t^2}{U}\sum_{xy\in\Lambda} P_\Lambda^{(1)}\,\vec{S}_x \cdot \vec{S}_y\,P_\Lambda^{(1)} - \tfrac{1}{4}U|\Lambda|P_\Lambda^{(1)} + O(t^3).$$

States & equilibrium states

A state is a linear functional on a C^* algebra that is positive and normalised.

An equilibrium state or Gibbs state is a state that satisfies certain extra conditions.

Plan:

- States & equilibrium states with finite-dimensional Hilbert space (i.e. finite volume).
- Extend notions to infinite volumes.

States on $B(\mathcal{H})$

$\mathcal{H}$: Hilbert space, $\dim \mathcal{H} < \infty$.

$B(\mathcal{H})$: space of operators (matrices) on $\mathcal{H}$.

Recall that $\|A\| = \sup_{v \in \mathcal{H}} \frac{\|Av\|}{\|v\|}$ and $A \geq 0 \iff \langle v, Av \rangle \geq 0 \ \forall v \in \mathcal{H}$.

A **state** on $\mathcal{H}$ is a positive, normalised linear functional on $\mathcal{B}(\mathcal{H})$; that is, it is a map $\langle \cdot \rangle : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ that is

(i) linear: $\langle sA + tB \rangle = s\langle A \rangle + t\langle B \rangle$ for all $s, t \in \mathbb{C}$ and $A, B \in \mathcal{B}(\mathcal{H})$;

(ii) positive: $\langle A^* A \rangle \geq 0$ for all $A \in \mathcal{B}(\mathcal{H})$;

(iii) normalised: $\langle \mathbb{1} \rangle = 1$.

Notation: States are usually denoted $\langle \cdot \rangle$. Sometimes $\rho(\cdot)$.

Fact: the norm of a state is 1: $\|\langle \cdot \rangle\| = \sup_{A \neq 0} \frac{|\langle A \rangle|}{\|A\|} = 1$.

If ρ is a density matrix (i.e. $\rho \geq 0$ and $\operatorname{Tr}\rho = 1$), then

$$\langle A \rangle \doteq \operatorname{Tr} \rho A$$

is clearly a state.

Proposition 3.1 (Riesz representation of states). *Let $\langle \cdot \rangle$ be a state on a Hilbert space $\mathcal{H}$. Then there exists a unique density operator ρ such that $\langle A \rangle = \operatorname{Tr} \rho A$ for all $A \in \mathcal{B}(\mathcal{H})$.*

<u>Proof:</u> Introduce Hilbert-Schmidt inner product:

$$\langle A, B \rangle \longmapsto \operatorname{Tr} A^* B$$

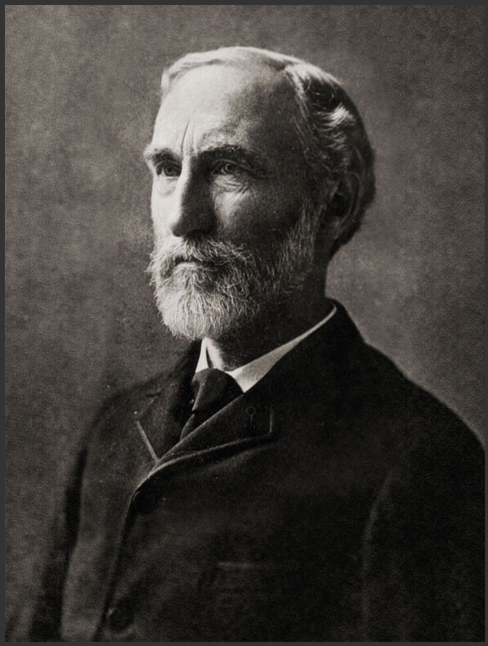
Then by Riesz, any linear functional is represented by a matrix ρ s.t.

$$\langle A \rangle = \langle \rho, A \rangle = \operatorname{Tr} \rho^* A.$$

If $A = |v\rangle\langle v|$: $0 \leq \langle |v\rangle\langle v| \rangle = \operatorname{Tr} \rho^* |v\rangle\langle v| = \langle v, \rho^* v \rangle$

$\Rightarrow \rho^* \geq 0 \Rightarrow \rho = \rho^* \geq 0$. $1 = \langle 1 \rangle = \operatorname{Tr} \rho 1 = \operatorname{Tr} \rho$. $\square$

Gibbs states on $\mathcal{B}(\mathcal{H})$



Given the hamiltonian $H = H^* \in \mathcal{B}(\mathcal{H})$,
and the inverse temperature $\beta \geq 0$,
consider the density matrix

$$\rho = \frac{1}{Z_\beta} e^{-\beta H}, \qquad Z_\beta = \operatorname{Tr} e^{-\beta H}$$

"partition function"

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathbb{C}^2$$

The Gibbs state is

$$\langle A \rangle = \langle A \rangle_{H,\beta} = \operatorname{Tr} \rho A = \frac{1}{Z_\beta} \operatorname{Tr} A e^{-\beta H}$$

Motivation: Not straightforward.

Average energy: $\langle H \rangle = \frac{1}{Z_\beta} \operatorname{Tr} H e^{-\beta H}$.

For large systems, it takes typical values, so the Gibbs state is essentially an average over configurations with correct energy.

Characterisation of Gibbs states

Main interest: these notions will extend to infinite volumes.

PROPOSITION 3.3. *The Gibbs state $\langle\cdot\rangle_{H,\beta}$ is the unique state $\langle\cdot\rangle = \mathrm{Tr}\,\cdot\,\rho$ satisfying any of the following four conditions:*

(a) Tangent condition: *Let $F_\beta(H) := -\frac{1}{\beta}\log \mathrm{Tr}\,\mathrm{e}^{-\beta H}$. Then $F_\beta(H+A) \leq F_\beta(\overset{H}{\cancel{A}}) + \langle A\rangle$ for all $A = A^* \in \mathcal{B}(\mathcal{H})$.*

(b) Gibbs variational principle: *The density matrix ρ minimizes the function $\mathcal{F}_\beta(\rho) := \mathrm{Tr}\,H\rho + \frac{1}{\beta}\mathrm{Tr}\,\rho\log\rho$.*

(c) KMS condition: *Define the time evolution*

Kubo-Martin-Schwinger

$$\alpha_t(A) = \mathrm{e}^{\mathrm{i}tH}\,A\,\mathrm{e}^{-\mathrm{i}tH}\,, \qquad t\in\mathbb{C}. \tag{3.14}$$

Then $\langle AB\rangle = \big\langle B\,\alpha_{\mathrm{i}\beta}(A)\big\rangle$ for all $A, B \in \mathcal{B}(\mathcal{H})$.

(d) RAS condition: *For all $A \in \mathcal{B}(\mathcal{H})$ such that $\langle AA^*\rangle > 0$,*

Roepstorff-Araki-Sewell

$$\langle A^*[H,A]\rangle \geq \frac{1}{\beta}\langle A^*A\rangle \log\frac{\langle A^*A\rangle}{\langle AA^*\rangle} \tag{3.15}$$

Remarks:

- $F_\beta(H)$ is the free energy.
- $\mathcal{F}_\beta(\rho)$ is also the free energy.

Proof of (a), (b), (d): exercises.

Proof of Prop. 3.3 (c):

PROPOSITION 3.3. *The Gibbs state $\langle\cdot\rangle_{H,\beta}$ is the unique state $\langle\cdot\rangle = \mathrm{Tr}\cdot\rho$ satisfying any of the following four conditions:*

(c) KMS condition: *Define the time evolution*

$$\alpha_t(A) = \mathrm{e}^{\mathrm{i}tH}\,A\,\mathrm{e}^{-\mathrm{i}tH}\,, \qquad t \in \mathbb{C}. \tag{3.14}$$

Then $\langle AB\rangle = \big\langle B\,\alpha_{\mathrm{i}\beta}(A)\big\rangle$ for all $A, B \in \mathcal{B}(\mathcal{H})$.

① $\Rightarrow$: $\langle A\rangle = \mathrm{Tr}\, A\, e^{-\beta H}\frac{1}{Z_\beta}$ then KMS

$$\langle B\,\alpha_{i\beta}(A)\rangle = \frac{1}{Z_\beta}\mathrm{Tr}\, B\, e^{-\beta H} A\, \cancel{e^{\beta H}}\, \cancel{e^{-\beta H}}$$

$$= \frac{1}{Z_\beta}\mathrm{Tr}\, AB\, e^{-\beta H} = \langle AB\rangle$$

② KMS $\Rightarrow$ Gibbs: let ρ s.t. $\langle A \rangle = \operatorname{Tr} \rho A$.

$$\operatorname{Tr}(\rho A)B \overset{\text{KM}}{=} \operatorname{Tr} \rho B e^{-\beta H} A e^{\beta H} = \operatorname{Tr}(e^{-\beta H} A e^{\beta H} \rho) B$$

then $\rho A = e^{-\beta H} A e^{\beta H} \rho \quad \forall A$

$$\Leftrightarrow \quad e^{\beta H} \rho A = A e^{\beta H} \rho \Leftrightarrow [e^{\beta H} \rho, A] = 0$$

Then $e^{\beta H} \rho = c \mathbb{1} \Rightarrow \rho = c e^{-\beta H}$

$\operatorname{Tr} \rho = 1 \rightarrow c = (\operatorname{Tr} e^{-\beta H})^{-1}$. $\square$

Next week: extend Gibbs states to infinite volumes.

- Space of "quasi-local operators".
- Infinite-volume free energy, entropy, evolution.