# Introduction to Quantum Spin Systems

## Lecture 2

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## Basic Setup

For concreteness, consider finite subsets $\Lambda \subset \mathbb{Z}^d$, and assume $\mathcal{H}_x \cong \mathbb{C}^n$, for all $x \in \mathbb{Z}^d$. The Hilbert space describing the total system is

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{H}_x.$$

The algebra of observables of the system is

$$\mathcal{A}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{B}(\mathcal{H}_x) = \mathcal{B}(\mathcal{H}_\Lambda).$$

If $X \subset \Lambda$, we have $\mathcal{A}_X \subset \mathcal{A}_\Lambda$, by identifying $A \in \mathcal{A}_X$ with $A \otimes \mathbb{1}_{\Lambda \setminus X} \in \mathcal{A}_\Lambda$. The algebra of local observables $\mathcal{A}_{\mathrm{loc}}$ is then defined by (inductive limit):

$$\mathcal{A}_{\mathrm{loc}} = \bigcup_{\Lambda \subset \mathbb{Z}^d} \mathcal{A}_\Lambda.$$

## The $C^*$-algebra $\mathcal{A}$

Since $\mathcal{A}_{\text{loc}}$ is built from the net of matrix algebras $\mathcal{B}(\mathcal{H}_\Lambda)$, it inherits a natural $^*$-operation and norm (note $\|A \otimes \mathbb{1}\| = \|A\|$) from them with the following basic properties:

- $\mathcal{A}_{\text{loc}}$ is an algebra with unit $\mathbb{1}$ ($\mathbb{1}^* = \mathbb{1}$, $\|\mathbb{1}\| = 1$);
- $A^{**} = A$, $(A + B)^* = A^* + B^*$, $(\lambda A)^* = \overline{\lambda} A^*$, $(AB)^* = B^* A^*$;
- the positive elements are defined as all $A$ of the form $B^* B$;
- $\|A^* A\| = \|A\|^2$, $\|A + B\| \leq \|A\| + \|B\|$, $\|AB\| \leq \|A\| \, \|B\|$, $\|\lambda A\| = |\lambda| \, \|A\|$, $\|A\| = 0 \Rightarrow A = 0$.

All these properties carry over from properties for bounded linear operators on a Hilbert space, although $\mathcal{A}_{\text{loc}}$ is not obviously a set of operators on a Hilbert space. By definition, a $C^*$-algebra is an algebra with all these properties which, in addition, is complete for the norm topology. Later we will use this compeltion denoted by $\mathcal{A}_{\mathbb{Z}^d} = \overline{\mathcal{A}_{\text{loc}}}$, or $\mathcal{A}$ for short.



## States

For any algebra of observables $\mathcal{A}$ as above (e.g., $\mathcal{A}_\Lambda$, $\mathcal{A}_{\text{loc}}$, or $\mathcal{A}_{\mathbb{Z}^d}$), a state on $\mathcal{A}$ is linear functional $\omega : \mathcal{A} \to \mathbb{C}$ with the following two properties:

Positivity: $\omega(A^* A) \geq 0$, for all $A \in \mathcal{A}$;

Normalization: $\omega(\mathbb{1}) = 1$.

finite dimensional, it yields the set of all the density matrices.

### Theorem

*Let* $\mathcal{H} = \mathbb{C}^n$ *and* $\omega$ *a state on* $\mathcal{B}(\mathcal{H})$*, then there exists a unique density matrix* $\rho \in \mathcal{B}(\mathcal{H})$ $(\rho \geq 0, \operatorname{Tr}\rho = 1)$ *such that* $\omega(A) = \operatorname{Tr}\rho A$*, for all* $A \in \mathcal{B}(\mathcal{H})$*.*

The proof is an exercise.

# Bloch sphere

Example/Exercise:
Let $\mathcal{H} = \mathbb{C}^2$. Then all states $\omega$ on $\mathcal{B}(\mathcal{H}) \cong M_2(\mathbb{C})$ are of the form

$$\omega(A) = \mathrm{Tr}\rho A, \quad \rho = \begin{pmatrix} r & \overline{\mu} \\ \mu & 1-r \end{pmatrix} \tag{1}$$

where $r \in [0,1]$ and $\mu \in \mathbb{C}$ s.t. $|\mu|^2 \leq r(1-r)$. The parameters have a simple interpretation in terms of the basic observables

$$(S^1, S^2, S^3) = \tfrac{1}{2}(\sigma^1, \sigma^2, \sigma^3) \tag{2}$$

$$\mathrm{Tr}\rho S^1 = \mathrm{Re}\,\mu, \quad \mathrm{Tr}\rho S^2 = \mathrm{Im}\,\mu, \quad \mathrm{Tr}\rho S^3 = r - \tfrac{1}{2} \tag{3}$$

Exercise: $\rho$ is a rank-1 projection and $\omega = \langle\psi, \cdot\psi\rangle$ for a unit vector $\psi \in \mathcal{H}$ iff $|\mu|^2 = r(1-r)$.



# General Properties of States

### Theorem

*Let $\omega$ be a state on $\mathcal{A}$. Then:*

1. $\omega(A^*) = \overline{\omega(A)}$
2. $|\omega(A^*B)|^2 \leq \omega(A^*A)\omega(B^*B)$ *(Cauchy-Schwarz ineq.)*
3. $|\omega(A)| \leq \|A\|$
4. $|\omega(A^*BA)| \leq \|B\|\omega(A^*A)$

For proofs of these properties in the case of arbitrary $\mathcal{A}$, see Bratteli & Robinson, vol 1.
The set of all states on a given algebra $\mathcal{A}$ is convex. The extreme points of this set are called pure states.

## Hamiltonian Dynamics

A quantum spin model is typically defined by specifying for a family of finite $\Lambda$, the Hamiltonian: $H_\Lambda = H_\Lambda^* \in \mathcal{A}_\Lambda$. Then, $U_t = e^{-itH_\Lambda}$, is unitary for all $t \in \mathbb{R}$.

The dynamics on $\mathcal{A}_\Lambda$ is defined by

$$\alpha_t(A) = U_t^* A U_t \tag{4}$$

The maps $\alpha_t$ have the following properties:

- $\alpha_t : \mathcal{A}_\Lambda \to \mathcal{A}_\Lambda$ is linear;
- $\alpha_t(AB) = \alpha_t(A)\alpha_t(B)$
- $\alpha_t(A^*) = \alpha_t(A)^*$
- $\alpha_t(\mathbb{1}) = \mathbb{1}$
- $\|\alpha_t(A)\| = \|A\|$, $\forall A \in \mathcal{A}_\Lambda$

These properties characterize each $\alpha_t$ as an automorphism of the $C^*$-algebra $\mathcal{A}_\Lambda$.



Furthermore, the family $\{\alpha_t \mid t \in \mathbb{R}\}$ has the properties

- $\alpha_0 = \mathrm{id}$;
- $\alpha_t \alpha_s = \alpha_{t+s}$, for all $t, s \in \mathbb{R}$;
- $\lim_{t\to 0} \|\alpha_t(A) - A\| = 0$, for all $A \in \mathcal{A}_\Lambda$

We say that $\{\alpha_t\}$ a strongly continuous one-parameter group of automorphisms of $\mathcal{A}_\Lambda$. This dynamics on observables is the so-called Heisenberg picture. $A_t = \alpha_t(A)$ satisfies the Heisenberg equation

$$\frac{d}{dt} A_t = i[H, A_t] \equiv i\delta(A_t) \tag{5}$$

and

$$\alpha_t = e^{it\delta} = e^{it[H,\cdot]} \tag{6}$$

$\delta$ is a derivation on $\mathcal{A}_\Lambda$: It is linear and $\delta(AB) = \delta(A)B + A\delta(B)$.

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The Schrödinger picture is given by $\psi_t = U_t\psi_0$, which is the solution of the Schrödinger equation:

$$\frac{d}{dt}\psi_t = -iH_\Lambda\psi_t$$

In the case of $\dim\mathcal{H} = \infty$, and $H$ a densely-defined (unbounded) self adjoint operator, this equation can still be solved by a group of unitaries $U_t = e^{-itH}$.

### Theorem (Stone's Theorem)

*Let $U_t$ be a strongly continuous one-parameter group ($\lim_{t\to 0} U_t\psi = \psi$, for all $\psi$) of unitaries on $\mathcal{H}$. Then there exists a s.a. operator $H$ with dense domain $\mathrm{Dom}(H)$ such that*

$$U_t = e^{-itH} \tag{7}$$

*and such that for all $\phi \in \mathrm{Dom}(H)$, $\lim_{t\to 0}\frac{U_t\phi-\phi}{t} = -iH\phi$*

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## The Heisenberg Model

Example:
For $x, y \in \mathbb{Z}^d$, let $|x - y|$ denote the lattice distance between $x$ and $y$. $x$ and $y$ are called nearest neighbors if $|x - y| = 1$. Let $\mathcal{H}_x = \mathbb{C}^2$, for all $x$.
The Hamiltonians of the spin-$1/2$ (homogeneous and isotropic) Heisenberg ferromagnet on $\Lambda$ is given by

$$H_\Lambda = -\sum_{x,y\in\Lambda,|x-y|=1} \mathbf{S}_x \cdot \mathbf{S}_y \tag{8}$$

where $\mathbf{S} = (S^1, S^2, S^3) = \frac{1}{2}(\sigma^1, \sigma^2, \sigma^3)$ and the subscript $x$ denotes that $S^i$ is considered as an element of $\mathcal{A}_{\{x\}}$.

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## Ground states and the spectral gap

Some of the first and most important questions to address about the Hamiltonians $H_\Lambda$ are the 1) what is the number of ground states, 2) what is the magnitude of the spectral gap above the ground state energy, and 3) what are the salient features of the ground states and low-lying excited states.
Ground state: eigenvector with eigenvalue $E_0 = \inf \mathrm{spec} H$.
Spectral gap above the ground state: if $\dim \mathcal{H}_\Lambda < \infty$, and $H$ has eigenvalues $E_0 < E_1 < E_2 < \ldots$, we define $\gamma = E_1 - E_0 > 0$. In general

$$\gamma = \sup\{\delta \geq 0 \mid \mathrm{spec} H_\Lambda \cap (E_0, E_0 + \delta) = \emptyset\} \geq 0 .$$

If $E_0$ is simple, one says that the system has a unique (or non-degenerate) ground state.

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## Back to the spin $1/2-$ Heisenberg Model

The Hamiltonian is

$$H_\Lambda = -J \sum_{|x-y|=1, x,y\in\Lambda} \mathbf{S}_x \cdot \mathbf{S}_y$$

with $J > 0$ ($J < 0$) corresponding to the (anti-)ferromagnet. It is useful the introduce $\sigma^\pm$ such that

$$\sigma^1 = \sigma^+ + \sigma^-, \quad \sigma^2 = i(\sigma^- - \sigma^+).$$

Then

$$\mathbf{S}_x \cdot \mathbf{S}_y = \frac{1}{2}(\sigma_x^+ \sigma_y^- + \sigma_x^- \sigma_y^+) + \frac{1}{4}\sigma_x^3 \sigma_y^3 = \frac{1}{2} t_{xy} - \frac{1}{4}\mathbb{1}.$$

where $t_{xy} \in \mathcal{A}_{\{x,y\}}$ acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$ as the swap of the two tensor factors: $t(u \otimes v) = v \otimes u$.

Clearly the ground states of the ferromagnetic model are the eigenvectors with smallest eigenvalue of the operator

$$\tilde{H}_\Lambda = - \sum_{|x-y|=1, x,y\in\Lambda} t_{xy}$$

Consider $\Lambda$ as a graph with $N$ vertices $x \in \Lambda$ and $E$ edges $(xy)$ given by the nearest neighbor pairs.

### Theorem

*Suppose $\Lambda$ considered as a graph is connected. Then, the smallest eigenvalue of $\tilde{H}_\Lambda$ is $-E$ and its eigenspace has dimension $N + 1$ and consist of all vectors symmetric under permutations of the vertices.*



## Proof

Let $\{e_-, e_+\}$ be an o.n. basis of $\mathbb{C}^2$, and $\lambda_0(A)$ the smallest eigenvalue of a matrix $A$.

Observation 1)

For any Hermitian operators, $\lambda_0(A + B) \geq \lambda_0(A) + \lambda_0(B)$. (For any hermitian matrix the lowest eigenvalue satisfies the variational principle $\lambda_0(A) = \inf_{\psi\neq 0}\langle A\rangle_\phi$. Thus $\lambda_0(A + B) = \inf_{\psi\neq 0}\langle A + B\rangle_\psi$, while for any $\psi$, $\langle A + B\rangle_\psi = \langle A\rangle_\psi + \langle B\rangle_\psi \geq \lambda_0(A) + \lambda_0(B)$, which proves the observation.) Apply this to $\tilde{H}$ to obtain $\lambda_0(\tilde{H}) \geq -E$.

Observation 2)

$$\tilde{H}(\bigotimes_{x\in\Lambda} e_+) = -E \bigotimes_{x\in\Lambda} e_+$$

which implies that $\lambda_0(H)$ does equal $-E$.

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Observation 3) If $\lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$ then $(A+B)\phi = \lambda_0(A+B)$ implies $A\phi = \lambda_0(A)\phi$ and $B\phi = \lambda_0(B)\phi$. (For a hermitian matrix $A$, $\psi$ is an eigenvector for $\lambda_0(A)$ iff $\langle A\rangle_\psi = \lambda_0(A)$. Now suppose $\lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$ and $\phi$ is a ground state for $A+B$. Then

$$\langle A\rangle_\phi + \langle B\rangle_\phi = \langle A+B\rangle_\phi = \lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$$

Also, $\langle A\rangle_\phi \geq \lambda_0(A)$ and $\langle B\rangle_\phi \geq \lambda_0(B)$. So we have $\langle A\rangle_\phi = \lambda_0(A)$ and $\langle B\rangle_\phi = \lambda_0(B)$. And this implies $A\phi = \lambda_0(A)\phi$ and $B\phi = \lambda_0(B)\phi$.) Apply this to determine $H\phi = -E\phi$ only if $t_{xy}\phi = \phi$ for all $(xy) \in \Lambda$.

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Observation 4) If $\Lambda$ is a connected graph then any permutation of its vertices, $\pi$, can be written as a product of transpositions $\tau_{xy}$ where $(xy)$ is an edge in the graph. Apply this to deduce that for any ground state $\phi$, $U_\pi\phi = \phi$ for all permutations $\pi$, where $U_\pi$ is the unitary determined by its action on simple tensors:

$$U_\pi(v_1 \otimes \cdots \otimes v_N) = v_{\pi_1} \otimes \cdots \otimes v_{\pi_N}$$

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So, all ground states have to be permutation-invariant vectors, and vice-versa if $U_\pi \phi = \phi$ for all $\pi$ then $t_{xy}\phi = \phi$ for all $x, y$ (because $t_{xy} = U_{\tau_{xy}}$). An o.n. basis of permutation invariant vectors is given by

$$\psi_k = \frac{1}{N!} \sum_{\pi \in \mathrm{Perm}(\Lambda)} U_\pi((\underbrace{e_- \otimes \cdots \otimes e_-}_{k}) \otimes \underbrace{(e_+ \otimes \cdots \otimes e_+)}_{N-k})$$

for $k = 0, 1, \cdots, N$.
This is also the maximum spin irreducible representation contained in $\otimes_{x \in \Lambda} \mathcal{D}^{(1/2)}$. More about that later.

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(Let $\mathcal{G}$ be the group generated by $\{\tau_{xy} : (xy) \in \Lambda\}$. Prove by induction that $\tau_{xy} \in \mathcal{G}$ for all $i$ and $j$, vertices in $\Lambda$. Induction is on

$$d(x, y) = \min\{n : (xx_2), (x_2x_3), \ldots, (x_{n-1}y) \in \Lambda\}$$

For $d(x, y) = 0$ it is trivial that $\tau_{xx} = id \in \mathcal{G}$. For the induction step assume that $\tau_{xy} \in \mathcal{G}$ whenever $d(x, y) \leq n$. If $d(x, y) = n + 1$ let $x_2, \cdots, x_n$ be a sequence s.t. $(xx_2), \ldots, (x_ny) \in \Lambda$. Then $\tau_{xx_n}, \tau_{x_ny} \in \mathcal{G}$ by the induction hypothesis. So $\tau_{xy} = \tau_{x_ny}\tau_{xx_n}\tau_{x_ny} \in \mathcal{G}$. Since the permutation group is generated by all transpositions, $\mathcal{G} = \mathrm{Perm}(\{x : x \in \Lambda\})$.)