Lecture I

Quantum many-body systems

Many-body problem in cond. matter & q. chemistry:

- N electrons w/ charge $-e$
- K nuclei w/ charge $P_k e$, $\sum P_k = N$, mass m_k.

→ Solve many-body Schrödinger eq. $H\psi = E\psi$,

$$H = -\frac{1}{2m_e}\sum_u \Delta_u^e - \sum_k \frac{1}{2m_k}\Delta_k^m + \sum_{u,u'}{}' \frac{e^2}{|r_u - r_{u'}|} + \sum_{u,k} \frac{-P_k e^2}{|r_u - R_k|} + \sum_{k,k'} \frac{P_k P_{k'} e^2}{|R_k - R_{k'}|}$$

→ describes solids, gases, liquids, molecules, ...

Huge no. of degrees of freedom → extremely complicated.

Approximations:

- Most electrons form filled shells

  → good approx.: ions + outer electrons.

• Nuclei much heavier than electrons:

Consider electrons in static potential of nuclei (and nuclei in eg. energy landscape of electrons):

→ Born-Oppenheimer-approx.

→ N-electron problem:

$$H = \frac{-1}{2m}\sum_{k=1}^{N} \Delta_k + \sum_{k,k'}{}' \frac{e^2}{|r_k - r_{k'}|} + \sum_k V(r_k)$$

(V: potential of nuclei)

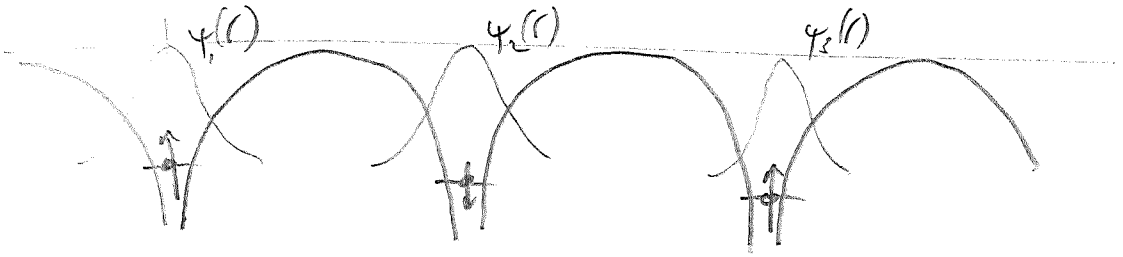
Solids: Nuclei form lattices at low enough temperatures:

→ periodic lattice potential $V(r)$.

Many conductive + magnetic props given by electrons in nuclear potential $V(r)$.

Specific scenario of interest:

1 electron / nucleus + deep potential $V(r)$:



→ Electrons tightly bound to "their" nucleus ("tight-binding approximation") → insulators.

Typ. happens with all and f electrons.

Spatial degree of freedom of electrons frozen.

Remaining DoF: spin of electrons ⟹ Quantum spin system.

(Note: There are other ways to get spin systems.)

What is the Hilbert space of such a system?

Electron orbitals (without spin) are $\psi_1(r), \psi_2(r), \dots$

Assume they are orthogonal: $\int \psi_i^*(r)\,\psi_j(r)\,dr = 0$.

Wavefunction for electron w/ spin $s = \uparrow, \downarrow$:

$$\Psi(r,s) = \underbrace{\psi(r)}_{\text{spatial part}} \otimes \underbrace{|\chi(s)\rangle}_{\text{spin part}}$$

$$|\chi(s)\rangle = \chi(\uparrow)\,|\uparrow\rangle + \chi(\downarrow)\,|\downarrow\rangle = \begin{pmatrix} \chi(\uparrow) \\ \chi(\downarrow) \end{pmatrix} \in \mathbb{C}^2$$

$$\leftrightarrow\quad \Psi(r,s) = \begin{pmatrix} \chi(\uparrow)\,\psi(r) \\ \chi(\downarrow)\,\psi(r) \end{pmatrix}.$$

N electrons: Slater determinant:

$$\Psi(r_1, s_1, r_2, s_2, \dots) = \sum_{\pi} \sigma(\pi)\, \psi_1(r_{\pi(1)})\, \psi_2(r_{\pi(2)}) \cdots \times$$

$$|\chi_1(s_{\pi(1)})\rangle \otimes |\chi_2(s_{\pi(2)})\rangle \otimes \dots \Big]$$

ψ_i orthogonal $\longrightarrow$ electron at site i ($=$ in state ψ_i)
is in spin state $|\chi_i\rangle \equiv |\chi_i(s)\rangle$.

Spatial part is fixed $\longrightarrow$ can be omitted!

<u>Interesting part:</u> Spin DoF

$$\Psi(s_1, \dots, s_N) = |\chi_1(s_1)\rangle \otimes |\chi_2(s_2)\rangle \otimes \dots$$

(s_i: spin of electron at site i)

<u>Basis states:</u>

Spin configurations $|\dots\uparrow,\uparrow,\uparrow\rangle, |\dots,\uparrow,\uparrow,\downarrow\rangle, |\dots,\uparrow,\downarrow,\uparrow\rangle, \dots$

$\longrightarrow$ all states $|s_1, s_2, \dots, s_N\rangle$ $\left(s_k = \uparrow,\downarrow \text{ or } s_k = 0,1\right)$.

Superposition principle:

Any state

$$|\phi\rangle = \sum_{s_i = 0,1} c_{s_1,\dots,s_N} |s_1, s_2 \dots s_N\rangle$$

is a valid state!

$\rightarrow$ 2^N dim. Hilbert space $\mathcal{H} = \mathbb{C}^{2^N}$ w/ basis $|s_1,\dots,s_N\rangle$.

$\mathcal{H}$ has a natural tensor product structure:

$$|s_1, s_2 \dots, s_N\rangle = |s_1\rangle \otimes |s_2\rangle \otimes \dots \otimes |s_N\rangle$$

($|s_1\rangle$: each component = 1 lattice site.)

$$\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2.$$

Vector notation & tensor prod. basis:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \leftarrow |00\rangle$$

$$|0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \leftarrow |01\rangle \leftarrow |10\rangle \leftarrow |11\rangle \dots \text{ etc.}$$

Note: Such tightly bound, localized spins are often responsible for magnetic behavior (in particular in insulators)

Up to now: no interactions → not so interesting.

How do we get interactions?

Many mechanisms:
- directly via overlap of WFs
- via intermediate atom + el. orbital
- via Sea of electrons (RKKY)
- ⋮

Important: Interactions typ. couple only nearby spins!

What could be a "typical" interaction of 2 spins?

Interaction Ham. of 2 spins:

$$h: \mathbb{C}^2 \otimes \mathbb{C}^2 \longrightarrow \mathbb{C}^2 \otimes \mathbb{C}^2.$$

h can be any function of the spin operators:

$$S_x = \frac{1}{2}\sigma_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad S_y = \frac{1}{2}\sigma_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad S_z = \frac{1}{2}\sigma_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$\vec{S} = (S_x, S_y, S_z).$$

On tensor products:

$$S_x^1 = S_x \otimes \mathbb{1} \qquad \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(S_x on 1'st spin) (also: II, Id)

$$S_x^2 = \mathbb{1} \otimes S_x \quad \text{etc.}$$

Attention: No preferred axis → rot. inv. Ham.!

→ Rot. inv. expression in $\vec{S}_1$ and $\vec{S}_2$.

$$\Rightarrow h = J_{12}\, \vec{S}_1 \cdot \vec{S}_2 = J_{12}\left(S_x \otimes S_x + S_y \otimes S_y + S_z \otimes S_z\right)$$

⇒ Heisenberg interaction! → Rot. comm.!

Explicit form:

$$h = \frac{1}{4}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} & \\ & \end{pmatrix} \otimes \begin{pmatrix} & \\ & \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$

$$= \frac{1}{4}\left[\begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix} + \begin{pmatrix} & & & -1 \\ & & 1 & \\ & 1 & & \\ -1 & & & \end{pmatrix} + \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}\right]$$

$$= \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} \begin{matrix} \leftarrow |00\rangle \\ \leftarrow |01\rangle \\ \leftarrow |10\rangle \\ \leftarrow |11\rangle \end{matrix}$$

Eigenvalues:

$$h|00\rangle = \frac{1}{4}|00\rangle$$

$$h|11\rangle = \frac{1}{4}|11\rangle$$

on $|01\rangle, |10\rangle$ subspace:

$$h' = \frac{1}{4}\begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \begin{matrix} \leftarrow |01\rangle \\ \leftarrow |10\rangle \end{matrix}$$

$$h\,\frac{|01\rangle \pm |10\rangle}{\sqrt{2}} = \frac{1}{4}\,\frac{-|01\rangle + 2|10\rangle \pm 2|01\rangle \mp |10\rangle}{\sqrt{2}}$$

$$= \begin{cases} \frac{1}{4} & \frac{|01\rangle + |10\rangle}{\sqrt{2}} \\ \frac{1}{4} \cdot & \frac{-3|01\rangle - 3|10\rangle}{\sqrt{2}} \end{cases}$$

$\Rightarrow$ triplet state $|00\rangle, |11\rangle, \frac{|01\rangle + |10\rangle}{\sqrt{2}}$ with spin 1

have $h|\psi\rangle = +\frac{1}{4}|\psi\rangle$

singlet state $\frac{|01\rangle - |10\rangle}{\sqrt{2}}$ with spin 0

has $h|\psi\rangle = -\frac{3}{4}|\psi\rangle$.

$J_{12} > 0$: antiferromagnetic interaction (energy of $|01\rangle + |10\rangle$ (a))

$J_{12} < 0$: ferromagnetic ——"—— (energy of $|00\rangle, |11\rangle, \ldots$ (a))

(N.B.: $|01\rangle + |10\rangle$ must also have low energy if we want that parallel spins in all directions have low e.)

Heisenberg model on lattice:

Interaction between all NN on lattice:

$$H = \sum_{\langle ij \rangle} h_{ij}$$

$\langle ij \rangle$ ← nearest neighbors

$$h_{ij} = \sum_{\alpha = x,y,z} \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes S_{i,\alpha} \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes S_{j,\alpha} \otimes \mathbb{1} \ldots$$

Lattices can be 3D, but also 1D or 2D (e.g. in layered Materials where interactions are only mediated in certain directions)

Interactions can also appear between NNN etc:

$$H = \sum J_{ij} \vec{S}_i \cdot \vec{S}_j \,, \quad J_{ij} \text{ rapidly decaying w/ distance } d(i,j).$$

General feature: interactions decay rapidly w/ distance!

Other interactions also possible, e.g.

Ising: $\sigma_z \otimes \sigma_z$

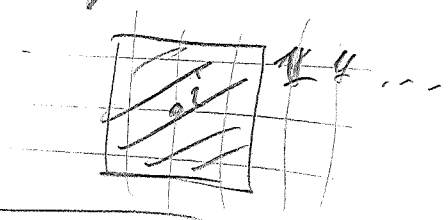
XY: $\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y$

XXZ: $\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \gamma \sigma_z \otimes \sigma_z$

General interactions: Local Hamiltonian

$h_i \equiv h_i \otimes \mathbb{1}$

h_i: acts on spins around i; $\mathbb{1}$: on all other spins.



$$H = \sum_i h_i .$$ ⟹ local spin system.

What are the consequences of locality in QIS systems?

[Note: Local fermionic models can be defined in a similar manner.]