Entanglement in Quantum Many-Body Systems

I. Background

1. The quantum many-body problem and quantum spin systems

Further reading: W. Nolting, A. Ramakanth: Quantum Theory of Magnetism (Springer 2009)

a) The quantum many-body problem

The non-relativistic quantum many body (QMB) problem (solids, molecules, chemical reactions, electric/magn./thermodynamic/mechanical properties of materials, ...):

Given:

N electrons w/ charge $-e$, mass m_e

K nuclei w/ charge $Z_k \cdot e$, $\sum Z_k = N$, mass M_k

solve the many-body Schrödinger equation

$$H\psi = E\psi,$$

$$H = \sum_n \left(-\frac{\hbar^2}{2m_e} \Delta_n^{el.} \right) + \sum_k \left(-\frac{\hbar^2}{2M_k} \Delta_k^{nucl.} \right) +$$

$$+ \sum_{n,n'} \frac{e^2}{|r_n - r_n'|} + \sum_{k,k'} \frac{Z_k Z_{k'} e^2}{|R_k - R_{k'}|} + \sum_{n,k} \frac{-Z_k e^2}{|r_n - R_k|}$$

Wave-function $\psi \equiv \psi(r_1, s_1; r_2, s_2; \ldots; R_1, S_1, R_2, S_2, \ldots)$ has huge number of degrees of freedom (DoF) $\rightarrow$ extremely complicated!

Use <u>approximations</u> to solve QMB problem:

- most electrons form <u>filled shells</u>: very stable
  $\rightarrow$ good approx: consider ions + outer electrons (i.e. <u>partly</u> filled shells)

- nuclei <u>much heavier</u> than electrons: For electrons, nuclei look almost <u>static</u>:
  $\Rightarrow$ <u>Born-Oppenheimer-approximation</u>:
  1) solve electron problem for <u>static</u> configuration

of nuclei $R_1, \dots, R_K$

$$H = \frac{-\hbar^2}{2m_e} \sum_n \Delta_n + \sum_{n,n'} \frac{e^2}{|r_n - r_{n'}|} + \sum_n V(r_n)$$

potential of nuclei.

$\Rightarrow$ ground state energy $E_{el}(R_1, \dots, R_K)$.

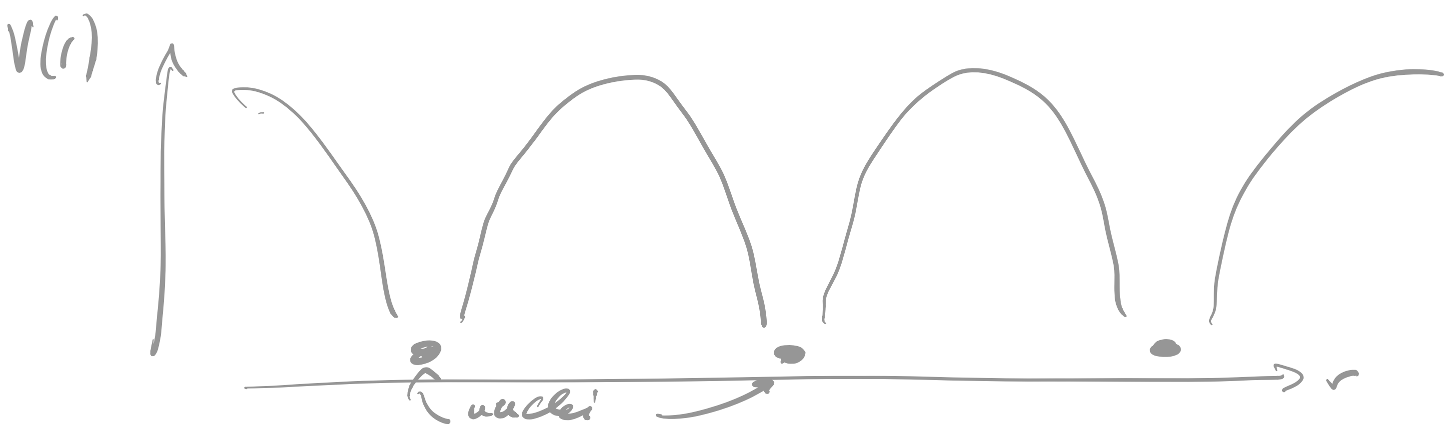
2) Solve nuclei in external potential E_{el}.

b) Lattice systems & quantum spin systems

Solids: Nuclei form lattices at low enough temperatures

$\Rightarrow$ periodic lattice potential $V(r)$ for electrons.

Electric & magnetic properties can be typically understood by studying behavior of electrons in nuclear potential $V(r)$.



In fact, not really a $\frac{1}{r}$ potential, since we have taken out fully filled orbitals.

In addition, there is electrons/orbitals forming the lattice bonds — these are also in a stable (low-energy) state and will not be relevant for electric/magn. props.

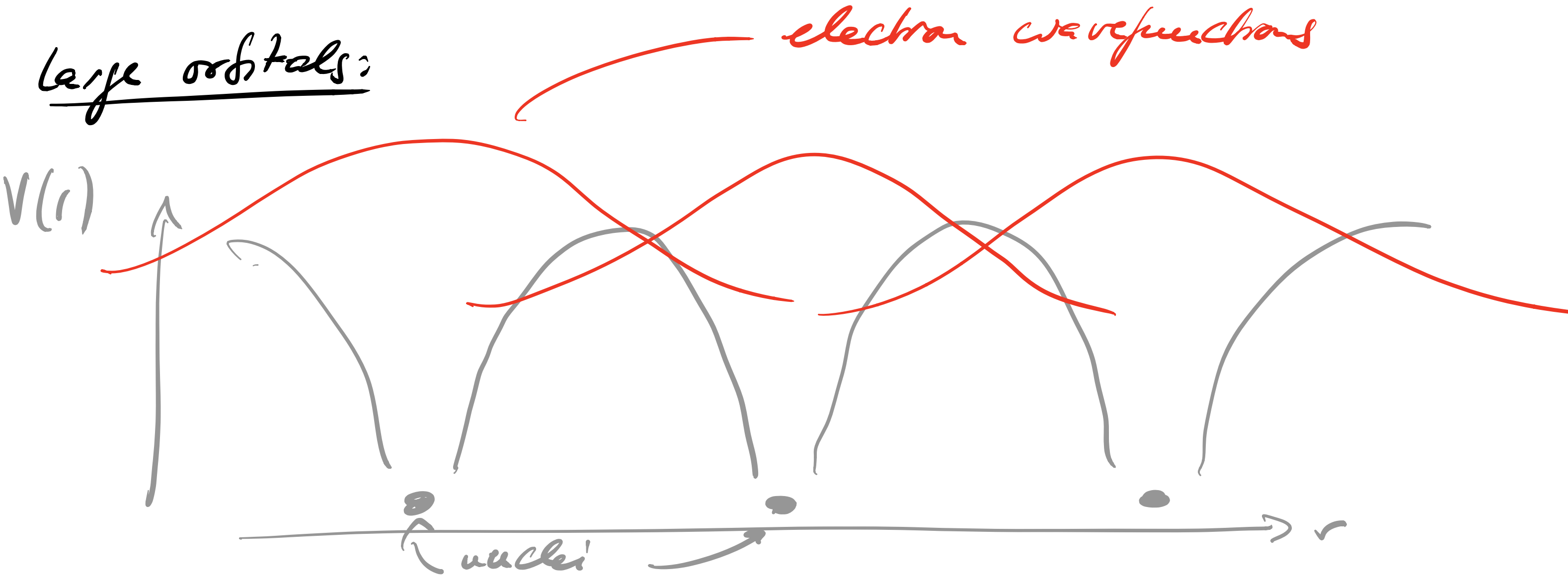
(Note: This can lead to changes in filled vs. partly filled orbitals.)

How do the additional electrons (non-filled shells, not essential for lattice bonds) behave?

Depends on orbital they occupy:

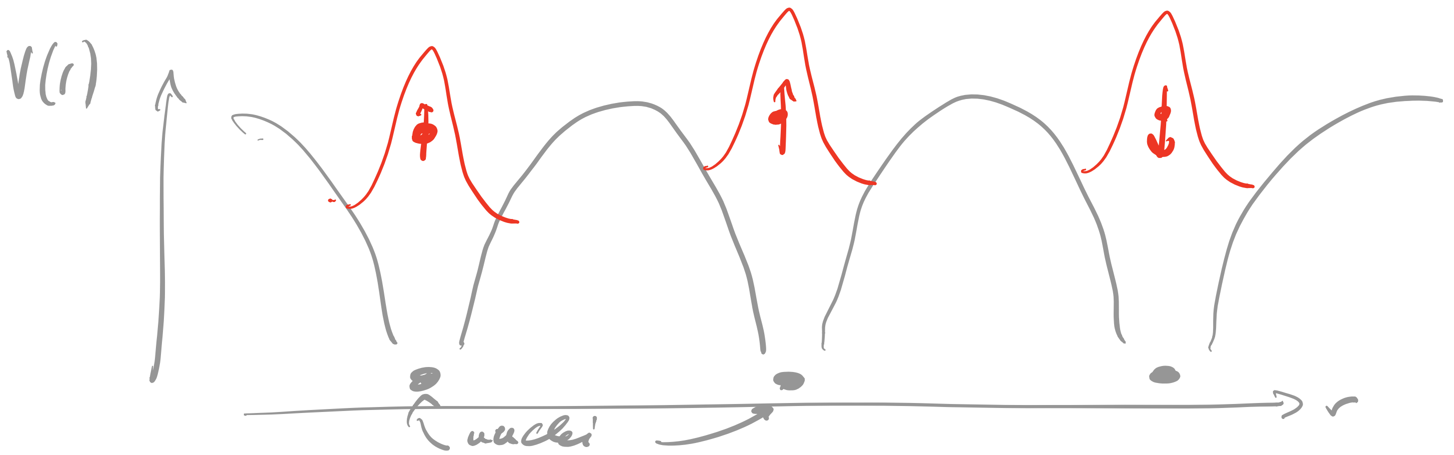
large orbital	small orbital
large principal q. number, thus typ. s, p orbitals.	small principal q. number, typ. d, f orbitals: transition group elements.

large orbitals:



large overlap of wavefunctions $\Rightarrow$ electrons can easily hop to next site $\Rightarrow$ metallic behavior
($\Rightarrow$ band theory!)

small orbitals:



small overlap of wavefunctions $\Rightarrow$ electrons static at "their" nucleus $\Rightarrow$ insulator.

Remaining degrees of freedom: Each electron contributes a spin-$\frac{1}{2}$ DoF

$\Longrightarrow$ **Quantum Spin System.**

(**Note**: Such spins are behind magnetic properties especially of insulators.)

Formally:

Wavefunction for one electron at position R_0:

$$\psi(r,s) = \psi_{R_0}(r) \cdot \chi(s)$$

spin part, $s = \uparrow, \downarrow$.

spatial part:

$$\psi_{R_0}(r) = \tilde{\psi}(r - R_0)$$

$$\left(\text{or:} \quad \psi = \begin{pmatrix} \psi_{R_0}(r) \cdot \chi(\uparrow) \\ \psi_{R_0}(r) \cdot \chi(\downarrow) \end{pmatrix} \right)$$

Note: $\psi_{R_i}(\cdot)$ is fixed by the orbital, but $\underline{\chi(s) \text{ is arbitrary!}}$

N electrons on lattice at $R_0, R_1, \ldots$:

(We can assume states at diff. positions R_i are orthogonal):

Slater determinant for N-electron wavefunction, using states $\psi_{R_1}(r) \cdot \chi_1(r), \psi_{R_2}(r) \cdot \chi_2(r), \ldots$:

$$\Psi(r_1, s_1; r_2, s_2; \dots) =$$

$$= \sum_{\pi} \sigma(\pi)\, \psi_{k_1}(r_{\pi(1)}) \cdot \psi_{k_2}(r_{\pi(2)}) \cdot \dots \cdot \chi_1(s_{\pi(1)}) \cdot \chi_2(s_{\pi(2)}) \cdot \dots$$

Since ψ_{k_i} are orthogonal: Each term in the sum associates electron $\pi(i)$ to position R_i.

The spin DoF $s_{\pi(i)}$ of this electron is in state χ_i.

Thus, we can meaningfully talk of the "spin of the electron at position R_i"!

Furthermore, since $\psi_{k_i}(\cdot)$ is fixed, we can omit it

$\Longrightarrow$ system fully described by spin degrees of freedom,

$$\Psi(s_1, \dots, s_N) = \chi_1(s_1) \cdot \chi_2(s_2) \cdot \dots \cdot \chi_N(s_N).$$

spin at lattice position S_i.

Note: The geometry, i.e. "where" S_i is located, is dictated by the geometry of the underlying lattice.

Note: There is other mechanisms to get a quantum spin system on a lattice, e.g.

- electrons which can freely hop but experience a strong Coulomb repulsion when they are at the same site ("Hubbard model"), in the limit of one electron per site ("half filling").

- optical lattices: periodic potential by standing laser waves where atoms are trapped. Internal states of atoms can make up a 2-level system (or d-level system).

c) Hilbert space of quantum spin systems

Quantum spin system:

$$\Psi(s_1, \dots, s_N) = \chi_1(s_1) \cdot \chi_2(s_2) \cdot \dots \cdot \chi_N(s_N)$$

$\rightarrow$ state obtained from independent spins (Slater det.)

What is the <u>Hilbert space</u> describing the spin system?

<u>Basis states:</u>

$$\chi_i(s) = \begin{cases} \delta_{s,\uparrow} & \text{"spin up state"} \\ \delta_{s,\downarrow} & \text{"spin down state"} \end{cases}$$

Denote this as kets:

$$|\uparrow\rangle, |\downarrow\rangle \quad ; \quad \text{or also } |0\rangle, |1\rangle$$

Then,
$$|\chi_i\rangle = \chi_i(\uparrow)|\uparrow\rangle + \chi_i(\downarrow)|\downarrow\rangle$$
$$= \chi_i(0)|0\rangle + \chi_i(1)|1\rangle \in \mathbb{C}^2$$

<u>Basis for 2 spins:</u>

$$\chi_1(s_1) \cdot \chi_2(s_2) = \begin{cases} \delta_{s_1,0}\,\delta_{s_2,0} = \delta_{s_1 s_2, 00} \\ \delta_{s_1,0}\,\delta_{s_2,1} = \delta_{s_1 s_2, 01} \\ \delta_{s_1 s_2, 10} \\ \delta_{s_1 s_2, 11} \end{cases}$$

or basis kets $\quad |0\rangle \otimes |0\rangle \equiv |0\rangle|0\rangle \equiv |00\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

$|0\rangle \otimes |1\rangle \equiv |0\rangle|1\rangle \equiv |01\rangle \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$|1\rangle \otimes |0\rangle \equiv |1\rangle|0\rangle \equiv |10\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$

$|1\rangle \otimes |1\rangle \equiv |1\rangle|1\rangle \equiv |11\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

General state:

$$|\phi\rangle = \phi_{00}|00\rangle + \phi_{01}|01\rangle + \phi_{10}|10\rangle + \phi_{11}|11\rangle$$

$$\in \mathbb{C}^2 \otimes \mathbb{C}^2 = \left(\mathbb{C}^2\right)^{\otimes 2} \cong \mathbb{C}^4$$

(Note: Contains states not of the form $\chi_1(s_1)\cdot\chi_2(s_2)$)

Basis for N spins:

$|s_1, s_2, \ldots, s_N\rangle$, with $s_i = 0, 1 \quad \forall i$:

$$\left.\begin{array}{l} |00 \ldots 00\rangle \\ |00 \ldots 01\rangle \\ |00 \ldots 10\rangle \\ \quad \vdots \\ |11 \ldots 11\rangle \end{array}\right\} \quad 2^N \text{ orthogonal basis vectors}$$

(Note: If written as vector, order components as here.)

Most general state

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

$$\in \underbrace{\mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2}_{N \text{ times}} = (\mathbb{C}^2)^{\otimes N} \cong \mathbb{C}^{(2^N)}$$

2^N - dimensional vector!

State of a spin system with N spins lives in an exponentially big Hilbert space of dimension 2^N!

More generally, if we have a d-level system, $d \geq 2$, at each lattice site (e.g. optical lattices, effective degrees of freedom), with basis $|0\rangle, \dots, |d-1\rangle$, the state is

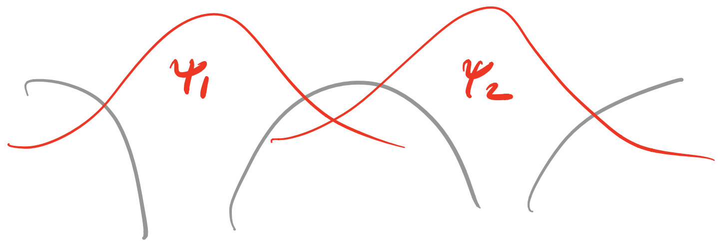
$$|\phi\rangle = \sum_{s_i=0}^{d-1} c_{s_1 \dots s_N} |s_1, \dots, s_N\rangle \in (\mathbb{C}^d)^{\otimes N} \cong \mathbb{C}^{(d^N)}$$

i.e., it lives in a d^N-dim. Hilbert space.

d) Interactions

To study the physics of a quant. system, we need to know its Hamiltonian – here, how the spins interact.

First, consider two spins:



also used in optical lattices!

One possible mechanism (not most common, but easiest to explain): Direct exchange.

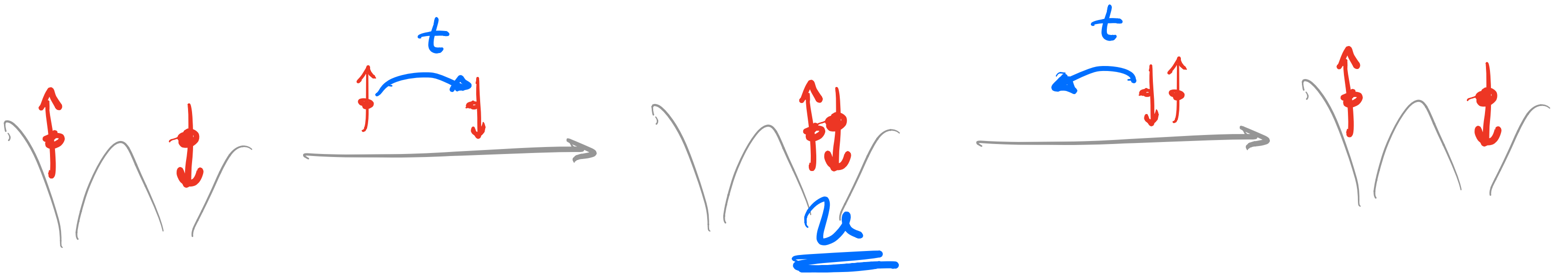
- orbitals ψ_1 and ψ_2 overlap
  $\Rightarrow$ possibility for electron to tunnel from $1 \leftrightarrow 2$
  with tunneling rate t.

- Consider a process where electron 1 tunnels to 2

- Can only happen if the two electrons form a singlet (Pauli exclusion principle),

$$|\phi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)$$

- If both electrons are at the same site, they experience strong Coulomb repulsion U.
- $U \gg t$: ground space has exactly one electron per site, but there is an energy correction from 2nd order perturbation theory:



correction from 2nd order perturbation theory:

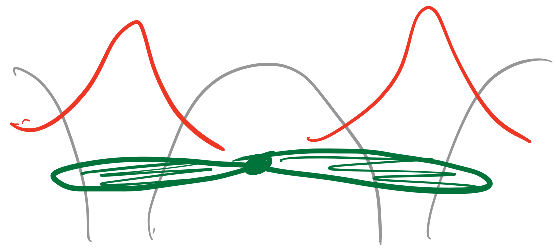
$$\Delta E = -\frac{t^2}{U}$$

- We thus find: energy of singlet state $|\phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ lower by $-\frac{t^2}{U}$

$\Rightarrow$ antiferromagnetic Heisenberg interaction.

The same, or similar, interactions (including ferromagnetic ones) can be obtained from a range of other mechanisms, e.g.

- intermediate orbitals which induce an effective coupling



- coupling through intermediate coupling to a band of electrons — the RKKY interaction (Ruderman - Kittel - Kasuya - Yosida)

What is the <u>general structure of interactions</u> in a quantum spin system?

→ <u>Locality</u>: interactions only couples nearby spin (or strength decays rapidly with distance)

→ <u>few-body</u>: interactions only couple a small number (typ. 2) spins.

→ <u>symmetry</u>: interactions generally have the symmetries of the setup (lattice, ...)

How does a general 2-body interaction look like?

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

Hamiltonian : 4×4 – matrix

We can express h using spin operators:

$$S^x = \frac{1}{2}\sigma^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad S^y = \frac{1}{2}\sigma^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};$$

$$S^z = \frac{1}{2}\sigma^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

and $\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

The spin operator S^α acting on site 2 is given by

$$S_2^\alpha = \mathbb{1} \otimes S^\alpha$$

$$\equiv \mathbb{1}_1 \otimes S_2^\alpha = \begin{array}{cc} \left(\begin{array}{c|c} 1\cdot S_2^\alpha & 0\cdot S_2^\alpha \\ \hline 0\cdot S_2^\alpha & 1\cdot S_2^\alpha \end{array}\right) & \begin{array}{l} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \end{array}$$

Sloppy notation!

$$= \left(\begin{array}{c|c} S_2^\alpha & \\ \hline & S_2^\alpha \end{array}\right)$$

and similarly:

$$S_1^\alpha = S^\alpha \otimes \mathbb{1} \equiv S_1^\alpha \otimes \mathbb{1}_2 ,$$

e.g. $$S_1^x = \frac{1}{2}\left(\begin{array}{c|c} 0\cdot\mathbb{1} & 1\cdot\mathbb{1} \\ \hline 1\cdot\mathbb{1} & 0\cdot\mathbb{1} \end{array}\right) = \frac{1}{2}\left(\begin{array}{c|c} 0 & \begin{smallmatrix}1 & 0 \\ 0 & 1\end{smallmatrix} \\ \hline \begin{smallmatrix}1 & 0 \\ 0 & 1\end{smallmatrix} & 0 \end{array}\right).$$

We can also act with S^α on 1 & S^β on 2:

$$S_1^\alpha \cdot S_2^\beta = S^\alpha \otimes S^\beta$$

$$\equiv S_1^\alpha \otimes S_2^\beta = \frac{1}{2}\left(\begin{array}{c|c} 0 & S_2^\beta \\ \hline S_2^\beta & 0 \end{array}\right).$$

e.g. $S_1^\alpha = S_1^x$

Examples:

$$S_1^x \cdot S_2^x = \frac{1}{4}\begin{pmatrix} 0 & & & 1 \\ & 0 & 1 & \\ & 1 & 0 & \\ 1 & & & 0 \end{pmatrix};$$

$$S_1^y \cdot S_2^y = \frac{1}{4}\begin{pmatrix} & & & -1 \\ & & 1 & \\ & 1 & & \\ -1 & & & \end{pmatrix};$$

$$S_1^z \cdot S_2^z = \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

Note: Rotation (in real space) transforms between S^x, S^y, S^z as it should. The general spin operator in direction $\vec{r} = (r_x, r_y, r_z)$, $\|\vec{r}\| = 1$, is

$$r_x \cdot S^x + r_y S^y + r_z S^z = \vec{r} \cdot \vec{S},$$

with $\vec{S} = (S^x, S^y, S^z)$.

What are some prototypical simple interactions?

- The derivation before — $|\phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ gets energy $-t^2/u$ — is:

$$h = \underbrace{-\frac{t^2}{u}|\phi\rangle\langle\phi|}_{\text{energy } -\frac{t^2}{u} \text{ to } |\phi\rangle,\ 0 \text{ to the other states}} = -\frac{t^2}{u}\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\frac{(0\ 1\ -1\ 0)}{\sqrt{2}}$$

$$= -\frac{t^2}{2u}\begin{pmatrix}0&&&\\&1&-1&\\&-1&1&\\&&&0\end{pmatrix} = \frac{t^2}{2u}\begin{pmatrix}0&&&\\&-1&1&\\&1&-1&\\&&&0\end{pmatrix}$$

- The only fully rotationally invariant interaction:

$$h = J\cdot\left(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z\right)$$

$$\equiv J\cdot\left(\vec{S}_1\cdot\vec{S}_2\right)$$

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

$$= \frac{J}{4}\begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}$$

$$= \frac{J}{4}\left[\begin{pmatrix} 0 & & & \\ & -2 & 2 & \\ & 2 & -2 & \\ & & & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}}_{\text{constant!}}\right]$$

$$= \frac{J}{2}\begin{pmatrix} 0 & & & \\ & -1 & 1 & \\ & 1 & -1 & \\ & & & 0 \end{pmatrix} + \frac{J}{4}$$

$\Rightarrow$ <u>same</u> as $-\frac{t^2}{u}|\phi\rangle\langle\phi|$ (up to constant)

$$\boxed{\text{Heisenberg interaction}}$$

$J>0$: antiferromagnetic

$J<0$: ferromagnetic

Eigenvalues of operator

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}:$$

$1 \times \left(-\frac{3}{4}\right)$, with eigenvector $\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = |01\rangle - |10\rangle$ total spin $= 0$

$3 \times \left(+\frac{1}{4}\right)$, with eigenvectors (total spin $= 1$)

$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle$ $\quad S_z = +1$

$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = |11\rangle$ $\quad S_z = -1$

$\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = |01\rangle + |10\rangle$. $\quad S_z = 0$

Important: To preserve rotational symmetry,

$\frac{|01\rangle + |10\rangle}{\sqrt{2}}$ must go with the ferromagnetic

states: classical intuition misleading!

$\Longrightarrow$ form of quantum correlations

(entanglement) plays an essential role!

Other important interactions:

Ising interaction: $h = S_1^x \cdot S_2^x$

(or $S_1^z \cdot S_2^z, \dots$)

XX interaction: $h = S_1^x \cdot S_2^x + S_1^y \cdot S_2^y$

XXZ interaction: $h = S_1^x \cdot S_2^x + S_1^y \cdot S_2^y + \Delta S_1^z \cdot S_2^z$

... those have a preferred axis/plane.

How do these act on the full N-spin Hilbert space?

$$|\phi\rangle = \sum c_{s_1 \dots s_N} |s_1, s_2, \dots, s_N\rangle$$

$h_{12} |\phi\rangle$ acts only on s_1, s_2, and leaves other s_i invariant:

$$h_{12} |\phi\rangle = \sum c_{s_1 \dots s_N} \left(h | s_1, s_2 \rangle \right) \otimes | s_3, s_4 \dots \rangle$$

$$= \sum c_{s_1 \dots s_N} \left(h_{12} \right)^{s_1' s_2'}_{s_1 s_2} | s_1', s_2', s_3, \dots \rangle$$

That is: h_{12} should be understood as

$$h_{12} \otimes \mathbb{1}_3 \otimes \mathbb{1}_4 \otimes \dots \otimes \mathbb{1}_N .$$

Or we can do this right at the level of spin operators,

$$S_i^\alpha = \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{i-1} \otimes S_i^\alpha \otimes \mathbb{1}_{i+1} \otimes \dots ,$$

and define h_{ij} using these S_i^α, e.g.,

$$h_{ij} = J \, \vec{S}_i \cdot \vec{S}_j .$$

Can couple arbitrary spins this way, but typ. Hamiltonian should be <u>local</u>.

Total Hamiltonian: Sum of all (local) terms,

$$H = \sum_k h_k \overset{\text{e.g.}}{=} \sum J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$

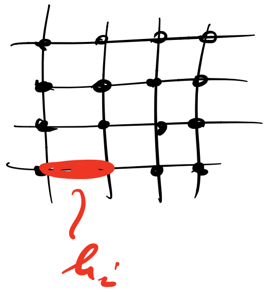
sum over all local terms

should decay with distance.

e) Study of quantum spin systems

Spin system:

$$\mathcal{H} = (\mathbb{C}^d)^{\otimes N} \; ; \quad \text{lattice geometry}$$



$$H = \sum_i h_i \quad \text{local / quasi-local interactions}$$

H is typically transl. invariant, i.e. $h_i \equiv h$, centered at position i – e.g. Heisenberg coupling, ...

time-indep. Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle; \qquad |\psi\rangle \in \mathcal{H}.$$

in particular: lowest eigenvalue E_0 and corresponding eigenvector $|\psi_0\rangle$:

ground state $|\psi_0\rangle$, ground state energy E_0

– describes system at sufficiently low temperatures.

Thermal state

$$\rho = \frac{e^{-\beta H}}{Z} \; ; \quad Z = \mathrm{tr}\left(e^{-\beta H}\right)$$

$$\beta = \frac{1}{kT}$$

significantly more complex than $|\psi_0\rangle$:
$2^N \times 2^N$ - matrix.

For T small enough: $\rho \approx |\psi_0\rangle\langle\psi_0|$.

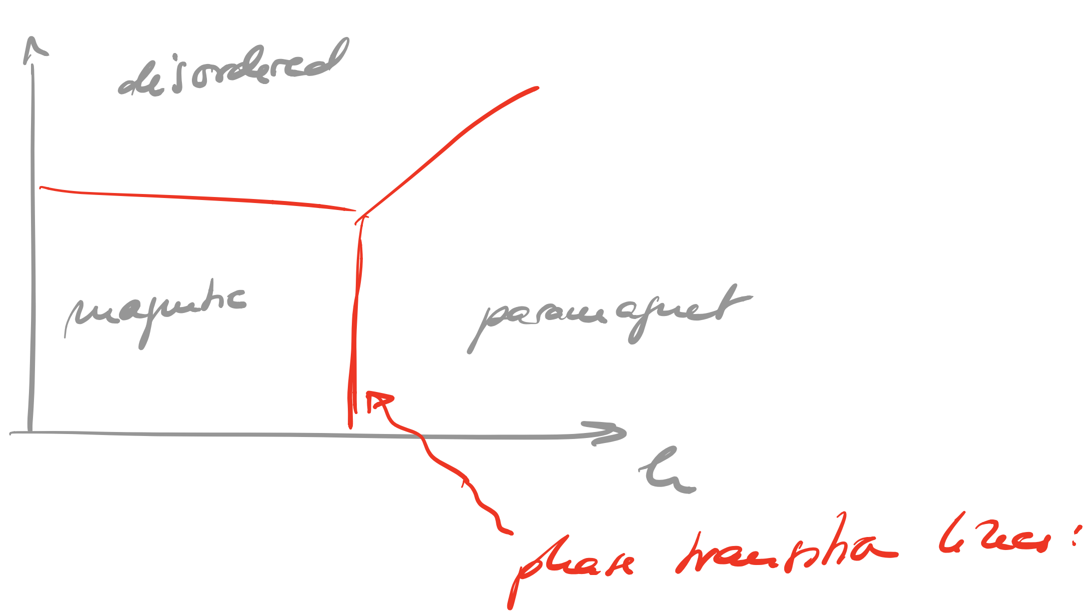
Key questions to ask about system (e.g. for ground or thermal state):

What type of order (phase) does system exhibit?

- long-range magnetic order
- no magnetic order
- other types of order ?!

... as a function of T, or of some parameter in H, such as different couplings, a magnetic field

$$H' = H - h \cdot \sum_i S_i^z \, , \quad \text{or} \quad H' = H - \sum_i \vec{h} \cdot \vec{S}_i \, , \ldots$$

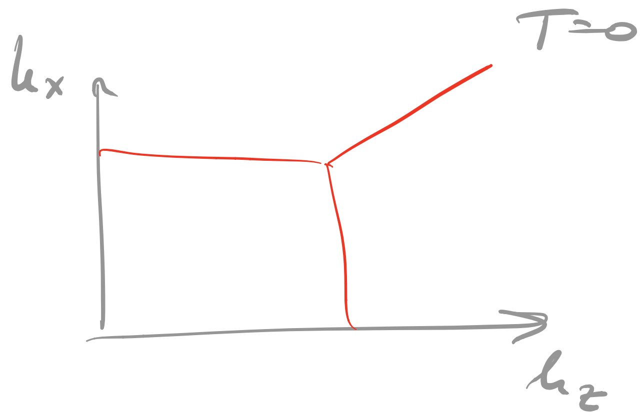


Where are the phase transitions?
What properties do they have?

<u>Focus: Quantum Matter</u> – materials where quantum effects play an <u>essential</u> role.

⇒ this is more prominent at low T
($kT \ll$ energy scales of H (cf. later))
(Why? → cf. later: at large T, quantum correlations – entanglement – vanish.)

⇒ Special interest in physics at $T=0$, i.e. ground state properties & phase diagram.



"quantum phases"

"quantum phase transitions"

(Important point: Are properties at T=0 stable against small T>0 ? → later!)

What properties are we interested in?

- magnetic order:

e.g. average magnetization

$$m = \frac{1}{N}\sum_i \langle \vec{S}_i \rangle = \begin{cases} = 0 \\ \neq 0 \end{cases} ?$$

$\neq 0$ ← ferromagnetic

or, more general,

$$m(k) = \frac{1}{N}\sum_j e^{ikj}\langle \vec{S}_j \rangle = ?$$

e.g. for 2D, $k = (\pi, \pi)$: "staggered magnetization", detects antiferromagnetic order.

- correlations between spins

* $\langle S_i^\alpha \cdot S_j^\beta \rangle$ – typically (transl. inv.) only a function of $i-j$, or even $|i-j|$,

* average $\frac{1}{N} \sum_{ij} \langle S_i^\alpha S_j^\beta \rangle$ ($= O(1)$ if correlations decay exponentially, $O(N)$ with long-rg. order)

* "structure factor" $S(k) = e^{ik(i-j)} \langle S_i^\alpha S_j^\beta \rangle$

→ encodes information about magnetic order

→ $S(k)$ can be measured with neutron scattering

→ behavior of correlations, e.g.

$$\langle S_i^\alpha S_j^\alpha \rangle \sim e^{-|i-j|/\xi}$$

gives <u>correlation length</u> ξ, which diverges phase trans. & gives extra info. about <u>type</u> of transition.

https://www.ericmfischer.com/project/exact-sampling-cluster-sampling/

- ground state energy E_0

By itself meaningless, but derivatives with respect to parameters (fields, ...) encode information

(cf. free energy $F = -kT \ln \underbrace{Z}_{=e^{-\beta H}}$)

e.g.: $H' = H + \lambda V$, e.g. $V = \sum S_i^z$:

$$\left.\frac{dE_0(H')}{d\lambda}\right|_{\lambda=0} = \left.\frac{d}{d\lambda}\right|_{\lambda=0} \left(\langle \psi_0(\lambda) | H + \lambda V | \psi_0(\lambda) \rangle \right)$$

$$= \langle \psi_0(0) | V | \psi_0(0) \rangle$$

(other terms vanish as $\frac{d|\psi_0\rangle}{d\lambda}$ must be orthogonal to $|\psi_0\rangle$ due to normalization)

- Finally, we might also be interested in other questions:
  - time evolution, e.g. after change of H ("quench"), or flipping a spin
    can be meas. w/ in-elastic neutron scattering

- excited states:

$$H|\psi_{k,E}\rangle = E_k\,|\psi_{k,E}\rangle$$

with momentum $\underset{\substack{\uparrow \\ \text{translation operator}}}{T}|\psi_{k,E}\rangle = e^{ik}|\psi_{k,E}\rangle$

- effects of disorder in H
- properties of thermal states
- ... and much more!

For the beginning, key questions will be:

- what is the ground state
- what are its properties

This will also form the basis for many of the other questions.

f) The spectral gap

What characterizes a phase transition?

- Divergence of correlation length
- discontinuity of derivatives of certain quantities.
- ...

Phase transition: Small change in parameters can give rise to large (sudden) change in physical properties – the system is unstable.

Inside a phase: System should only react weakly to small perturbations, i.e. the properties and thus the system are stable against perturbations.

How can we characterize (in-)stability to small perturbations $H \longrightarrow H' = H + \varepsilon V$ in a simple way?

Perturbation theory:

H: ground state $|\psi\rangle$ w/ energy E_0,
ex. states $|\phi_i\rangle$ w/ energy E_i (sorted: $E_i \leq E_{i+1}$)

H': ground state $|\psi'\rangle$

$$|\psi'\rangle = \underbrace{-\varepsilon \sum_i \frac{|\phi_i\rangle\langle\phi_i|V|\psi\rangle}{E_i - E_0}}_{\text{change in state!}} + |\psi\rangle + \ldots$$

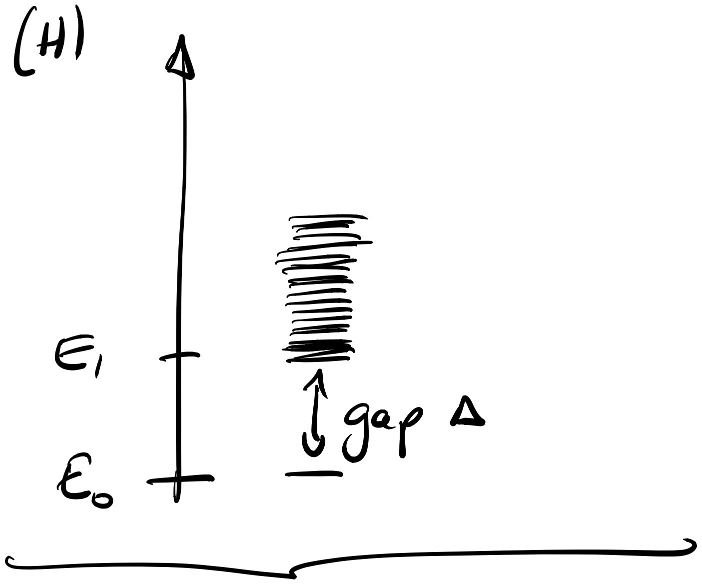
$$\| |\psi'\rangle - |\psi\rangle \| = \varepsilon \cdot \Big| \sum_i \frac{|\phi_i\rangle\langle\phi_i| V|\psi\rangle}{\underbrace{E_i - E_0}_{\geq E_1 - E_0 =: \Delta}} \Big|$$

$$\leq \frac{\varepsilon}{\Delta} \| V|\psi\rangle \|$$

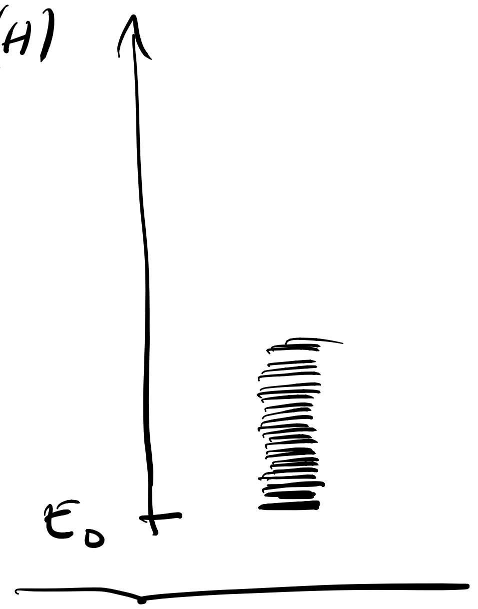
(& higher orders scale with $\left(\frac{\varepsilon}{\Delta}\right)^k$!)

$\Rightarrow$ If the "energy gap" (or: "spectral gap", or "gap") of H is <u>sufficiently large</u>, then

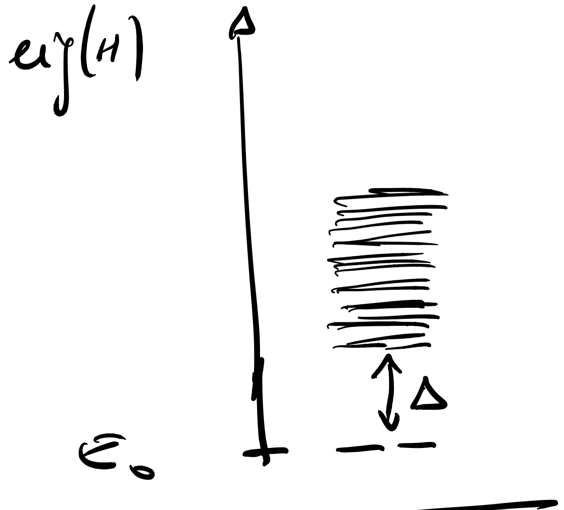
$$\frac{\varepsilon}{\Delta} \ll 1 \quad \text{for} \quad \varepsilon \ll 1 .$$



gapped Hamiltonian



gapless Hamiltonian



gapped with <u>degenerate ground state</u>

Definition: We call a Hamiltonian (better, a family of Hamiltonians)

$$H = \sum_{i=1}^{N} h_i$$

on a lattice of size N **gapped** if the gap $E_1(N) - E_0(N) = \Delta(N)$ on a lattice of size N is lower bounded:

$$\Delta(N) \geq \Delta > 0$$

$$(\text{typ. } \Delta(N) \longrightarrow \Delta).$$

We call Δ the **gap (or energy gap, spectral gap)** of H.

This can also be extended to systems with k degenerate (or almost degenerate, as $N \to \infty$) ground states; then, $\Delta(N) = E_{k+1}(N) - E_k(N)$.

Gapless (or critical) systems are those where

$$\Delta(N) \longrightarrow 0 \quad \left(\text{often, } \Delta(N) \sim \frac{1}{\mathrm{poly}(N)}\right).$$

We can define (gapped) quantum phases as regions in parameter space where H is gapped, and the boundaries (transitions) between them as the lines where H is gapless.

Intuition – cf. above: A gap ensures stability of the phase, as the prefactor $\left(\frac{\varepsilon}{\Delta}\right)^k$ in the perturbation series vanishes.

But this is not rigorous, since typ. V is extensive (e.g.: $H' = H + \varepsilon \underbrace{\sum \sigma_i^z}_{\equiv V}$),

and thus $\| V|\psi\rangle \| \propto N$. Thus, higher order terms can in fact get larger (as the bounds scale as $\left(\frac{\varepsilon}{\Delta}\right)^k N^k!$)

Should still be true if the terms in V don't "conspire".

Proofs of such stability possible in some cases (see, e.g., https://arxiv.org/abs/1001.0344).

g) Setup:

- Quantum spin system $\mathcal{H} = (\mathbb{C}^d)^{\otimes N}$.
- Local Hamiltonian $H = \sum h_i$.
- Determine properties of ground state & spectral properties of H.

Q: How can we deal with the exp. dimension d^N of the underlying Hilbert space $\mathcal{H}$?

Observation: $H = \sum_{i=1}^{N} h_i$ specified by $O(N)$ parameters & we care about ground state $\Rightarrow$ only a small fraction of states in $\mathcal{H}$ actually relevant!

What singles out the relevant states?

$\Rightarrow$ The structure of their q. correlations – entanglement!