

Tensor network methods in many-body physics

I. Introduction

1. The quantum many-body problem

a) The quantum many-body problem

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

Given:

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

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

solve the many-body Schrödinger equation

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

$$H = \sum_u \left(-\frac{\hbar^2}{2m_e} \Delta_u^{el.} \right) + \sum_k \left(-\frac{\hbar^2}{2m_k} \Delta_k^{nuc.} \right) +$$

$$+ \sum_{u, u'} \frac{e^2}{|r_u - r_{u'}|} + \sum_{k, k'} \frac{Z_k Z_{k'} e^2}{|R_k - R_{k'}|} + \sum_{u, k} \frac{-Z_k e^2}{|r_u - R_k|}$$

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

Use approximations to solve QTB problem:

- most electrons form filled shells: very stable
 $\rightarrow$ good approx; consider ions + outer electrons
 (i.e. partly filled shells)
- nuclei much heavier than electrons: For electrons,
 nuclei look almost static:
 $\Rightarrow$ Born-Oppenheimer approximation:
 1) solve electron problem for static 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 $E_e(R_1, \dots, R_K)$.

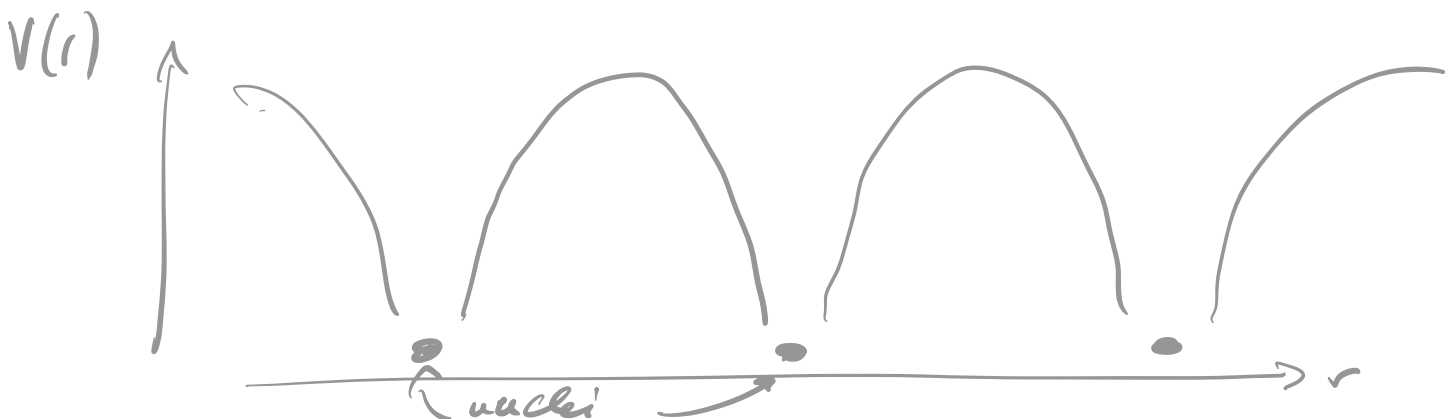
2) Solve nuclei in external potential E_e .

6) 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 bands — these are also in a stable (low-energy) state and will not be relevant for electronic/phys. props.

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

Depends on orbital they occupy:

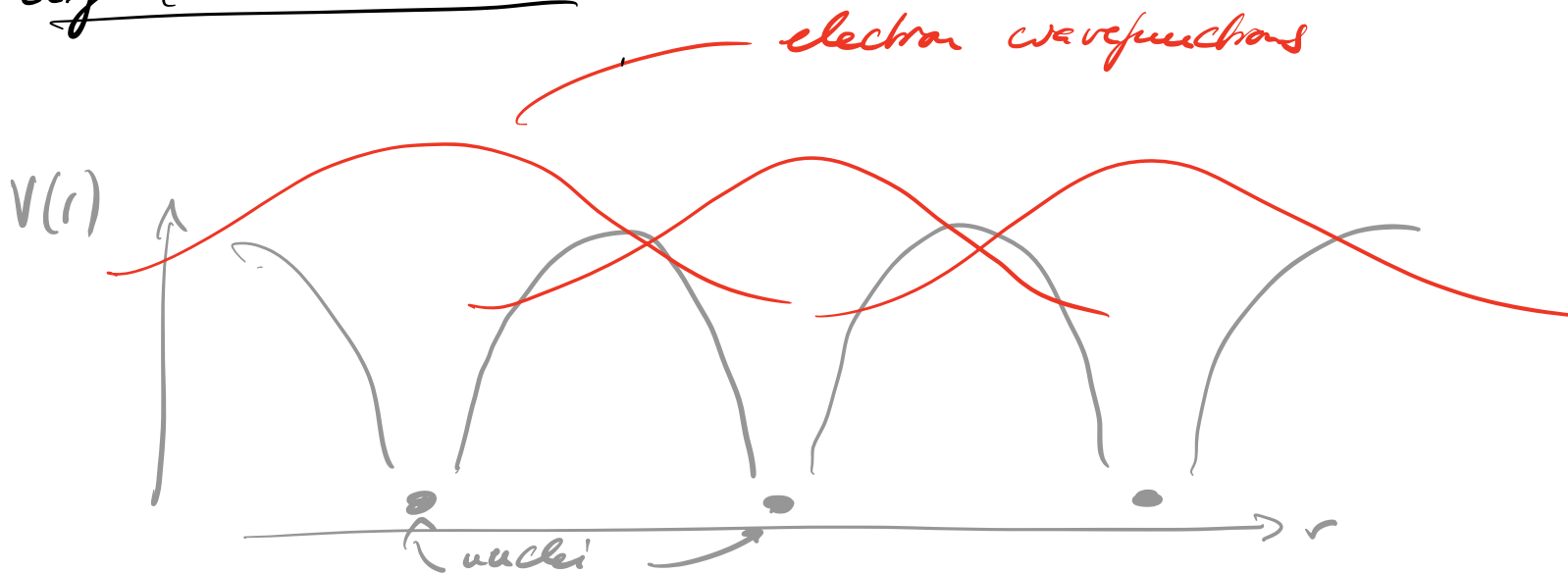
↙
Large orbital

large principal q. number,
thus typ. s, p orbitals.

↘
small orbital

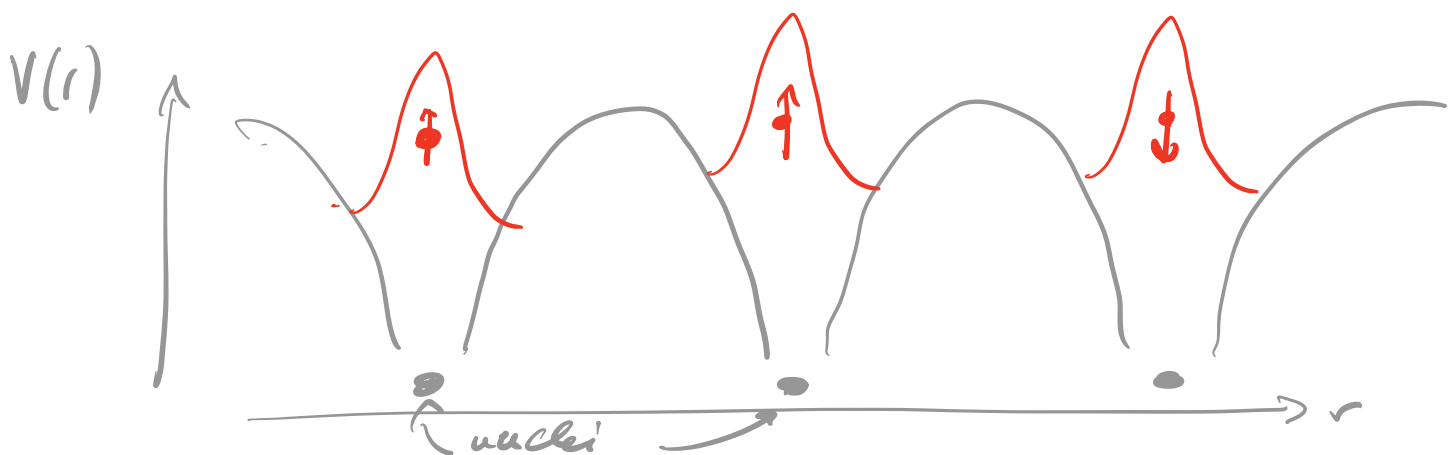
small principal q. number,
typ. d, f orbitals:
transition group elements.

large (delocalized) orbitals:



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

small (localized) 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. Since the electron orbitals at different positions are localized (= essentially orthogonal), we can meaningfully talk of the "spin at lattice site x ".

Quantum Spin System.

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

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).

2. Quantum Spin Systems

a) Hilbert space of quantum spin systems

What Hilbert space (i.e., wavefunction) do we need to describe a quantum spin system?

A single spin can be in two states,

$$|\uparrow\rangle \text{ or } |\downarrow\rangle.$$

We will often use the notation

$$|0\rangle \equiv |\uparrow\rangle \quad \text{and} \quad |1\rangle \equiv |\downarrow\rangle.$$

We can also use a spin notation

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

A general state of one quantum spin is then

$$|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle \in \mathbb{C}^2$$

For two spins, we then have basis states

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

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

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

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

"lexicographic"
ordering:
 $\begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$

A general state of two qubits is then of the form

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

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

(Note: This contains states not of the form $|\phi_1\rangle \otimes |\phi_2\rangle$!)

Basis for N spins:

$$|s_1, s_2, \dots, s_N\rangle, \quad \text{with } s_i = 0, 1 \quad \forall i:$$

$$|00 \dots 00\rangle$$

$$|00 \dots 01\rangle$$

$$|00 \dots 10\rangle$$

$$\vdots$$

$$|11 \dots 11\rangle$$

2^N 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

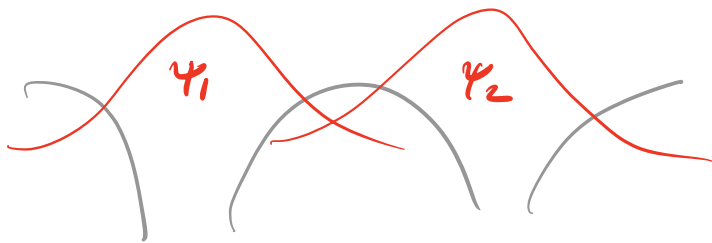
$$|\phi\rangle = \sum_{s_i=0}^{d-1} c_{s_1, \dots, s_N} |s_1, \dots, s_N\rangle \in \underbrace{(\mathbb{C}^d)^{\otimes N}}_{\mathbb{C}^{(d^N)}}$$

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

b) Interactions

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

First, consider two spins:



also used in
optical lattices!

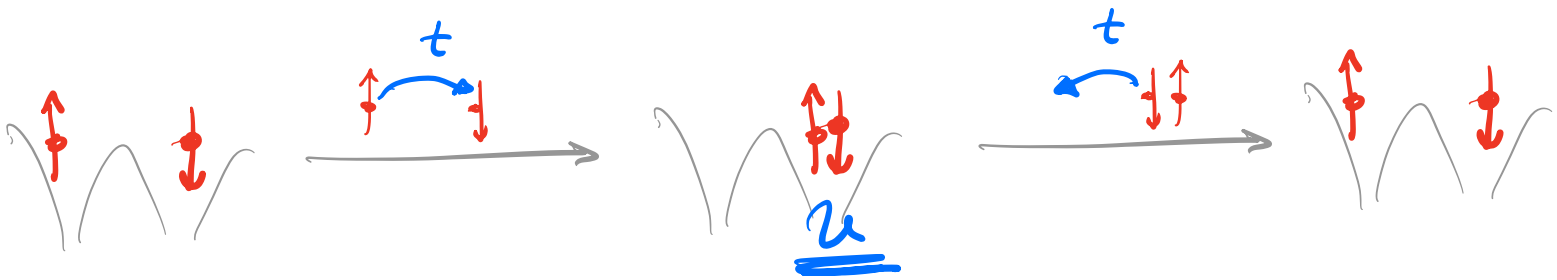
One possible mechanism (not most common, but easiest to explain): Direct exchange.

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

- Considers a process where electron 1, tunnels to 2
- Can only happen if the two electrons form a singlet (Pauli exclusion principle),

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

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



correction from 2nd order perturbation theory:

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

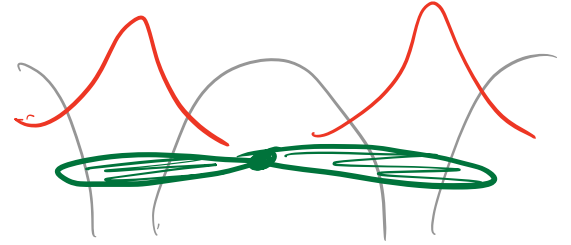
- We thus find: energy of singlet state

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \text{ lower by } -\frac{t^2}{U}$$

$\Rightarrow$ 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)

Further reading: W. Nolting, A. Kamakuchi:

Quantum Theory of Magnetism (Springer 2009)

What is the general structure of interactions in a quantum spin system?

- locality: interactions only couple nearby spins (or strength decays rapidly with distance)
- few-body: interactions only couple a small number (typ. 2) spins.

→ symmetry: interactions generally have the symmetries of the setup (lattice, ...)

How does a general 2-body interaction look like?

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

↖ Hamiltonian: 4×4 -matrix

We can express h using spin operators:

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

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

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

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

$$\begin{aligned}
 S_2^\alpha &\equiv \mathbb{1} \otimes S^\alpha \\
 &\equiv \mathbb{1}_1 \otimes S_2^\alpha = \begin{pmatrix} 1 \cdot S_2^\alpha & 0 \cdot S_2^\alpha \\ 0 \cdot S_2^\alpha & 1 \cdot S_2^\alpha \end{pmatrix} \begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix} \\
 &= \begin{pmatrix} S_2^\alpha & \\ & S_2^\alpha \end{pmatrix}
 \end{aligned}$$

↑
shorthand notation

and similarly:

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

$$\text{e.g., } S_1^x = \frac{1}{2} \begin{pmatrix} 0 \cdot \mathbb{1} & 1 \cdot \mathbb{1} \\ 1 \cdot \mathbb{1} & 0 \cdot \mathbb{1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

We can also act with S^x on 1 & S^y on 2:

$$\begin{aligned}
 S_1^\alpha \cdot S_2^\beta &= S^\alpha \otimes S^\beta \\
 &\equiv S_1^\alpha \otimes S_2^\beta = \frac{1}{2} \begin{pmatrix} 0 & S_2^\beta \\ S_2^\beta & 0 \end{pmatrix}.
 \end{aligned}$$

↑
shorthand notation w/out $\otimes$

↑
e.g., $S_1^\alpha = S_1^x$

Examples:

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

$$S_1^y, S_2^y = \frac{1}{4} \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix};$$

$$S_1^z, S_2^z = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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

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

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

What are some prototypical simple interactions? Chapter 1, Pg. 16

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

$$E = -\frac{t^2}{u} |\phi\rangle\langle\phi| = -\frac{t^2}{u} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \frac{(0 \ 1 \ -1 \ 0)}{\sqrt{2}}$$

energy $-\frac{t^2}{u}$ to $|\phi\rangle$,
0 to the other states

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

- The only fully rotationally invariant interaction:

$$H = J \cdot (S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z)$$
$$\equiv J \cdot (\vec{S}_1 \cdot \vec{S}_2)$$

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

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

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

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

$\Rightarrow$ same as $-\frac{t^2}{u} |\phi \times \phi|$ (up to constant)

Heisenberg interaction

$J > 0$: antiferromagnetic

$J < 0$: ferromagnetic

Eigenvalues of operator

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

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

$$3 \times \left(+\frac{1}{4}\right), \text{ with eigenvectors } \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle \quad \left. \begin{array}{l} \text{total spin} \\ S_{\text{tot}} = 1 \\ S_z = +1 \end{array} \right\}$$

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = |11\rangle \quad \left. \begin{array}{l} S_z = -1 \end{array} \right\}$$

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

Important: To preserve rotational symmetry,

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

states: classical intuition misleading!

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

... these 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:

$$\begin{aligned} h_{12} |\phi\rangle &= \sum c_{s_1 \dots s_N} (h_{12} |s_1, s_2\rangle) \otimes |s_3, s_4, \dots\rangle \\ &= \sum c_{s_1 \dots s_N} (h_{12})_{s_1 s_2}^{s'_1 s'_2} |s'_1, s'_2, s_3, \dots\rangle \end{aligned}$$

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 local ($\rightarrow$ mechanism behind net.)

Total Hamiltonian: Sum of all (local) terms,

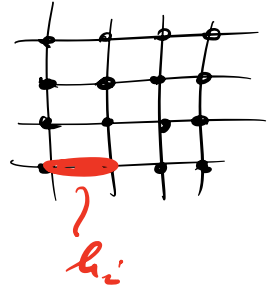
$$H = \sum_k h_k \stackrel{\text{e.g.}}{=} \sum J_{ij} \vec{S}_i \cdot \vec{S}_j$$

sum over all local terms $\rightarrow$ J_{ij} should decay with distance.

c) 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, ...

true - indep. Schrödinger equation

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

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

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

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

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

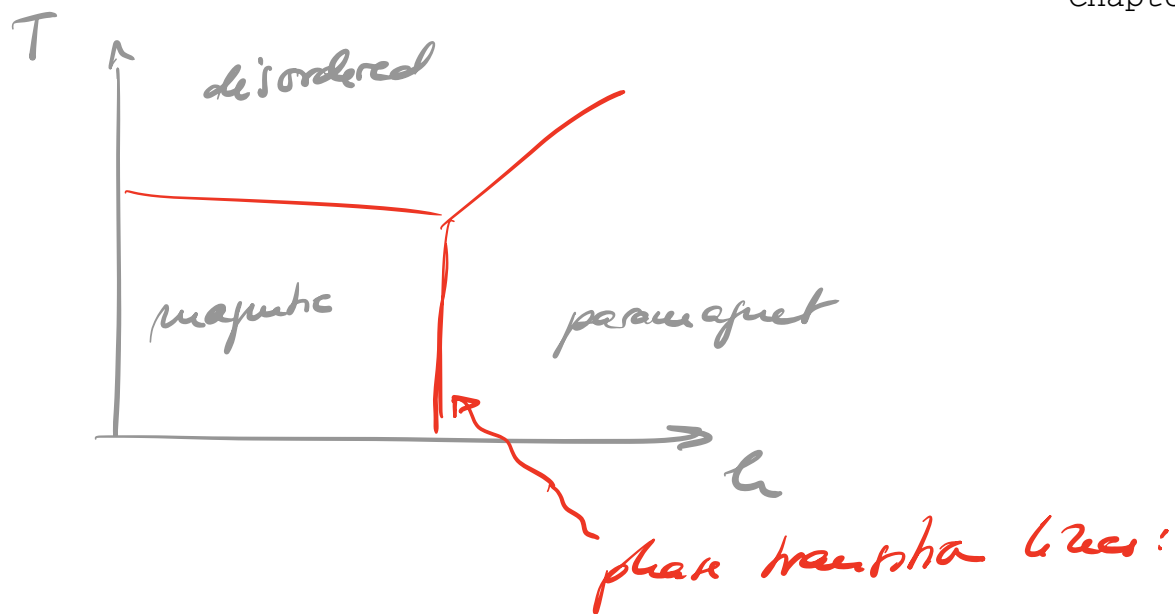
(e.g. for ground or Thermal State):

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 n
 H , such as different couplings, a magnetic field

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



Where are the phase transitions?

What properties do they have?

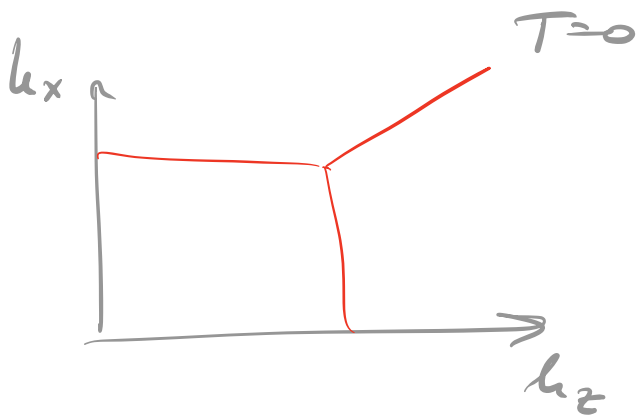
Focus: Quantum Matter - materials where quantum

effects play an essential 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 $T>0$? $\rightarrow$ later!)

What properties are we interested in?

- magnetic order:

e.g. average magnetization

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

$\uparrow$ ferromagnetic

or, more general,

$$\vec{m}(\mathbf{k}) = \frac{1}{N} \sum_{j'} e^{i\mathbf{k} \cdot \mathbf{r}_{j'}} \langle \vec{S}_{j'} \rangle = ?$$

e.g. for 2D, $\mathbf{k} = (\bar{u}, \bar{u})$: "staggered magnetization",
detects antiferromagnetic order.

• correlations between spins

* $\langle S_i^\alpha \cdot S_j^\beta \rangle$ — for transl. invariant systems,
this only depends on $i-j$,
or (if we also have reflection sym.) on $|i-j|$.

* average $\frac{1}{N} \sum_{i,j} \langle S_i^\alpha S_j^\beta \rangle$ $\left(\begin{array}{l} = 0(1) \text{ if correlations} \\ \text{decay exponentially,} \\ O(N) \text{ with long-r. order} \end{array} \right)$

* "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 correlation length ξ , which diverges

phase trans. & gives extra info. about

type of transition.

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

(cf. free energy $F = -kT \ln Z$)

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 kipping a spring
 can be meas. w/ in-elastic neutron scattering

- excited states:

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

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

- effects of disorder on 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.

d) 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 (small) 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 $H \rightarrow H' = H + \epsilon V$ 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 $|\psi'\rangle$

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

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

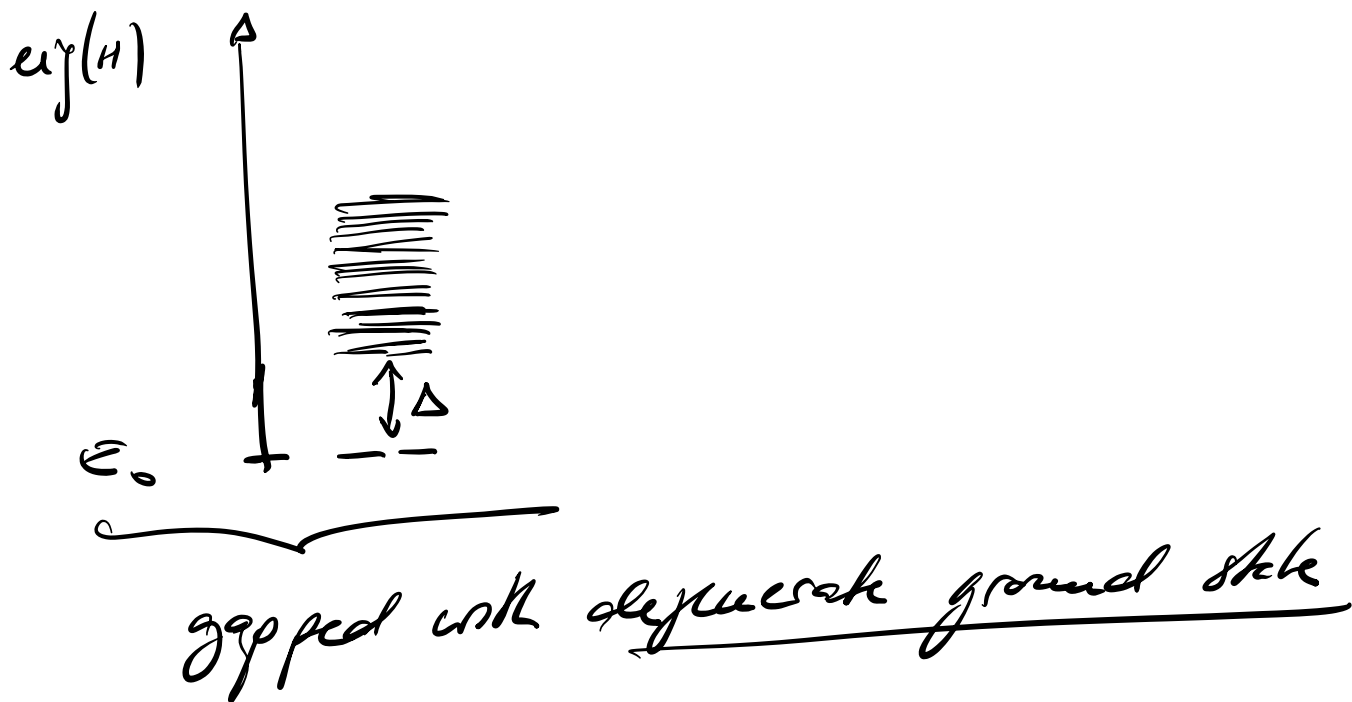
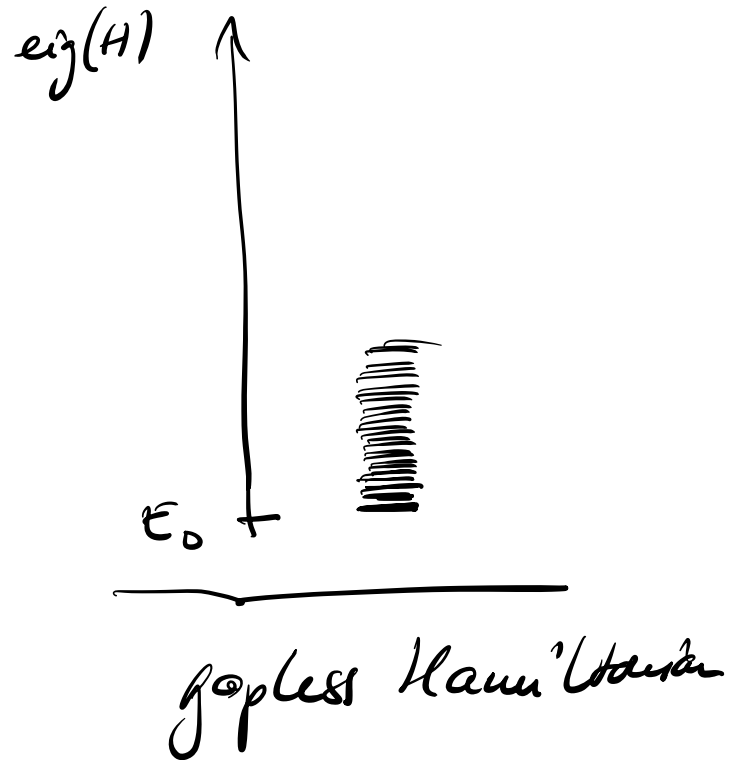
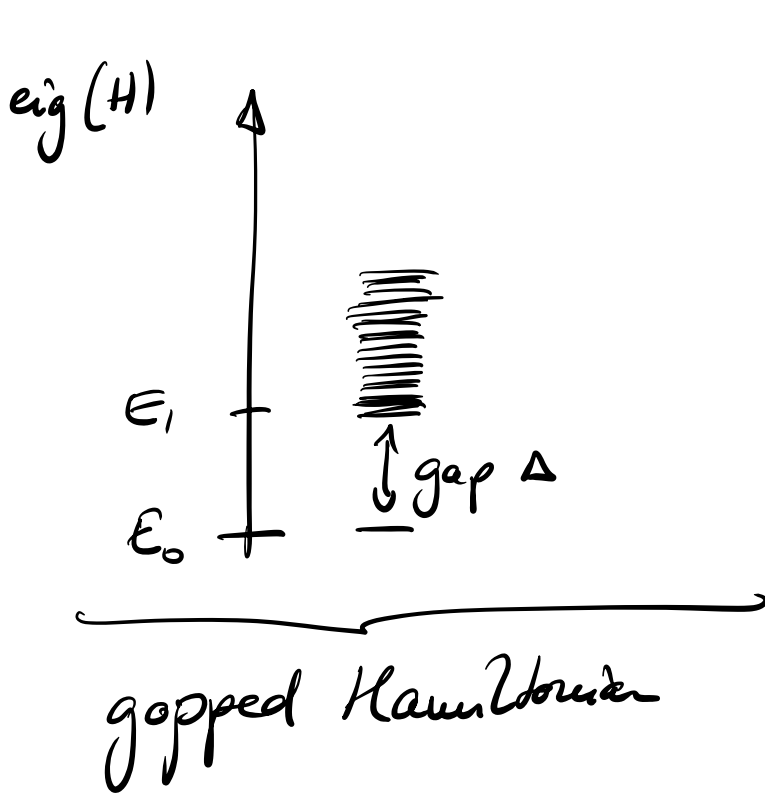
$$\leq \frac{\varepsilon}{\Delta} \| V |\psi\rangle \|$$

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

$\Rightarrow$ If the "energy gap" (or: "spectral gap",

or "gap" of H is sufficiently large, then

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



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Definition: We call a Hamiltonian (set, 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:

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

(typ, $\Delta(N) \rightarrow \Delta$),

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 $N \rightarrow \infty$) ground states; then, $\Delta(N) = E_{k+1}(N) - E_k(N)$.

Gapless (or critical) systems are those where $\Delta(N) \rightarrow 0$ (often, $\Delta(N) \sim \frac{1}{\text{poly}(N)}$).

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 $(\frac{\epsilon}{\Delta})^k$ in the perturbation series vanishes.

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

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

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

Proofs of such stability possible in certain cases
under some additional reasonable assumptions:

$$H'(\epsilon) = H + \epsilon \sum_i V_i$$

is still gapped for small enough ϵ , and
the ground states of H and $H'(\epsilon)$ only
differ inside a "light cone" whose size
depends on ϵ and Δ (up to small corrections):
Thus, the properties of the ground state do not
change abruptly, and in particular, no long-range
correlation can appear (or disappear).

(Further reading:

<https://arxiv.org/abs/1001.0344>

for the stability of the gap, and

<https://arxiv.org/abs/cond-mat/0503554>

for the consequence that the state only changes
inside a "light cone".)

A further consequence of a gap is that for low temperature,

$$\rho(T) = \frac{e^{-\beta H}}{\text{tr}(e^{-\beta H})} \approx |\psi_0\rangle\langle\psi_0|,$$

with $|\psi_0\rangle$ the ground state (this requires an extra reasonable assumption on the density of states) — i.e., we don't need to cool to $T=0$ to be (effectively) in the ground state.

e) Summary: Setup & Questions

- 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 n is actually relevant!

What singles out the relevant states?

$\Rightarrow$ The structure of $\ker q$, correlations — entanglement!