Lectures 9 & 10

- Quantum phase transitions
  - Introduction
  - Quantum Ising model
- Quantum critical phenomena
  - Connection to classical criticality
- Exact solution of quantum Ising chain
  - Critical behaviour

Sachdev (1999/2011)

Quantum statistical mechanics

basis of states s for each site: $|s\rangle_i$

basis for global state of N sites:

$$|\{s_i\}\rangle = |s_1, s_2, \ldots s_N\rangle = \prod_i^N |s_i\rangle_i$$

general state of N sites:

$$|\Psi\rangle = \sum_{\{s_i\}} \psi_{\{s_i\}} \, |\{s_i\}\rangle$$

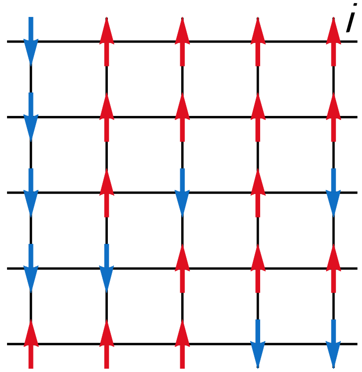
Hamiltonian $\mathcal{H}$ (operator in N-site Hilbert space) with eigenstates:

$$\mathcal{H}\,|n\rangle = E_n\,|n\rangle$$

e.g., spin-$\frac{1}{2}$ d.o.f.: basis states $|\uparrow\rangle_i$, $|\downarrow\rangle_i$

basis states correspond to classical configurations

$$\text{e.g., spins } s_i = \begin{cases} +1 & \uparrow \\ -1 & \downarrow \end{cases}$$



partition function $Z = \mathrm{Tr}\,\mathrm{e}^{-\mathcal{H}/T} = \sum_n \mathrm{e}^{-E_n/T}$ $\quad (k_\mathrm{B} = 1)$

free energy $F = \langle\mathcal{H}\rangle - TS = -T\log Z$

zero-T limit: (any operator Q)

$$\langle Q\rangle = \langle \mathrm{g.s.}|Q|\mathrm{g.s.}\rangle \qquad |\mathrm{g.s.}\rangle \equiv |0\rangle$$

$$F = \langle\mathcal{H}\rangle = E_{\mathrm{g.s.}} \qquad E_{\mathrm{g.s.}} \equiv E_0$$

Quantum Ising model

transverse-field quantum Ising model: $\langle ij \rangle$: nearest neighbours

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$

- each site i has spin-$\frac{1}{2}$ d.o.f.
- $\hat{\sigma}_i^\mu$: operators obeying $[\hat{\sigma}_i^\mu, \hat{\sigma}_j^\nu] = -2\mathrm{i}\epsilon_{\mu\nu\rho}\hat{\sigma}_i^\rho \delta_{ij}$ $\quad s, s' \in \{+1, -1\}$
- in $\hat{\sigma}^z$ basis, $|\uparrow\rangle_i$, $|\downarrow\rangle_i$, $\hat{\sigma}_i^\mu |s\rangle_i = (\boldsymbol{\sigma}^\mu)_{ss'} |s'\rangle_i$ $\quad \boldsymbol{\sigma}^\mu$: Pauli matrix

$$\hat{\sigma}_i^z |\uparrow\rangle_i = +|\uparrow\rangle_i \qquad \hat{\sigma}_i^z |\downarrow\rangle_i = -|\downarrow\rangle_i$$
$$\hat{\sigma}_i^x |\uparrow\rangle_i = |\downarrow\rangle_i \qquad \hat{\sigma}_i^x |\downarrow\rangle_i = |\uparrow\rangle_i$$

Quantum Ising model has symmetry under spin-flip operator $U = \prod_i \hat{\sigma}_i^x$

i.e., $[\mathcal{H}, U] = 0$

$$\hat{\sigma}_i^z \xrightarrow{U} U\hat{\sigma}_i^z U^{-1} = -\hat{\sigma}_i^z$$
$$\hat{\sigma}_i^z \hat{\sigma}_j^z \xrightarrow{U} \hat{\sigma}_i^z \hat{\sigma}_j^z$$
$$\hat{\sigma}_i^x \xrightarrow{U} \hat{\sigma}_i^x$$

Quantum paramagnet

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - Jg\sum_i \hat{\sigma}_i^x$$

$$\left.\begin{array}{l}\hat{\sigma}_i^x|\uparrow\rangle_i = |\downarrow\rangle_i \\ \hat{\sigma}_i^x|\downarrow\rangle_i = |\uparrow\rangle_i\end{array}\right\} \hat{\sigma}_i^x|\rightarrow\rangle_i = +|\rightarrow\rangle_i \text{ where } |\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

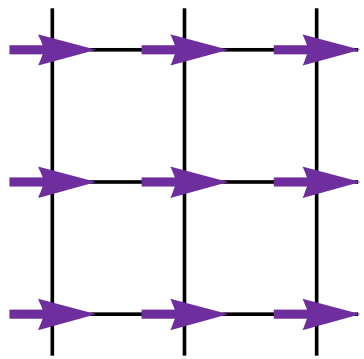
For $g \to +\infty$, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$

spins align with applied field: "quantum paramagnet"

g.s. is symmetric under spin flip: $U|\text{g.s.}\rangle = |\text{g.s.}\rangle$

$\langle\text{g.s.}|\hat{\sigma}_i^z|\text{g.s.}\rangle = 0$ $\qquad U = \prod_i \hat{\sigma}_i^x$

product state, so no correlations: $\langle\text{g.s.}|\hat{\sigma}_i^z\hat{\sigma}_j^z|\text{g.s.}\rangle = \delta_{ij}$



For large finite g, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$ + perturbative corrections in $1/g$

correlations $\langle\text{g.s.}|\hat{\sigma}_i^z\hat{\sigma}_j^z|\text{g.s.}\rangle \sim \mathrm{e}^{-|\boldsymbol{x}_i-\boldsymbol{x}_j|/\xi}$ with $\xi \to 0$ for $g \to \infty$

"kinetic energy (i.e., off-diagonal term) wins"

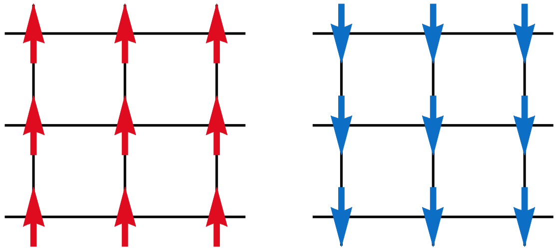
("kinetic" / "potential" depends on choice of basis)

Ferromagnetic phase

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$

For $g = 0$, two degenerate ground states: $|\Uparrow\rangle = \prod_i |\uparrow\rangle_i$ and $|\Downarrow\rangle = \prod_i |\downarrow\rangle_i$

spins align with each other: ferromagnet



both states break spin-flip symmetry ($U|\Uparrow\rangle = |\Downarrow\rangle$)

$\langle \text{g.s.}|\hat{\sigma}_i^z|\text{g.s.}\rangle = 1$

product state: $\langle \text{g.s.}|\hat{\sigma}_i^z \hat{\sigma}_j^z|\text{g.s.}\rangle = \langle \text{g.s.}|\hat{\sigma}_i^z|\text{g.s.}\rangle \langle \text{g.s.}|\hat{\sigma}_j^z|\text{g.s.}\rangle = 1$

For $g = 0^+$, superpositions $|\Uparrow\rangle \pm |\Downarrow\rangle$ are e'states, but splitting $\to 0$ as $N \to \infty$

$N = \infty$: macroscopic superpos'ns unstable; take $|\Uparrow\rangle$, $|\Downarrow\rangle$ as degenerate g.s.

for small g and $N = \infty$, $|\text{g.s.}_+\rangle = \prod_i |\uparrow\rangle_i +$ perturbative corrections in g

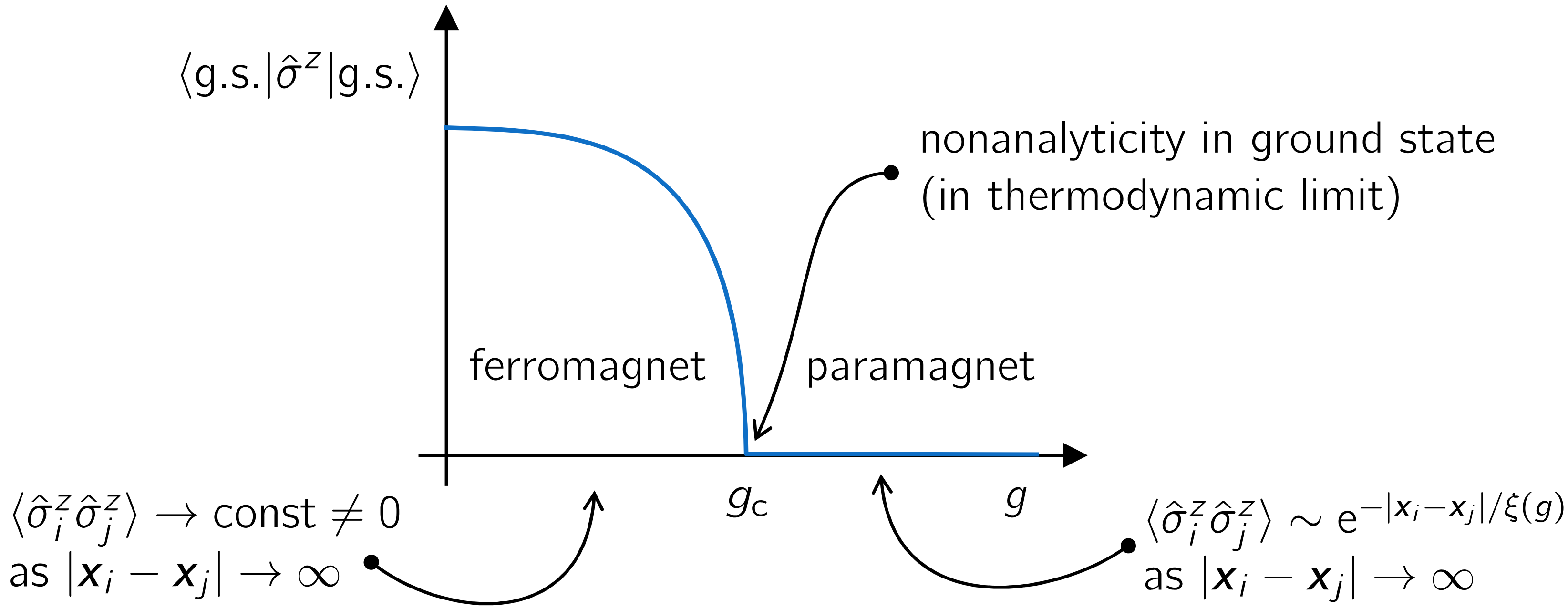
$|\text{g.s.}_-\rangle = \prod_i |\downarrow\rangle_i +$ perturbative corrections in g

"potential energy (i.e., diagonal term) wins"

Quantum phase transition

phase transition in ground state of quantum system

$$\text{e.g., } \mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$



continuous (second-order) phase transition:

$\langle \text{g.s.} | \hat{\sigma}^z | \text{g.s.} \rangle \to 0$ continuously as $g \to g_c$

$\xi(g) \to \infty$ as $g \to g_c$

Path integral for partition function

at temperature $T = 1/\beta$, partition function

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}}$$

$$= \sum_{\boldsymbol{s}} \langle \boldsymbol{s} | \mathrm{e}^{-\beta\mathcal{H}} | \boldsymbol{s} \rangle$$

for any (orthonormal) basis $\{|\boldsymbol{s}\rangle\}$

split operator $\mathrm{e}^{-\beta\mathcal{H}}$ into M pieces $\mathrm{e}^{-a\mathcal{H}}$ with $Ma = \beta$:

$$Z = \sum_{\boldsymbol{s}_0} \langle \boldsymbol{s}_0 | \underbrace{\mathrm{e}^{-a\mathcal{H}} \mathrm{e}^{-a\mathcal{H}} \cdots \mathrm{e}^{-a\mathcal{H}}}_{M} | \boldsymbol{s}_0 \rangle$$

$$\sum_{\boldsymbol{s}} |\boldsymbol{s}\rangle\langle\boldsymbol{s}| = 1$$

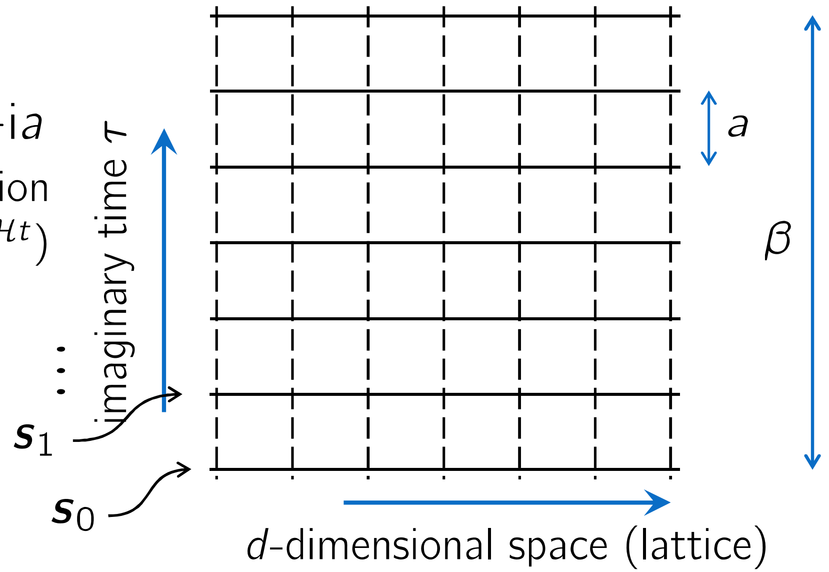
$$= \sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}} \langle \boldsymbol{s}_0 | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_1 \rangle \langle \boldsymbol{s}_1 | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_2 \rangle \langle \boldsymbol{s}_2 | \cdots | \boldsymbol{s}_{M-1} \rangle \langle \boldsymbol{s}_{M-1} | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_0 \rangle$$

$\mathrm{e}^{-a\mathcal{H}}$: evolution by "imaginary time" $t = -\mathrm{i}a$

(real-time evolution operator $\mathrm{e}^{-\mathrm{i}\mathcal{H}t}$)

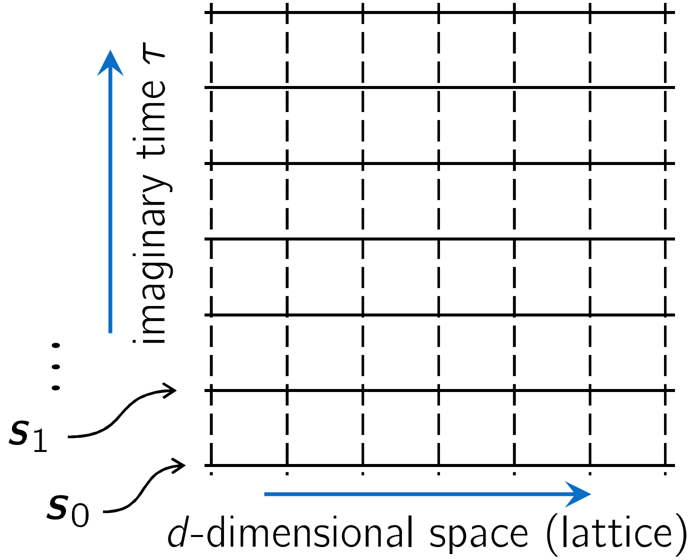
$\sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}}$: sum over trajectories

"path integral" representation of Z



Quantum–classical mapping

$$Z = \sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}} \langle \boldsymbol{s}_0 | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_1 \rangle \langle \boldsymbol{s}_1 | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_2 \rangle \langle \boldsymbol{s}_2 | \cdots | \boldsymbol{s}_{M-1} \rangle \langle \boldsymbol{s}_{M-1} | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}_0 \rangle$$



choose basis states $|\boldsymbol{s}\rangle$ corresponding
to classical configurations $\boldsymbol{s}$

define $\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}') = -\log \langle \boldsymbol{s} | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}' \rangle = [\mathcal{E}(\boldsymbol{s}', \boldsymbol{s})]^*$

$$Z = \sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}} \mathrm{e}^{-\sum_{i=0}^{M-1} \mathcal{E}(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})}$$

where $\boldsymbol{s}_M \equiv \boldsymbol{s}_0$ (periodicity in τ)

cf. classical statistical system with reduced Hamiltonian E_{cl}
on $(d+1)$-dimensional lattice (with p.b.c.)

$$E_{\mathrm{cl}} = \sum_i [E_1(\boldsymbol{s}_i) + E_2(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})]$$

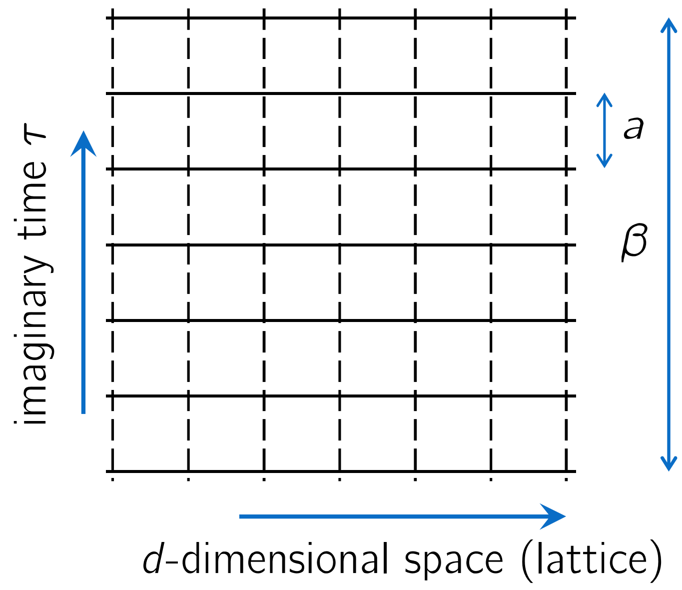
E_1: layer configuration energy
E_2: interaction between adjacent layers

$$= \sum_i \left\{ \frac{1}{2} [E_1(\boldsymbol{s}_i) + E_1(\boldsymbol{s}_{i+1})] + E_2(\boldsymbol{s}_i, \boldsymbol{s}_{i+1}) \right\} = \sum_{i=0}^{M-1} E(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})$$

if $\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}')$ is real, interpret Z as partition f'n for classical $(d+1)$-dimensional system

QC mapping: General case

quantum	classical
imaginary time τ	extra spatial dimension τ
inverse temperature $\beta = \frac{1}{T}$	system size L_τ in τ direction
imaginary-time evolution $e^{-a\mathcal{H}}$	Boltzmann weight (transfer matrix) $e^{-\mathcal{E}(\boldsymbol{s},\boldsymbol{s}')} = \langle \boldsymbol{s} \| e^{-a\mathcal{H}} \| \boldsymbol{s}' \rangle$
sum over trajectories ("path integral")	sum over configurations (canonical ensemble)
quantum critical phenomena at $T = 0$ in d dimensions	classical critical phenomena in $d + 1$ dimensions



- at zero temperature, $\beta = 1/T = \infty$: imaginary-time direction is infinite
- n.b., distinct from relationship between classical stochastic dynamics (in d dimensions) and quantum mechanics (in d dimensions)

QC mapping: Ising model

transverse-field quantum Ising model: $\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$

define $\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}') = -\log \langle \boldsymbol{s} | \mathrm{e}^{-a\mathcal{H}} | \boldsymbol{s}' \rangle$

$$Z = \sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \dots, \boldsymbol{s}_{M-1}} \mathrm{e}^{-\sum_{i=0}^{M-1} \mathcal{E}(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})}$$

use $\hat{\sigma}_i^z$ basis, $|\uparrow\rangle_i$, $|\downarrow\rangle_i$:

$$|\boldsymbol{s}\rangle = |\{s_1, s_2, \dots s_N\}\rangle = \prod_i^N |s_i\rangle_i,$$

for sufficiently small a, use $\mathrm{e}^{a(A+B)} = \mathrm{e}^{aA} \mathrm{e}^{aB} [1 + \mathcal{O}(a)]$

$$\begin{aligned}
\langle \boldsymbol{s} | \, \mathrm{e}^{-a\mathcal{H}} \, | \boldsymbol{s}' \rangle &\approx \langle \boldsymbol{s} | \, \mathrm{e}^{aJg \sum_i \hat{\sigma}_i^x} \mathrm{e}^{aJ \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z} \, | \boldsymbol{s}' \rangle \\
&= \langle \boldsymbol{s} | \, \mathrm{e}^{aJg \sum_i \hat{\sigma}_i^x} \, | \boldsymbol{s}' \rangle \, \mathrm{e}^{aJ \sum_{\langle ij \rangle} s_i' s_j'} \\
&= \mathrm{e}^{aJ \sum_{\langle ij \rangle} s_i' s_j'} \prod_i \langle s_i | \, \mathrm{e}^{aJg \hat{\sigma}^x} \, | s_i' \rangle \\
&= [A(aJg)]^N \mathrm{e}^{aJ \sum_{\langle ij \rangle} s_i' s_j' + B(aJg) \sum_i s_i s_i'}
\end{aligned}$$

$$\langle s | \mathrm{e}^{\alpha \hat{\sigma}^x} | s' \rangle = A(\alpha) \mathrm{e}^{B(\alpha) s s'}$$

$$B(\alpha) = -\tfrac{1}{2} \log \tanh \alpha$$

$$\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}') = -aJ \sum_{\langle ij \rangle} s_i' s_j' - B(aJg) \sum_i s_i s_i' + \text{const}$$

QC mapping: Ising model

transverse-field quantum Ising model: $\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$

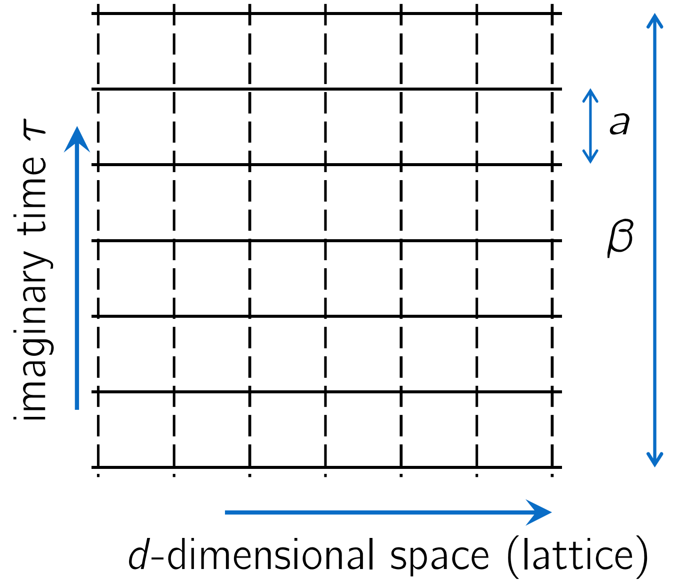
$$Z = \sum_{\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{M-1}} \mathrm{e}^{-\sum_{i=0}^{M-1} \mathcal{E}(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})}$$

For $a \to 0$, $\quad B(\alpha) = -\frac{1}{2} \log \tanh \alpha$

$$\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}') = -aJ \sum_{\langle ij \rangle} s_i' s_j' - B(aJg) \sum_i s_i s_i'$$

layer configuration energy

interaction between adjacent layers



- Transverse-field Ising model in d dimensions maps to highly anisotropic ($a \to 0$) classical Ising model in $d+1$ dimensions
- By universality, quantum Ising model has identical critical properties to isotropic classical Ising model in $d+1$ dimensions

Quantum Ising chain

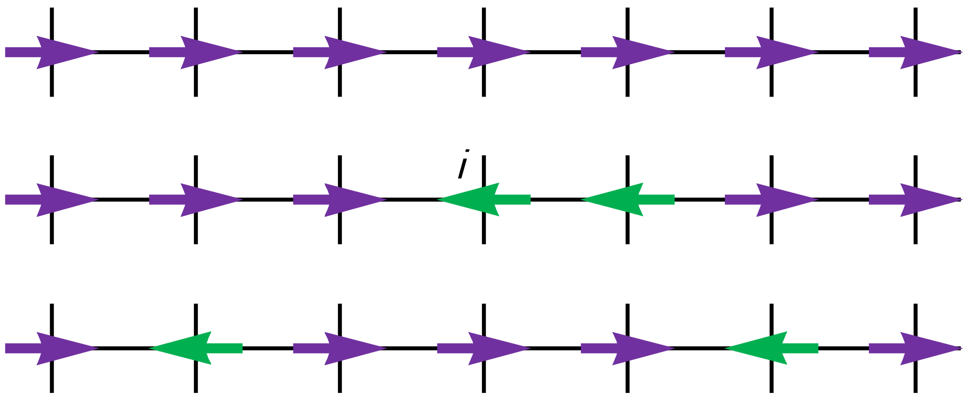
transverse-field quantum Ising model in 1D:

$$\mathcal{H} = -J \sum_i \left[\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + g \hat{\sigma}_i^x \right]$$

(related to 2D classical Ising model, so ordering transition at g_c)

for $g = \infty$, $|\text{g.s.}\rangle = \prod_i |{\rightarrow}\rangle_i$

excited states have flipped spins



for large g, use perturbation theory, with $\delta\mathcal{H} = \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$

$\delta\mathcal{H}$ creates flipped spins in pairs & hops them between sites

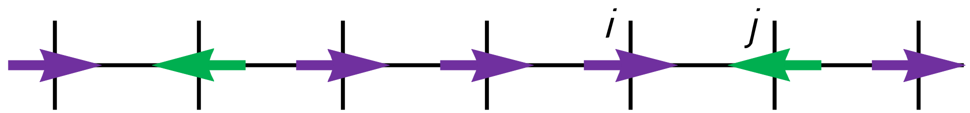
$$|{\rightarrow}\rangle = \frac{1}{\sqrt{2}} \left(|{\uparrow}\rangle + |{\downarrow}\rangle \right) \qquad \hat{\sigma}^z |{\rightarrow}\rangle = |{\leftarrow}\rangle$$

$$|{\leftarrow}\rangle = \frac{1}{\sqrt{2}} \left(|{\uparrow}\rangle - |{\downarrow}\rangle \right) \qquad \hat{\sigma}^z |{\leftarrow}\rangle = |{\rightarrow}\rangle$$

so treat flipped spins as particles

Jordan–Wigner transformation

Treat flipped spins as particles



either:

- as bosons—but then need interactions to forbid two flipped spins on one site

$$\hat{\sigma}^x_i = 1 - 2n_i \qquad n_i = 0$$

$$\hat{\sigma}^z_i = b_i + b_i^\dagger \qquad n_j = 1$$

- as fermions—double occupation automatically forbidden, *but* fermion operators anticommute on different sites:

$$\{c_i, c_j^\dagger\} = \delta_{ij}$$

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = \delta_{ij}$$

$$[\hat{\sigma}^\mu_i, \hat{\sigma}^\nu_j] = -2\mathrm{i}\epsilon_{\mu\nu\rho}\hat{\sigma}^\rho_i\delta_{ij}$$

Jordan–Wigner transformation (in 1D): add a string of minus signs

$$\hat{\sigma}^x_i = 1 - 2n_i \qquad n_j = c_j^\dagger c_j$$

$$\hat{\sigma}^z_i = -(c_i + c_i^\dagger)\prod_{j<i}(1 - 2n_j)$$

including this string, $[\hat{\sigma}^x_i, \hat{\sigma}^z_j] = 0$ for $i \neq j$, as required

Ising chain: Exact spectrum

transverse-field quantum Ising model in 1D: $\mathcal{H} = -J \sum_i \left[\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + g\hat{\sigma}_i^x\right]$

JW transformation: $\hat{\sigma}_i^x = 1 - 2n_i \qquad n_j = c_j^\dagger c_j$

$$\hat{\sigma}_i^z = -(c_i + c_i^\dagger) \prod_{j<i} (1 - 2n_j)$$

$$\begin{aligned}
\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z &= (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger) \prod_{j<i} (1 - 2n_j) \prod_{j'<i+1} (1 - 2n_{j'}) \\
&= (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger)(1 - 2n_i) \qquad \{c_i, c_j^\dagger\} = \delta_{ij} \\
&= (-c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger) \qquad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = \delta_{ij}
\end{aligned}$$

result: quadratic Hamiltonian in terms of fermion operators

$$\mathcal{H} = -J \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i - 2g c_i^\dagger c_i + g\right)$$

(see practice problems)

diagonalize with FT and unitary transformation: $c_k = u_k \gamma_k + \mathrm{i} v_k \gamma_{-k}^\dagger \qquad \{\gamma_k, \gamma_k^\dagger\} = \delta_{k,k'}$

$$\mathcal{H} = \sum_k \varepsilon_k (\gamma_k^\dagger \gamma_k - \tfrac{1}{2})$$

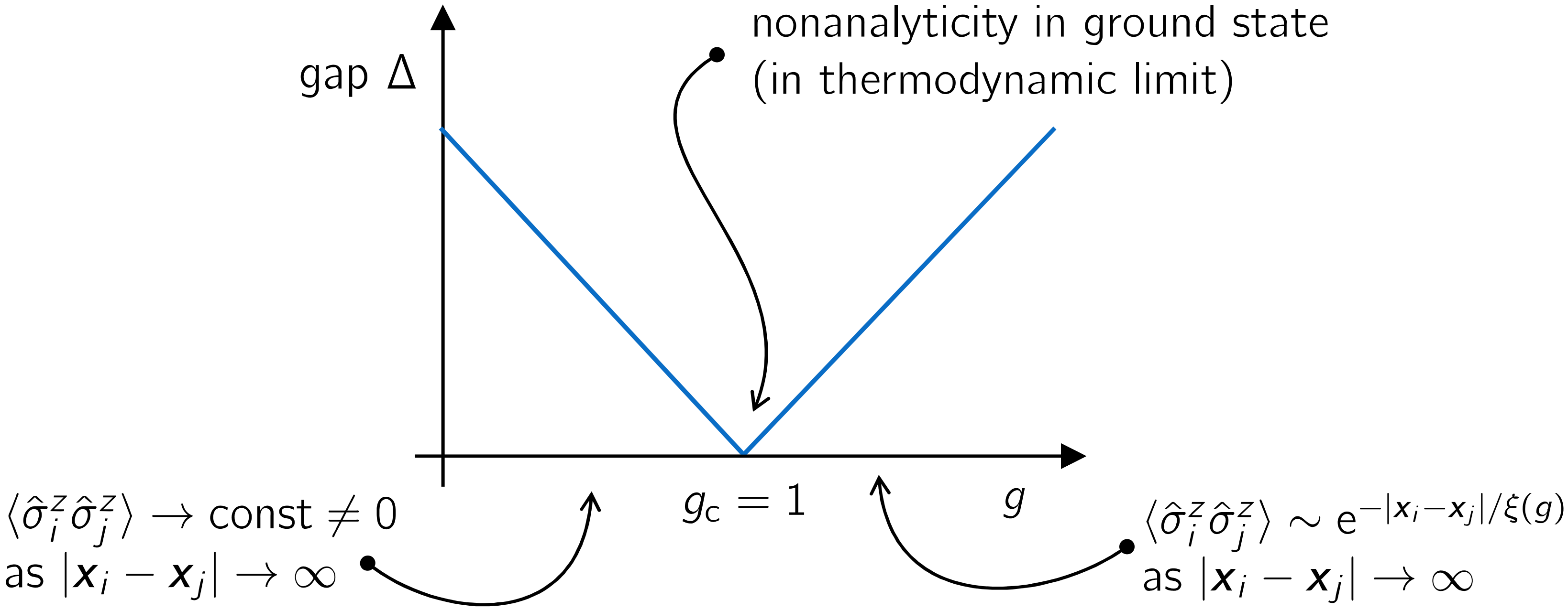
ground state $|\text{g.s.}\rangle$: $\gamma_k |\text{g.s.}\rangle = 0$ (all k)

$$\varepsilon_k = 2J\sqrt{1 + g^2 - 2g\cos k}$$

gap $\Delta = E_1 - E_{\text{g.s.}} = \varepsilon_0 = 2J|1 - g|$

Ising chain: Quantum phase transition

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x = \sum_k \varepsilon_k (\gamma_k^\dagger \gamma_k - \tfrac{1}{2})$$



$$\varepsilon_k = 2J\sqrt{1 + g^2 - 2g\cos k}$$

$$\Delta = 2J|1-g| \sim |g - g_c|^{z\nu}$$

critical exponent $z\nu = 1$

Sachdev (1999/2011)