Quantum Spin Chains and Topology

PH 543: Advanced Statistical Mechanics

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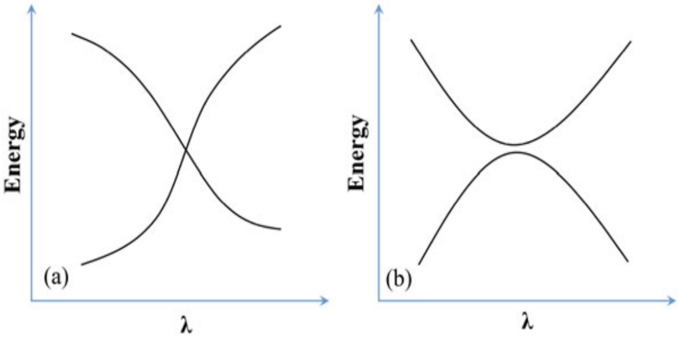
Quantum Phase Transitions

- Quantum Phase Transitions arise due to singularities in the ground state energies of a system as a function of some coupling parameter.
- This phase transition can be characterized by looking at the separation between the ground state and the first excited state.
- At the critical value of the coupling constant, the two states either intersect or come closest to each other

Quantum Phase Transitions



(a) Level crossing and (b) avoided level crossing of the ground state of a quantum Hamiltonian. Figure adapted from [BBJ22].

Transverse Field Ising Model

- Let us look at the TFIM Hamiltonian defined as

$$H_I = -Jg \sum_i \hat{\sigma}_i^x - J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z \tag{1}$$

- The ground state is dependent on the value of the coupling constant g. We have two extreme cases : $g >> 1$, $g << 1$.
- $g >> 1$: The eigenstate will be an eigenvector of $\hat{\sigma}_i^x$.

$$|1_x\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle) \tag{2}$$

$$|-1_x\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle) \tag{3}$$

Transverse Field Ising Model

- $g << 1$: The eigenstate will be an eigenstate of $\hat{\sigma}_i^z$
- The first excited state will be the one with one particle out of order.
- The form of the energy gap between first and ground state is different in the two limits

$$\epsilon_k = Jg[1 - \frac{2}{g}\cos(ka) + \mathcal{O}(\frac{1}{g^2})] \qquad g >> 1 \tag{4}$$

$$\epsilon_k = J(2 - 2g\cos(ka) + \mathcal{O}(g^2)) \qquad g << 1 \tag{5}$$

Transverse Field Ising Model

We can solve exactly for the energy of the first excited state by using the nearest neighbor nature of the interaction.

$$\epsilon_k = 2J(1 + g^2 - 2g\cos(k))^{\frac{1}{2}} \tag{6}$$

The minimum gap here is thus

$$\epsilon_0 = 2J|1 - g| \tag{7}$$

We can clearly see that this quantity becomes zero at $g = 1$ making $g = 1$ the critical point. This gap also behaves as expected in the two extreme limits.

Revisting the TFIM

We know the TFIM model exhibits a phase transition at $g = 1$.

$$H_I = -Jg \sum_i \hat{\sigma}_i^x - J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z \tag{8}$$

Let's explore the physics of this phase transition further.

The Jordan-Wigner transformation

- The JW mapping is a key tool in the study of phase transitions in quantum spin chains.
- The idea is to map the spin algebra to the fermionic algebra.
- **Spin algebra**

$$\sigma^{+} \left|\downarrow\right\rangle = \left|\uparrow\right\rangle ; \ \sigma^{-} \left|\uparrow\right\rangle = \left|\downarrow\right\rangle \tag{9}$$

  where $\sigma^{\pm} := 1/2(\sigma^x \pm \iota\sigma^y)$ are the raising and lowering operators.
- **Fermionic algebra**

$$c^{\dagger} \left|0\right\rangle = \left|1\right\rangle ; \ c \left|1\right\rangle = \left|0\right\rangle \tag{10}$$

  where $\left|1\right\rangle, \left|0\right\rangle$ denote the presence or absence of a fermion. Also, $c, c^{\dagger}$ are the fermionic annhilation and creation operators satisying the fermionic CCRs

$$\{c_i, c_j\} = \{c_i^{\dagger}, c_j^{\dagger}\} = 0; \ \{c_i, c_j^{\dagger}\} = \delta_{ij} \tag{11}$$

  where i, j are site indices.

The Jordan-Wigner transformation

- We identify the isomorphism
$$|\uparrow\rangle \sim \bullet, \quad |\downarrow\rangle \sim \circ \tag{12}$$
- Thus, should we transform $\sigma^+ \to c^\dagger$ and $\sigma^- \to c$?
- **Issue**: The $\sigma^\pm$ satisfy $[\sigma_i^-, \sigma_j^+] = [\sigma_i^+, \sigma_j^-] = 0 \forall i \neq j$. Hard-core bosons!
- We must ensure that the fermionic CCRs are satisfied.Jordan and Wigner [noa] paved the way:
$$c_i := \left(\Pi_{j<i}\sigma_i^z\right)\sigma_i^- \tag{13}$$
$$c_i^\dagger := \left(\Pi_{j<i}\sigma_i^z\right)\sigma_i^+ \tag{14}$$
- This is invertible,
$$\sigma_i^z = 1 - 2c_i^\dagger c_i \tag{15}$$
$$\sigma_i^+ = \left(\Pi_{j<i}(1 - 2c_j^\dagger c_j)\right) c_i^\dagger \tag{16}$$
$$\sigma_i^- = \left(\Pi_{j<i}(1 - 2c_j^\dagger c_j)\right) c_i \tag{17}$$

JW transforming the TFIM

- Rotating the spin-frame by 90^o we can write the mapping as,

$$\sigma_i^x = 1 - 2c_i^\dagger c_i \tag{18}$$

$$\sigma_i^z = -\left(\Pi_{j<i}(1 - 2c_j^\dagger c_j)\right)(c_i + c_i^\dagger) \tag{19}$$

- With this, we transform the Ising model as [Chh21],

$$\mathcal{H} = 2gJ\sum_i c_i^\dagger c_i - J\sum_i (c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger) - J\sum_i (c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1}) \tag{20}$$

- This is very similar to the Hamiltonian of the **Kitaev chain**

$$\mathcal{H}_{Kitaev} = -\mu\sum_i c_i^\dagger c_i - t\sum_{\langle ij\rangle} c_i^\dagger c_j - \Delta\sum_i c_i c_{i+1} + h.c. \tag{21}$$

  and is exact for $\Delta = t$. **Superconducting physics**.
- Quasiparticle domain-wall and spin-flip excitations now manifest as Bugoliubov excitations.

Spectrum of the Kitaev chain

- Transforming to k-space, we can write the Kitaev Hamiltonian as

$$\mathcal{H}_k = \sum_k \left[(\mu - 2t) c_k^\dagger c_k + \iota \Delta \sin(k) (c_{-k} c_k + c_k^\dagger c_{-k}^\dagger) \right] \tag{22}$$

- If we define,

$$\Psi_k := \begin{pmatrix} c_{-k} \\ c_k^\dagger \end{pmatrix} \tag{23}$$

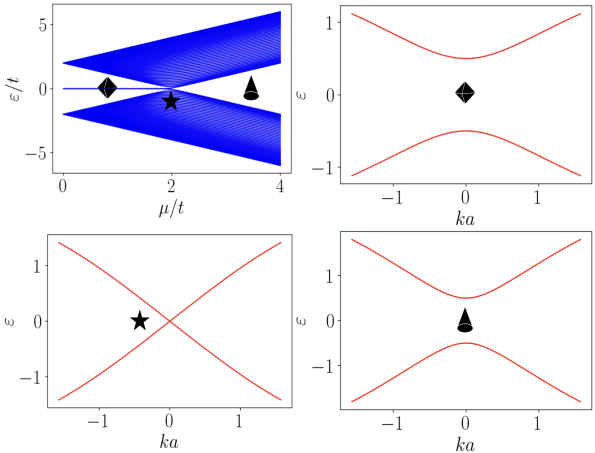
- Then we can write the k-space Hamiltonian as,

$$\mathcal{H}_k = \sum_k \Psi_k^\dagger \begin{pmatrix} \mu/2 - t\cos k & -\iota\Delta \sin k \\ \iota \Delta \sin k & -(\mu/2 - t\cos k) \end{pmatrix} \Psi_k \tag{24}$$

- This gives us the energy spectrum

$$\varepsilon_k = \pm \sqrt{(\mu/2 - t\cos k)^2 + \Delta^2 \sin^2 k} \tag{25}$$

Spectrum of the Kitaev chain



Kitaev spectrum. Note the Dirac cone at $k = 0$ for the critical point $g = 1 = \mu/2t$

Something unusual → topology and Majoranas.

- The diagonalized spectrum shows zero-energy modes for $\mu < 2t$, but the bulk, showed by the band-structure is gapped for all $\mu \neq 2t$! **How**?
- This is *topology*. The edge-modes must lie at the boundaries . The bulk Hamiltonian gives information about the behaviour at the edge. This is the **bulk-edge correspondence**.
- Let us see this formally. Define

$$\gamma_j^+ := c_j^\dagger + c_j; \quad \gamma_j^- := \iota(c_j - c_j^\dagger) \tag{26}$$

to be the Majorana operators, which describe particles which are their own anti-particles.
- Also, order the operators as:

$$\gamma_1, \gamma_2, \ldots, \gamma_{2N-1}, \gamma_{2N} \equiv \gamma_1^+, \gamma_2^-, \gamma_3^+, \gamma_3^-, \ldots, \gamma_N^+, \gamma_N^- \tag{27}$$

Majorana representation

Unpaired case

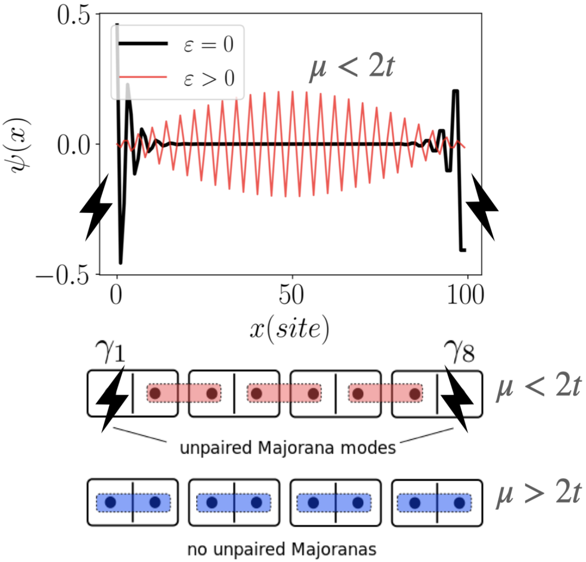
$$\mathcal{H}_{unpaired} = (\iota/2)\mu \sum_{i=1}^{N} \gamma_{2i-1}\gamma_{2i} \quad (\mu > 0 \text{ and } \Delta = 0 = t) \tag{28}$$

Paired case

$$\mathcal{H}_{paired} = \iota t \sum_{i=1}^{N-1} \gamma_{2i+1}\gamma_{2i} \quad (\Delta = t, \mu = 0) \tag{29}$$

Majoranas are robust modes. Due to (i) P-H symmetry, and (ii) lack of bulk zero-energy excitations. $\rightarrow$ *topological quantum computing*!

Majorana representation



Topology?

Two perspectives:

1. Write the Bloch Hamiltonian as
$$\mathcal{H}(\mathbf{k}) = \vec{d}(\mathbf{k}) \cdot \vec{\sigma} \tag{30}$$
   In our case,
   - $d_z(k) = \mu/2 - t \cos k$
   - $d_y(k) = \Delta \sin k$
2. Parametrized Hamiltonians $\mathcal{H}(g)$. *Adiabatically disconnected* unless gap closure happens $\rightarrow$ topological invariants!

More formally, we need to deal with Berry phases, Berry curvatures, and TKNN numbers. Topological invariants are discontinuous.

Entanglement (briefly)

- Coupled with the recent developments in the areas of quantum information and computation, there have been significant research efforts in using entanglement and related quantities like quantum discord, coherent information, quantum fidelty have been used to study QPTs [BBJ22].
- Important
  1. classifying multistate systems, wherein one needs a separate order parameter for each state
  2. lack of a local order parameter or symmetry-breaking in some QPTs
- Central quantity of study:

$$\mathcal{E}(|\Psi\rangle) = -Tr[\rho_A \log \rho_A] = S(\rho_A) \tag{31}$$

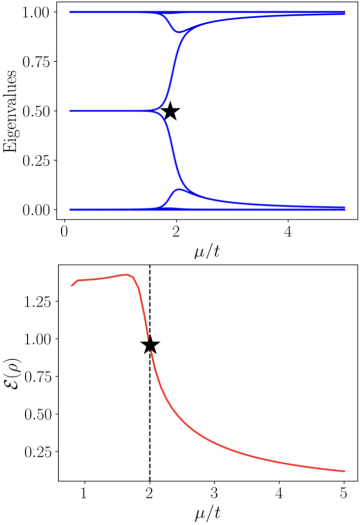
- For fermionic systems,

$$\langle c_i^\dagger c_j \rangle = \langle \Psi | c_i^\dagger c_j | \Psi \rangle \tag{32}$$

- We can get the EE from the partial correlation matrix C_A with eigenvalues ζ_i [KM22]

$$\mathcal{E}(|\Psi\rangle) = -Tr[\rho_A \log \rho_A] = S(\rho_A) = \sum [-\zeta_i \log \zeta_i - (1-\zeta_i) \log (1-\zeta_i)] \tag{33}$$

Entanglement (briefly)



Thus...

A simple model tells us about:

- the TFIM
- the JW mapping
- quasiparticle excitations
- topology
- entanglement (for QPTs)

$\rightarrow$...**workhorse** of theoretical understanding of many concepts of many-body physics, phase transitions, and entanglement theory.

Quantum mechanics at finite temperature

$$\begin{array}{c}\text{Conventional quantum mechanics}\\ \Big\downarrow \text{Temperature}\\ \text{Quantum statistical mechanics}\end{array}$$

Quantum statistical mechanics

Grand partition function,

$$\mathcal{Z}_q(\beta, \mu) = \mathrm{Tr}\left\{ e^{-\beta(\hat{H}-\mu\hat{N})} \right\}, \tag{34}$$

where $\hat{H}$ is the Hamiltonian, $\hat{N}$ is the number operator.

The trace is over the whole Hilbert space of the problem ($\sum_m \langle m|\cdots|m\rangle$).

Lattice field theory

$$\text{Latticization} \Longrightarrow \text{discretization of the path integral}$$

$$\text{Quantum field theory} \xrightarrow[\text{Euclideanization}]{\text{Latticization}} \text{classical statistical mechanical problem}$$

Path integral formulation of quantum mechanics I

The probability amplitude for a particle to travel from (x_i, t_i) to (x_f, t_f) is given by the kernel,

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}\left[x(t)\right] e^{\frac{i}{\hbar} S[x(t)]}. \tag{35}$$

The integral can be interpreted as some sort of a "sum over paths",

$$\mathcal{D}\left[x(t)\right] \sim \prod_j \mathrm{d}x(t_j)\,. \tag{36}$$

This is equivalent to the wavefunction formalism $(\{E_n, \phi_n\})$,

$$K(x_f, t_f; x_i, t_i) = \sum_n e^{\frac{i}{\hbar} E_n (t_f - t_i)} \phi_n^*(x_f) \phi_n(x_i). \tag{37}$$

Path integral formulation of quantum mechanics II

As a generating functional for correlation functions, the partition function is given by,

$$Z = \int \mathcal{D}\left[\{\phi\}\right] e^{\frac{i}{\hbar} S(\{\phi\})}. \tag{38}$$

Introducing an auxiliary function $J(x)$, we define our generating functional as,

$$Z[J] = \int \mathcal{D}\left[\{\phi\}\right] \exp\left\{ \frac{i}{\hbar} \left[S(\{\phi\}) + \int_{x_i}^{x_f} \mathrm{d}^4 x \, J(x)\phi(x) \right] \right\}. \tag{39}$$

The n-point correlation functions are then given by the functional derivatives,

$$G_n(x_1, \ldots, x_n) = (-i\hbar)^n \frac{1}{Z[0]} \left. \frac{\delta^{\mathrm{n}} Z}{\delta J(x_1) \cdots \delta J(x_n)} \right|_{J=0}. \tag{40}$$

Quantum to classical mapping: Wick rotation

The highly oscillatory e^{iS_M} in (38) is Wick-rotated into a damping exponential e^{-S_E},

$$t \to -i\tau, \qquad S_M \to iS_E, \qquad e^{iS_M} \to e^{-S_E}, \qquad \tau \in [0, \beta]. \tag{41}$$

Partition functions of QFTs are considered to be imaginary-time versions of statistical mechanical partition functions.

Upon euclideanization and discretization, the vacuum-to-vacuum amplitude takes the form,

$$Z \sim \int \prod_j \mathrm{d}\phi_j \, e^{-S_E(\{\phi_j\})}, \tag{42}$$

which resembles the classical statistical mechanical partition function.

Quantum to classical mapping

Thus the QFT partition function in (38) can be understood as a sum of "transition" amplitudes, but in the Euclidean imaginary time evolution,

$$
\begin{aligned}
Z &= \mathrm{Tr}\left\{ e^{-\beta(\hat{H}-\mu\hat{N})} \right\} \\
&= \sum_a \int \mathcal{D}\left[\phi_a\right] \, \langle \phi_a | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi_a \rangle \,,
\end{aligned} \tag{43}
$$

with the periodic boundary condition $\phi(x,0) = \phi(x,\beta)$.

Wick rotation (41) enables us to identify imaginary time $\tau/\hbar$ of the lattice field theory with inverse temperature β of the classical statistical mechanical system

The classical limit of quantum statistical mechanics I

Quantum partition function for a particle of mass m in a potential $V(x)$ in the imaginary-time formalism is written as [Sha17],

$$Z(\beta) = \int \mathrm{d}x \int_{x}^{x} \mathcal{D}[x] \exp\left\{ -\frac{1}{\hbar} \int_{0}^{\beta\hbar} \mathrm{d}\tau \left(\frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}\tau} \right)^{2} + V[x(\tau)] \right) \right\}. \tag{44}$$

The kinetic energy for a particle to return to its starting position x, having been displaced by Δx, in $\beta\hbar$ time is of the order,

$$\sim \frac{m}{2} \left(\frac{\Delta x}{\beta\hbar} \right)^{2}. \tag{45}$$

The Boltzmann factor then becomes of the order,

$$\sim \exp\left\{ -\frac{m}{\hbar} \left(\frac{\Delta x}{\beta\hbar} \right)^{2} \beta\hbar \right\}. \tag{46}$$

The classical limit of quantum statistical mechanics II

In the "classical" limit, $\beta\hbar \to 0$, all Δx incursions must be exponentially suppressed, i.e.,

$$\Delta x \sim \sqrt{\frac{\beta}{m}}\hbar. \tag{47}$$

This is called the *thermal wavelength*.
Assuming the potential to be varying over length scales appreciably bigger than Δx, we can approximate (44) by,

$$\begin{aligned} Z(\beta) &\sim \int \mathrm{d}x\, e^{-\beta V(x)} \int_x^x \mathcal{D}[x] \exp\left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau\, \frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}\tau} \right)^2 \right\} \\ &= \int \mathrm{d}x\, e^{-\beta V(x)} \sqrt{\frac{m}{2\pi\beta\hbar^2}}, \end{aligned} \tag{48}$$

where the last equality follows from the transition amplitude for a free particle,

$$W(q_s, t_s, q_t, t_t) = \sqrt{\frac{m}{2\pi i\hbar(t_t - t_s)}}\, e^{\frac{i}{\hbar}\frac{m(q_t - q_s)^2}{2(t_t - t_s)}}\,. \tag{49}$$

The classical limit of quantum statistical mechanics III

Comparing (48) with the classical partition function,

$$\begin{aligned} Z &= A \int \mathrm{d}x \int \mathrm{d}p \, \exp\left\{-\beta \left(\frac{p^2}{2m} + V(x)\right)\right\} \\ &= A \sqrt{\frac{2\pi m}{\beta}} \int \mathrm{d}x \, e^{-\beta V(x)}. \end{aligned} \tag{50}$$

Comparing (48) and (50), we have that,

$$A = \frac{1}{2\pi\hbar} = \frac{1}{h}, \tag{51}$$

which explains the origin of the deceptively spurious pre-factor of Planck's constant h to the classical partition function.

The inverse map: classical to quantum I

Consider classical 1D Ising model in the absence of an external magnetic field,

$$H_c = -\frac{K}{\beta}\sum_{<ij>}(s_i s_j - 1), \quad s_i = \pm 1. \tag{52}$$

The transfer matrix would be,

$$T = I + e^{-2K}\sigma_x. \tag{53}$$

For an N-site chain,

$$Z = \mathrm{Tr}\left\{T^N\right\} = (1 - e^{-2K})^N + (1 + e^{-2K})^N. \tag{54}$$

In the $N \to \infty$ limit, the correlation length approaches,

$$\xi = -a \ln \tanh K \approx \frac{ae^{2K}}{2} \;(K \gg 1). \tag{55}$$

The inverse map: classical to quantum II

In the scaling limit ($\xi \gg a$), H_c has the same partition function as,

$$H_q = -\frac{\Delta}{2}\sigma_x, \tag{56}$$

at inverse temperature $\beta = \dfrac{Na}{\xi\Delta}$.

This is the quantum thermal partition function of a single Ising spin.

Zero temperature quantum system maps to an infinite classical chain and an infinitely correlated classical chain corresponds to a continuum quantum system.

And that's a wrap!

Thank you :)

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