Quantum many-body systems (8.513 fa19)
Lecture note 2

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https://stellar.mit.edu/S/course/8/fa19/8.513/index.html

The first step to build a theory: how to label states?

One particle states

- How to label states of one boson in 1D space? $\to |x\rangle$. The most general state $|\phi\rangle = \int \mathrm{d}x \psi(x)|x\rangle$
- Energy eigenstates (momentum eigenstates) $|k\rangle = \int \mathrm{d}x \mathrm{e}^{\mathrm{i}\, kx}|x\rangle$, where wave vector $k = \text{int.} \times \frac{2\pi}{L}$. (The space is a 1D ring of size L)

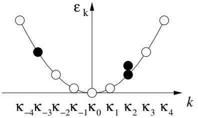
- Momentum $= p = \hbar k$.
- Energy $= \epsilon_k = \frac{\hbar^2 k^2}{2M}$ (Or $\epsilon_k = \hbar|k|c$ for massless photons)

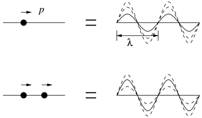
Many-particle states

- Label all zero-, one-, two-, three-, ... boson states:
  $|\emptyset\rangle$
  $|k_1\rangle$
  $|k_1, k_2\rangle$, $k_1 \leq k_2$ ($|k_1, k_2\rangle = |k_2, k_1\rangle$ for identical particles)
  $|k_1, k_2, k_3\rangle$, $k_1 \leq k_2 \leq k_3$
  ... ...
- Label all zero-, one-, two-, three-, ... boson states
  (The **second quantization** – quantum field theory of bosons):
  $n_k \equiv$ the number of bosons with wave vector k.
  $|\{n_k = 0\}\rangle$ is the ground state. $|\{n_k \neq 0\}\rangle$ is an excitated state.
  $|\{n_k = 0\}\rangle = |\emptyset\rangle$. No boson
  $|\{n_{k_1} = 1, \text{others } = 0\}\rangle = |k_1\rangle$. One boson
  $|\{n_{k_1} = 1, n_{k_2} = 1, \text{others } = 0\}\rangle = |k_1, k_2\rangle = |k_2, k_1\rangle$.
  $|\{n_{k_1} = 1, n_{k_2} = 1, n_{k_3} = 1, \text{others } = 0\}\rangle = |k_1, k_2, k_3\rangle = |k_2, k_3, k_1\rangle = \cdot\cdot$
  $|\{n_{k_1} = 2, n_{k_2} = 1, \text{others } = 0\}\rangle = |k_1, k_1, k_2\rangle = |k_1, k_2, k_1\rangle = \cdots$.

A many-boson system with no interaction $=$ a collection of decoupled harmonic oscillators

n_k $\to$ the occupation number of the bosons on orbital-k.





- If we ignore the interaction between bosons $|\{n_k\}\rangle$ is an energy eigenstate with energy $E = \sum_k n_k \epsilon_k$
- The above energy can be viewed as the total energy of a collection of decoupled harmonic oscillators. The oscillators are labeled by $k = \text{int.} \times \frac{2\pi}{L}$. The oscillator labeled by k has a frequency $\omega_k = \epsilon_k/\hbar$.
- A collection of decoupled harmonic oscillators $=$ vibration modes of a vibrating string. The two polarizations of bosons $\to$ two directions of string vibrations

  $\to$ **quantum field theory** of 1D boson gas.

Many-body Hamiltonian for non-interacting bosons

For 1D non-interacting bosons (with $0, 1, 2, 3, \cdots$ bosons)

$$\hat{H} = \sum_k (\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2})\hbar\omega_k, \quad \hbar\omega_k = \epsilon_k = \frac{\hbar^2 k^2}{2m}, \quad k = \text{int.} \times \frac{2\pi}{L}$$

raising-lowering operator

$$\hat{a}_k = \sqrt{\frac{m\omega_k}{2\hbar}}(\hat{x}_k + \frac{\mathrm{i}}{m\omega_k}\hat{p}_k), \qquad [\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{k,k'}$$

$$\hat{a}_k^\dagger \hat{a}_k |n_k\rangle = n_k |n_k\rangle, \qquad \hat{a}_k^\dagger |n_k\rangle = |n_k + 1\rangle, \quad \hat{a}_k |n_k\rangle = |n_k - 1\rangle.$$

- All the energy eigenstates are labeled by $|\{n_k\}\rangle = \bigotimes_k |n_k\rangle$.
  The total energy $E_{\text{tot}} = \sum_k (n_k + \frac{1}{2})\epsilon_k$.
  The total particle number $N = \sum_k n_k$.
  $\hat{a}_k^\dagger, \hat{a}_k$ are also creation-annihilation operator of bosons.

Many-body Hamiltonian for bosons on lattice

- Infinite problem on quantum field theory:
  The vaccum energy $E_0 = 0$ or $E_0 = \sum_k \frac{1}{2}\epsilon_k$?
  The right answer $E_0 = \sum_k \frac{1}{2}\epsilon_k = \infty$
- Non-interacting bosons on a lattice

  For 1D non-interacting bosons (with $0, 1, 2, 3, \cdots$ bosons)

$$\hat{H} = \sum_{k\in BZ} (\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2})\epsilon_k, \quad \epsilon_k = 2t[1 - \cos(ka)],$$

$$k = \text{int.} \times \frac{2\pi}{L} \in [-\frac{\pi}{a}, \frac{\pi}{a}].$$

- The vacuum energy now is finite

$$E_0 = \sum_{k\in BZ} \frac{1}{2}\epsilon_k = L\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\mathrm{d}k}{2\pi} 2t[1 - \cos(ka)] = L\frac{2t}{a} = 2tN.$$

Many-body Hamiltonian for interacting bosons on lattice

- The total particle number operator

$$\hat{N} = \sum_{k \in BZ} \hat{a}_k^\dagger \hat{a}_k = \sum_i \hat{\varphi}_i^\dagger \hat{\varphi}_i, \qquad [\hat{\varphi}_i, \hat{\varphi}_j^\dagger] = \delta_{ij}.$$

$$\hat{a}_k = \sum_{x_i} N^{-1/2} \mathrm{e}^{\mathrm{i}\, k x_i} \hat{\varphi}_i, \quad x_i = a\ i, \quad i = 1, \cdots, N;$$

- $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ is the number operator for bosons on orbital k.
- $\hat{n}_i = \hat{\varphi}_i^\dagger \hat{\varphi}_i$ is the number operator for bosons on site i. $\hat{\varphi}_i^\dagger, \hat{\varphi}_i$ are creation-annihilation operator of bosons at site-i.

- Many-body Hamiltonian for interacting bosons

$$H = \sum_k (\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2})\epsilon_k - \sum_i \mu \hat{n}_i + \sum_{i \leq j} V_{ij} \hat{n}_i \hat{n}_j$$

$$= \sum_k \frac{1}{2}(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_k \hat{a}_k^\dagger)\epsilon_k - \sum_i \mu \hat{\varphi}_i^\dagger \varphi_i + \sum_{i \leq j} V_{ij} \hat{\varphi}_i^\dagger \hat{\varphi}_i \hat{\varphi}_j^\dagger \hat{\varphi}_j$$

$$= \sum_i \left[t(\hat{\varphi}_i^\dagger \hat{\varphi}_i + \hat{\varphi}_i \hat{\varphi}_i^\dagger) - t(\hat{\varphi}_{i+1}^\dagger \hat{\varphi}_i + \hat{\varphi}_i^\dagger \hat{\varphi}_{i+1}) \right] - \sum_i \mu \hat{\varphi}_i^\dagger \varphi_i + \sum_{i \leq j} V_{ij} \hat{\varphi}_i^\dagger \hat{\varphi}_i \hat{\varphi}_j^\dagger \hat{\varphi}_j$$

Hard-core bosons and spin-1/2 systems

- Assume on-site interaction $V_{ij} = U\delta_{ij}, \quad \mu = U + 2B + t$.
  The low energy sector for interaction $U\hat{n}_i\hat{n}_i - \mu\hat{n}_i, \quad U \to +\infty$
  $\to n_i = 0, 1\ (\downarrow, \uparrow)$ or

$$n_i = \frac{\sigma_i^z - 1}{2}, \quad \hat{\varphi}_i = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma_i^- = \frac{\sigma_i^x - \mathrm{i}\sigma_i^y}{2}.$$

  Many-body Hamiltonian for interacting bosons = a spin-1/2 system

$$\begin{aligned} H &= \sum_i \Big[-t(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) - B\sigma_i^z \Big] \\ &= \sum_i \Big[-J(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) - B\sigma_i^z \Big], \qquad J = \frac{1}{2}t \end{aligned}$$

- Phase diagram:

$B < 0 : |\downarrow \cdots \downarrow\rangle \qquad B \sim 0 : |\rightarrow \cdots \rightarrow\rangle \qquad B > 0 : |\uparrow \cdots \uparrow\rangle$

$\longrightarrow B$

0-boson/site Superfluid 1-boson/site (Mott insulator)

Many-body Hamiltonian

- Consider a system formed by two spin-1/2 spins. The spin-spin interaction: $H = J(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z)$.
  where $\sigma_i^{x,y,z}$ are the Pauli matrices acting on the i^{th} spin.
  $J < 0 \to$ ferromagnetic, $J > 0 \to$ antiferromagnetic.
  Is H a two-by-two matrix? In fact
  $H = -J[(\sigma^x \otimes I)\cdot(I \otimes \sigma^x) + (\sigma^y \otimes I)\cdot(I \otimes \sigma^y) + (\sigma^z \otimes I)\cdot(I \otimes \sigma^z)]$
  H is a four-by-four matrix:
  $$\sigma_1^z\sigma_2^z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \sigma_1^x\sigma_2^x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \sigma_1^x\sigma_2^z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$
- $\sigma_i^z = I \otimes \cdots \otimes I \otimes \sigma^z \otimes I \otimes \cdots \otimes I$ is a $2^{N_{\text{site}}}$-dimensional matrix
  Example: An 1D ring formed by L spin-1/2 spins:
  $$H = -\sum_{i=1}^{L} \sigma_i^x \sigma_{i+1}^x - h\sum_{i=1}^{L} \sigma_i^z$$
  – transverse Ising model. H is a $2^L \times 2^L$ matrix.

Hard-core bosons and spin-1 systems

- Assume on-site interaction to have a form $U[(n_i - 1)^4 - (n_i - 1)^2]$. The low energy sector for the interaction: $n_i = 0, 1, 2$ $(\downarrow, 0, \uparrow)$ or

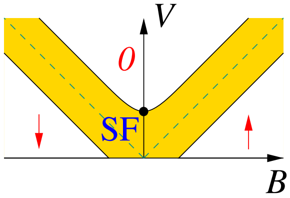
$$n_i = S_i^z - 1, \quad \hat{\varphi}_i = S_i^- .$$

Many-body Hamiltonian for interacting bosons = a spin-1 system

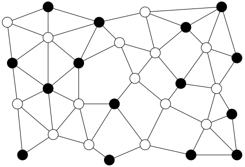
$$H = \sum_i \Big[- t(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) - BS_i^z + V(S_i^z)^2 \Big]$$
$$= \sum_i \Big[- J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - BS_i^z + V(S_i^z)^2 \Big].$$

- B-V phase diagrame ($J = 1$, superfliud: $\langle S^x \rangle, \langle S^y \rangle \neq 0$)

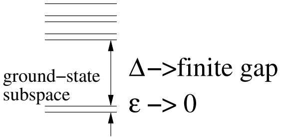
The filled dot represent a different critical point with (emergent) particle-hole symmetry



Condensed matter: A local many-body quantum system



- A many-body quantum system
  $= $ Hilbert space $\mathcal{V}_{tot}$ + Hamiltonian H
  - The locality of the Hilbert space:
    $\mathcal{V}_{tot} = \otimes_{i=1}^{N} \mathcal{V}_i$
  - The i also label the vertices of a graph
- A local Hamiltonian $H = \sum_x H_x$ and H_x are local hermitian operators acting on a few neighboring $\mathcal{V}_i$'s.
- A quantum state, a vector in $\mathcal{V}_{tot}$:
  $|\Psi\rangle = \sum \Psi(m_1, ..., m_N)|m_1\rangle \otimes ... \otimes |m_N\rangle$,
  $|m_i\rangle \in \mathcal{V}_i$
- A gapped Hamiltonian has the following spectrum as $N \to \infty$
  (eg $H = -\sum(J\sigma_i^z\sigma_{i+\delta}^z + h\sigma_i^x)$)

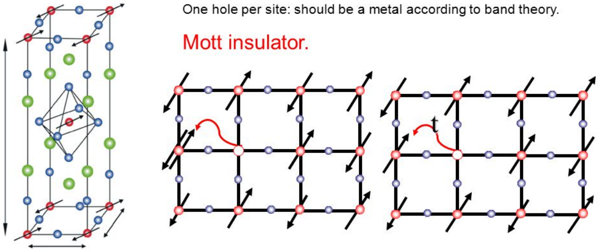


Mott insulator and spin system (magnetic system)

Four states per site $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

$E_{\text{site}} = U n_\uparrow n_\downarrow + \mu(n_\uparrow + n_\downarrow) = \frac{1}{2} U (n_\uparrow + n_\downarrow - 1)^2$ if $\mu = -\frac{1}{2} U$.

CuO plane: strongly-correlated electron system



Cu^{2+} O^{2-} La^{3+}

Undoped CuO_2 plane: Mott Insulator due to e^- - e^- interaction Virtual hopping induces AF exchange $J=4t^2/U$

CuO_2 plane with doped holes:

$La^{3+} \to Sr^{2+}$: $La_{2-x}Sr_xCuO_4$

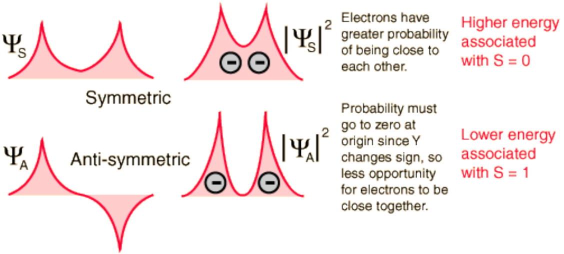
- What is the effective spin interaction?

Exchange interaction

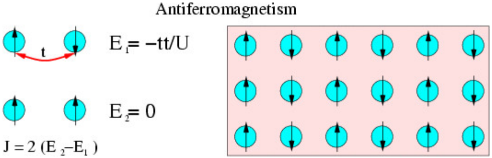
- Ferromagnetic exchange:

  $|\Psi\rangle = \Psi_A(x_1, x_2)|\uparrow\uparrow\rangle$, $|\Psi\rangle = \Psi_S(x_1, x_2)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

  Plot as function $x_1 - x_2$ with fixed $x_1 + x_2 = 0$



- Antiferromagnetic superexchange



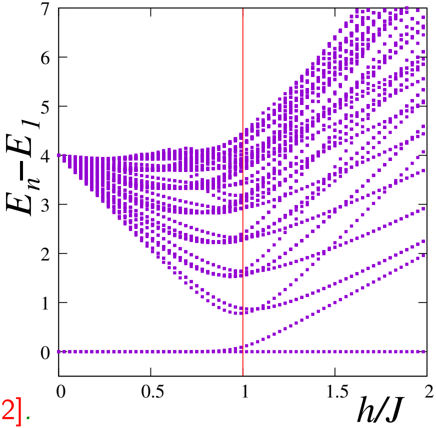
Many-body spectrum using Octave (Matlab or Julia)

Transverse Ising model on a ring of L site:

$$H = -J \sum_{i=1}^{L} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=1}^{L} \sigma_i^z$$

H is an 2^L-by-2^L matrix, whose eigenvalues can be computed via the following Octave code (the code also run in Matlab or Julia with minor modifications):

```
X=sparse([0,1;1,0]); Z=sparse([1,0;0,-1]); XX=kron(X,X);
L=13; h=1.0; J=1.0
H=-kron(kron(X, speye(2^(L-2)) ),X);
for i=1:L-1
  H=H - kron( speye(2^(i-1)), kron(J*XX, speye(2^(L-1-i)))) ;
end
for i=1:L
  H=H - kron( speye(2^(i-1)), kron(h*Z, speye(2^(L-i)))) ;
end
eigs( H , 10, 'sa') # compute the lowest 10 eigenvalues
```



The 100 lowest energy eigenvalues for $L = 16$, as functions of $h/J \in [0, 2]$.

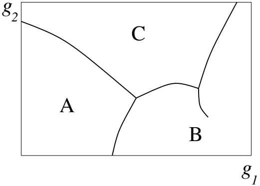
Quantum phases and quantum phase transitions

- Phases are defined through phase transitions.

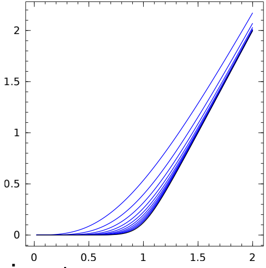
  What are phase transitions?

  As we change a parameter g in Hamiltonian $H(g)$, the ground state energy density $\epsilon_g = E_g/V$ or the average of a local operator $\langle \hat{O} \rangle$ may have a singularity at g_c: the system has a phase transition at g_c.

  The Hamiltonian $H(g)$ is a smooth function of g. How can the ground state energy density ϵ_g be singular at a certain g_c?



$E_2 - E_1$ of trans. Ising for $L = 3, \cdots, 13$



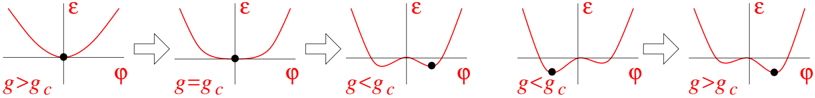
- There is no singularity for finite systems. Singularity appears only for infinite systems.
- Spontaneous symmetry breaking is a mechanism to cause a singularity in ground state energy density ϵ_g.
  $\to$ Spontaneous symmetry breaking causes phase transition.

Symmetry breaking theory of phase transition

It is easier to see a phase transition in the semi classical approximation of a quantum theory.

- Variational ground state $|\Psi_\phi\rangle$ for H_g is obtained by minimizing energy $\epsilon_g(\phi) = \frac{\langle\Psi_\phi|H_g|\Psi_\phi\rangle}{V}$ against the variational parameter ϕ. $\epsilon_g(\phi)$ is a smooth function of ϕ and g. How can its minimal value $\epsilon_g \equiv \epsilon_g(\phi_{min})$ have singularity as a function of g?
- Minimum splitting $\to$ singularity in $\frac{\partial^2\epsilon_g}{\partial g^2}$ at g_c. Second order trans. State-B has less symmetry than state-A. State-A $\to$ State-B: spontaneous symmetry breaking.

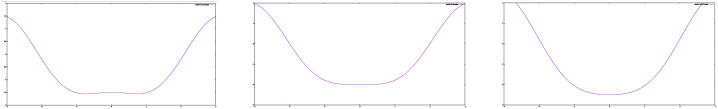
- For a long time, we believe that
phase transition = change of symmetry
the different phases = different symmetry.



- Minimum switching $\to$ singularity in $\frac{\partial\epsilon_g}{\partial g}$ at g_c. First order trans.

Example: meanfield symmetry breaking transition

Consider a transverse field Ising model $H = \sum_i -J\sigma_i^x \sigma_{i+1}^x - h\sigma_i^z$
Use trial wave function $|\Psi_\phi\rangle = \otimes_i |\psi_i\rangle$, $|\psi_i\rangle = \cos\frac{\phi}{2}|\uparrow\rangle + \sin\frac{\phi}{2}|\downarrow\rangle$
to estimate the ground state energy
$\langle\Psi_\phi|H|\Psi_\phi\rangle = -\sum\langle\psi_i|\sigma_i^x|\psi_i\rangle\langle\psi_{i+1}|\sigma_{i+1}^x|\psi_{i+1}\rangle - h\sum\langle\psi_i|\sigma_i^z|\psi_i\rangle$.
$= (2J\cos\frac{\phi}{2}\sin\frac{\phi}{2})^2 - h(\cos^2\frac{\phi}{2} - \sin^2\frac{\phi}{2}) = \sin^2\phi - h\cos\phi$
Phase transition at $h/J = 2$. ($h/J = 1.5, 2.0, 2.5$)



Order parameter and symmetry-breaking phase transition

ϕ or σ_i^x are order parameters for the Z_2 symm.-breaking transition:

- Under Z_2 (180° S^z rotation), $\phi \to -\phi$ or $\sigma_i^x \to -\sigma_i^x$
- In symmetry breaking phase $\phi = \pm\phi_0$, $\langle\sigma_i^x\rangle = \pm$.

In symmetric phase $\phi = 0$, $\langle\sigma_i^x\rangle = 0$. (**Classical picture**)

Ginzberg-Landau theory of continuous phase transition

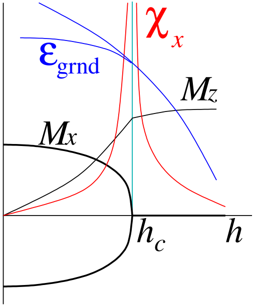
- Quantum Z_2-Symmetry: generator $U = \prod_j \sigma^z_j$, $U^2 = 1$.
  Symmetry trans.: $U\sigma^z_i U^\dagger = \sigma^z_i$, $U\sigma^x_i U^\dagger = -\sigma^x_i$, $U\sigma^y_i U^\dagger = -\sigma^y_i$.
  $\to UHU^\dagger = H$. If $H|\psi\rangle = E_{\text{grnd}}|\psi\rangle$, then $UH|\psi\rangle = E_{\text{grnd}}U|\psi\rangle \to$
  $UHU^\dagger U|\psi\rangle = E_{\text{grnd}}U|\psi\rangle \to HU|\psi\rangle = E_{\text{grnd}}U|\psi\rangle$
  Both $|\psi\rangle$ and $U|\psi\rangle$ are ground states of H:
  Either $|\psi\rangle \propto U|\psi\rangle$ (symmetric) or $|\psi\rangle \not\propto U|\psi\rangle$ (symm.-breaking).
- Trial wave function $|\Psi_\phi\rangle = \bigotimes_i (\cos\frac{\phi}{2}|\uparrow\rangle_i + \sin\frac{\phi}{2}|\downarrow\rangle_i)$:
  $U|\Psi_\phi\rangle = |\Psi_{-\phi}\rangle \to$
  $\langle\Psi_\phi|H|\Psi_\phi\rangle = \langle\Psi_\phi|U^\dagger UHU^\dagger U|\Psi_\phi\rangle = \langle\Psi_{-\phi}|H|\Psi_{-\phi}\rangle \to$
  $\epsilon(h,\phi) = \epsilon(h,-\phi)$
- If $|\Psi_{\phi=0}\rangle$ is the ground state $\to$ symmetric phase.
  If $|\Psi_{\phi\neq 0}\rangle$ is the ground state $\to$ symmetry breaking phase.
- Near the phase transition ϕ is small $\to$

$$\epsilon(h,\phi) = \epsilon_0(h) + \frac{1}{2}a(h)\phi^2 + \frac{1}{4}b(h)\phi^4 + \cdots$$

  Transition happen at $a(h_c) = 0$.

Properties near the $T = 0$ (quantum) phase transition

- Ground state energy density:
  $\phi = 0,\ \epsilon_{\text{grnd}}(h) = \epsilon_0(h)$ if $a(h) > 0$
  $\phi = \pm\sqrt{\frac{-a}{b}},\ \epsilon_{\text{grnd}}(h) = \epsilon_0(h) - \frac{1}{4}\frac{a(h)^2}{b}$ if $a(h) < 0$
  $\epsilon_{\text{grnd}}(h)$ is non-analytic at the transition point: $a(h) = a_0(h - h_c)$:
  $$\epsilon_{\text{grnd}}(h) = \begin{cases} \epsilon_0(h), & h > h_c \\ \epsilon_{\text{grnd}}(h) = \epsilon_0(h) - \frac{1}{4}\frac{a_0(h-h_c)^2}{b}, & h < h_c \end{cases}$$
- Magnetization in z-direction: $M_z = \frac{\partial \epsilon_{\text{grnd}}(h)}{\partial h}$.
  $M_z = \frac{\partial \epsilon_0(h)}{\partial h}, \quad h > h_c$
  $M_z = \frac{\partial \epsilon_0(h)}{\partial h} - \frac{1}{2}\frac{a_0(h-h_c)}{b}, \quad h < h_c$
- Magnetic susceptibility in x-direction:
  Magnetization in x-dir.: $M_x = \langle \sigma^x \rangle = \sin\phi$
  From $\epsilon(h, \phi, h_x) = \frac{1}{2}a(h)\phi^2 - h_x\phi + \cdots$
  $\to M_x = \phi = \frac{1}{a(h)} \to \chi_x = \frac{1}{a(h)}$



Quantum picture of continuous phase transition

No symmetry breaking in quantum theory according to a theorem: If $[H, U] = 0$, then H and U share a commom set of eigenstates.

In particular, the ground state $|\Psi_{\text{grnd}}\rangle$ of H, is an eigenstate of U: $U|\Psi_{\text{grnd}}\rangle = \mathrm{e}^{\mathrm{i}\theta}|\Psi_{\text{grnd}}\rangle$. No symmetry breaking.

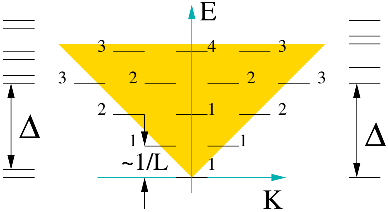
In our above discussion based on semi classical approximation, $|\Psi_\phi\rangle$ and $|\Psi_{-\phi}\rangle$ are not degenerate ground states. The true ground state is $|\Psi_{\text{grnd}}\rangle = |\Psi_\phi\rangle + |\Psi_{-\phi}\rangle$ which do not break the symmetry.

- **Quantum picture**: Symmetry-breaking phase has $\langle\Psi_{\text{grnd}}|\sigma_i^x|\Psi_{\text{grnd}}\rangle = 0$ for the true ground state. But the ground states are nearly degenerate: $|\Psi_{\text{grnd}}\rangle = |\Psi_\phi\rangle + |\Psi_{-\phi}\rangle$ and $|\Psi'_{\text{grnd}}\rangle = |\Psi_\phi\rangle - |\Psi_{-\phi}\rangle$ has an exponentially small energy separation $\Delta \sim \mathrm{e}^{-L/\xi}$.

Discrete-symmetry-breaking phase has exponentially nearly degenerate ground states, which are locally deferent.

Collective mode of order parameter ϕ: guess

- From the energy $\epsilon(h,\phi) = \epsilon_0(h) + \frac{1}{2}a(h)\phi^2 + \frac{1}{4}b(h)\phi^4 + \cdots$
  $\to$ Restoring force $f = -a\phi - b\phi^3$ $\to$ EOM $\rho\ddot{\phi} = -a\phi - b\phi^3$.
- $k \neq 0$ mode: $\epsilon(h,\phi) = \frac{1}{2}g(\partial_x\phi)^2 + \frac{1}{2}a(h)\phi^2 + \frac{1}{4}b(h)\phi^4 + \cdots$
  Restoring force $f = g\partial_x^2\phi - a\phi - b\phi^3$
  $\to$ EOM $\rho\ddot{\phi} = g\partial_x^2\phi - a\phi - b\phi^3$. *Where does ρ come from?*
- Dispersion of collective mode:
  $\omega_k = \sqrt{\frac{gk^2+a}{\rho}}$.
  Energy gap:
  $\Delta = \sqrt{\frac{a(h)}{\rho}} = \sqrt{\frac{a_0(h-h_c)}{\rho}}$.
  At the critical point:
  Gapless = diverging susceptibility



Continuous quantum phase transition between gapped phases = gap closing phase transition

Continuous quantum phase transition between gapless phases : more low energy modes at the critical point.

Collective mode of order parameter ϕ: calculate

Consider a transverse field Ising model $H = -\sum_i (J\sigma_i^x \sigma_{i+1}^x + h\sigma_i^z)$.

Trial wave function $|\Psi_{\phi_i}\rangle = \otimes_i |\phi_i\rangle$, $|\phi_i\rangle = \frac{|\uparrow\rangle + \phi_i|\downarrow\rangle}{\sqrt{1+|\phi_i|^2}}$

$$\langle \sigma_i^x \rangle = \frac{\phi_i + \phi_i^*}{1+|\phi_i|^2}, \quad \langle \sigma_i^z \rangle = \frac{1-|\phi_i|^2}{1+|\phi_i|^2}.$$

- Average energy

$$\bar{H} = -\sum_i \Big[J \frac{(\phi_i + \phi_i^*)(\phi_{i+1} + \phi_{i+1}^*)}{(1+|\phi_i|^2)(1+|\phi_{i+1}|^2)} + h \frac{1-|\phi_i|^2}{1+|\phi_i|^2} \Big]$$

Geometric phase term

$$\langle \phi_i | \frac{\mathrm{d}}{\mathrm{d}t} | \phi_i \rangle = \frac{\phi_i^* \dot{\phi}_i}{1+|\phi_i|^2} + \frac{\mathrm{d}}{\mathrm{d}t} \#$$

Phase space Lagrangian (for $\phi_i = q_i + \frac{\mathrm{i}}{2} p_i$ small, and $\hbar = 1$)

$$L = \langle \Phi_{\phi_i} | \mathrm{i} \tfrac{\mathrm{d}}{\mathrm{d}t} - H | \Phi_{\phi_i} \rangle = \textstyle\sum_i \mathrm{i} \phi_i^* \dot{\phi}_i + J(\phi_i + \phi_i^*)(\phi_{i+1} + \phi_{i+1}^*) - 2h|\phi_i|^2$$

$$= \textstyle\sum_i \big[p_i \dot{q}_i + 4J q_i q_{i+1} - 2h(q_i^2 + \frac{1}{4} p_i^2) \big]$$

Collective mode of order parameter ϕ: calculate

EOM:

$$\dot q_i = \frac{\partial \bar H}{\partial p_i} = \frac{h}{2} p_i,, \qquad \dot p_i = -\frac{\partial \bar H}{\partial q_i} = 4J(q_{i+1} + q_{i-1}) - 4hq_i$$

in k-space ($q_i = \sum_k N^{-1/2} \mathrm{e}^{\mathrm{i}\, kia} q_k,\ p_i = \sum_k N^{-1/2} \mathrm{e}^{\mathrm{i}\, kia} p_k$):

$$\dot q_k = \frac{h}{2} p_k,, \qquad \dot p_k = 4(J\mathrm{e}^{\mathrm{i}\, ka} + J\mathrm{e}^{-\mathrm{i}\, ka} - h) q_k$$

k label harmonic oscillators with EOM

$$\ddot q_k = 2h[2\cos(ka) - h] q_k \quad \to \quad -\omega_k^2 = 2h[2J\cos(ka) - h]$$

The dispersion of the collective mode

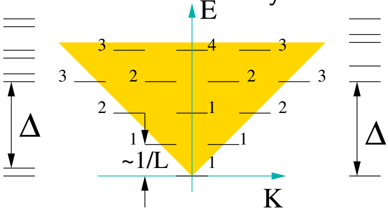
$$\omega_k = \sqrt{2h[h - 2J\cos(ka)]}$$

- For $h > 2J$, gap $= \sqrt{2h(h-2J)}$.
  For $h = 2J$, gapless mode with velocity $v = 2aJ$ and $\omega_k = v|k|$.

Many-body spectrum at the critical point

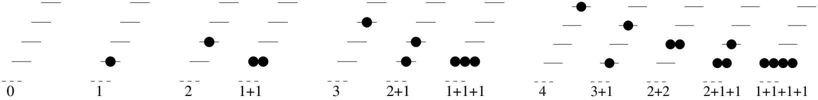
- At the critical point, the gapless excitation is described by a real scaler field ϕ (or q_i) with EOM:

$$\ddot{\phi} = v^2 \partial_x^2 \phi.$$



= an oscillator for every $k = \frac{2\pi}{L} n$
= a wave mode with $\omega_k = v|k|$
= a boson with $\epsilon(p) = v|p|$

- Many-body spectrum for right movers:



1 1 2 3 5

Do not count for the $k = 0$ orbital.

- Total energy and total momentum for right movers $E = vK$.

Magic at critical point: Emergence of Lorentz invariance $\epsilon = vk$. Emergence of independent right-moving and left-moving sectors (extra degeneracy in mony-body spectrum): conformal invariance

The property of $\boldsymbol{k} = 0$ mode

- Now consider transverse Ising model in d dimensions ($g \sim J, h$)
$$L = \sum_{\boldsymbol{i}} \sum_{\mu = x, y, \cdots} \left[p_{\boldsymbol{i}} \dot{q}_{\boldsymbol{i}} + 4J q_{\boldsymbol{i}} q_{\boldsymbol{i}+\mu} \right] - \sum_{\boldsymbol{i}} \left[2h(q_{\boldsymbol{i}}^2 + \frac{1}{4} p_{\boldsymbol{i}}^2) - g q_{\boldsymbol{i}}^4 \right]$$
The transition point now is at $h = 2dJ$
- At the critical point $h = 2dJ$,
the $\boldsymbol{k} = 0$ mode is described by the Lagrangian
$$\begin{aligned} L &= Np\dot{q} - \frac{N}{2} hp^2 - Ngq^4 \\ &= \tilde{p}\dot{\tilde{q}} - \frac{h}{2}\tilde{p}^2 - \frac{g}{N}\tilde{q}^4, \qquad \tilde{p} = \sqrt{N}p, \quad \tilde{q} = \sqrt{N}q. \end{aligned}$$
- The zero-point energy from the $\boldsymbol{k} = 0$ mode $\tilde{p}\tilde{q} \sim 1 \to \tilde{q} \sim N^{1/6}$
$$\frac{h}{2}\tilde{p}^2 + \frac{g}{N}\tilde{q}^4 \sim \frac{h}{2}\tilde{q}^{-2} + \frac{g}{N}\tilde{q}^4 \sim JN^{-1/3}$$
The non-linear term is important for $\boldsymbol{k} = 0$ mode.

\- The zero-point energy from the $\boldsymbol{k}$ mode (ignoring the non-linear term) $Jk \sim JN^{-1/d}|_{k \sim N^{-1/d}}$

The non-linear effect for $\boldsymbol{k}$ mode

- At the critical point $h = 2dJ$,
  the $\boldsymbol{k}$ mode is described by the Lagrangian

$$L = Np\dot{q} - JN\boldsymbol{k}^2 q^2 - \frac{N}{2}hp^2 - Ngq^4$$
$$= \tilde{p}\dot{\tilde{q}} - J\boldsymbol{k}^2\tilde{q}^2 - \frac{h}{2}\tilde{p}^2 - \frac{g}{N}\tilde{q}^4, \qquad \tilde{p} = \sqrt{N}p, \quad \tilde{q} = \sqrt{N}q.$$

- The zero-point energy from the $\boldsymbol{k}$ mode $\tilde{p}\tilde{q} \sim 1 \to \tilde{p} \sim 1/\tilde{q} \sim \sqrt{k}$

$$J\boldsymbol{k}^2\tilde{q}^2 + \frac{h}{2}\tilde{p}^2 + \frac{g}{N}\tilde{q}^4 \sim Jk + \frac{h}{2}k + \frac{g}{Nk^2}$$

  The non-linear term is important if

$$\frac{g}{Nk^2} > Jk \quad \text{or} \quad k < \frac{1}{N^{1/3}}$$

- Since the smallest k is $\frac{1}{N^{1/d}}$. For $d > 3$ there is no $\boldsymbol{k}$ satisfying the above condition (except $\boldsymbol{k} = 0$). We can ignore the non-linear term
- For $d \leq 3$, we cannot ignore the non-linear term.

Quantum fluctuations: relevant/irrelevant perturbations

EOM of Z_2 order parameter for the $d+1$D-transverse Ising model

$$\rho\ddot{\phi} = g\partial_{\boldsymbol{x}}^2\phi + a\phi + b\phi^3$$

Is the $b\phi^3$ term importent at the transition point $a = 0$?

- The action $S = \int \mathrm{d}t\mathrm{d}^d\boldsymbol{x}\ [\frac{1}{2}\rho(\dot{\phi})^2 - \frac{1}{2}g(\partial_{\boldsymbol{x}}\phi)^2 - \frac{1}{2}a\phi^2 - \frac{1}{4}b\phi^4]$

- Treating the above as a quantum system with quatum fluctuations, the term $\frac{1}{4}b\phi^4$ is irrelevant if dropping it does not affect the low energy properties at critical point $a = 0$. Otherwise, it is revelvent.

- Rescale t to make $\rho = g$ and rescale ϕ to make $\rho = g = 1$.

- Consider the fluctuation at length scale ξ. The action for such fluctuation is $S_\xi = \int \mathrm{d}t\ [\frac{1}{2}\xi^d(\dot{\phi})^2 - \frac{1}{2}\xi^{d-2}\phi^2 - \frac{1}{4}b\xi^d\phi^4]$

  $\rightarrow$ Oscillator with mass $M = \xi^d$ and spring constant $K = \xi^{d-2}$.
  Oscillator frequency $\omega = \sqrt{K/M} = 1/\xi$.
  Potential energy for quantum fluctuation $E = \frac{1}{2}\omega = \frac{1}{2}\xi^{d-2}\phi^2$.
  Fluctuation $\phi^2 = \xi^{1-d}$.

  Compare $\xi^{d-2}\phi^2$ and $b\xi^d\phi^4$: $\frac{b\xi^d\phi^4}{\xi^{d-2}\phi^2} = b\xi^{3-d}$ for $\xi \to \infty$.

  The $b\phi^4$ term is irrelevant for $d > 3$. Relevant for $d < 3$

Simple rules to test relevant/irrelevant perturbations

- After rescaling t to make $\rho = g$ and rescaling ϕ to make $\rho = g = 1$, the action becomes $S = \int \mathrm{d}t\mathrm{d}^d x \; [\frac{1}{2}(\dot{\phi})^2 - \frac{1}{2}(\partial_x\phi)^2 - \frac{1}{2}a\phi^2 - \frac{1}{4}b\phi^4]$
- **Estimate from dimension analysis**:
  $[t] = [L]$, $[S] = [L]^0$.
  $[\phi] = [L]^{\frac{1-d}{2}}$, $[a] = L^{-2}$, $[b] = [L]^{d-3}$

- **Counting dimensions**:
  $[t] = -1$, $[S] = 0$.
  $[\phi] = \frac{d-1}{2}$, $[a] = 2$, $[b] = 3 - d$.
- From the scaling dimensions, we can see that the quantum fluctuations are given by $\phi^2 = L^{1-d}$, and the dimensionless ratio of $L^d \frac{1}{L^2}\phi^2$ and $L^d b\phi^4$ terms is given by $\frac{bL^d\phi^4}{L^{d-2}\phi^2} = bL^{3-d}$

  The $b\phi^4$ term is irrelevant if $[b] < 0$. Relevant if $[b] > 0$.
  The $a\phi^2$ term is always relevant since $[a] = 2 > 0$.

Specific heat at the critical point

- Thermal energy density

$$\epsilon_T = \int_{-\infty}^{+\infty} \frac{\mathrm{d}k}{2\pi} \frac{v|k|}{\mathrm{e}^{v|k|/k_B T} - 1} = 2\frac{k_B^2 T^2}{2\pi v} \int_0^{+\infty} \mathrm{d}x \frac{x}{\mathrm{e}^x - 1} = \frac{k_B^2 T^2}{v} \frac{\pi}{6}$$

where $\int_0^{+\infty} \mathrm{d}x \frac{x}{\mathrm{e}^x - 1} = \frac{\pi^2}{6}$

- Specific heat

$$c_T = \frac{\partial \epsilon_T}{\partial T} = k_B \frac{k_B T}{v} \frac{\pi}{3} = \left(\frac{\pi}{6} k_B \frac{k_B T}{v}\right)_R + \left(\frac{\pi}{6} k_B \frac{k_B T}{v}\right)_L$$

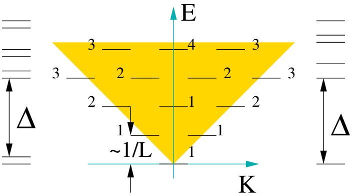
- *The above result is incorrect. The correct one is*

$$c_T = \left(\frac{1}{2}\frac{\pi}{6} k_B \frac{k_B T}{v}\right)_R + \left(\frac{1}{2}\frac{\pi}{6} k_B \frac{k_B T}{v}\right)_L$$

- $\frac{1}{2} = c$ is called the **central charge** = number of modes.
- Many-body spectrum for one right-moving mode ($c = 1$):
$1, 1, 2, 3, 5, 7, 11, \cdots$ = partition number

Specific heat away from the critical point

Away from the critical point, the boson dispersion becomes $\epsilon_k = \sqrt{v^2k^2 + \Delta^2}$ where Δ is the many-body spectrum gap on a **ring** (the energy to create a single boson).



many-body spectrum = spectrum of the set of the oscillators ($\times 2$ in the symmetry breaking phases)

Specific heat

$$c \sim T^\alpha \mathrm{e}^{-\frac{\Delta}{k_B T}}$$

The above result is correct in the symmetric phase, but incorrect in the symmetry breaking phase. The correct one is

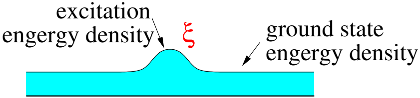
$$c \sim T^\alpha \mathrm{e}^{-\frac{\Delta/2}{k_B T}}$$

What really is a quasiparticle? $\to$ factor 1/2

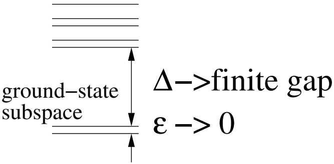
The answer is very different for gapped system and gapless systems. Here, we only consider the definition of quasiparticle for gapped systems.

Consider a many-body system $H_0 = \sum_x H_x$, with ground state $|\Psi_{\text{grnd}}\rangle$.

- a point-like excitation above the ground state is a many-body wave function $|\Psi_\xi\rangle$ that has an energy bump at location ξ:
energy density $= \langle\Psi_\xi|H_{\boldsymbol{x}}|\Psi_\xi\rangle$



More precisely, point-like excitations at locations ξ_i are something that can be trapped by local traps δH_{ξ_i}: $|\Psi_{\xi_i}\rangle$ is the gapped ground state of $H_0 + \sum_i \delta H_{\xi_i}$ – the Hamiltonian with traps.



Local and topological excitations

Consider a many-body state $|\Psi_{\xi_1,\xi_2,\cdots}\rangle$ with several point-like excitations at locations ξ_i.

Can the first point-like excitation at ξ_1 be created by a local operator O_{ξ_1} from the ground state: $|\Psi_{\xi_1,\xi_2,\cdots}\rangle = O_{\xi_1}|\Psi_{\xi_2,\cdots}\rangle$?

$|\Psi_{\xi_1,\xi_2,\cdots}\rangle$ = the ground state of $H_0 + \delta H_{\xi_1} + \delta H_{\xi_1} + \cdots$

$|\Psi_{\xi_2,\cdots}\rangle$ = the ground state of $H_0 + \delta H_{\xi_1} + \cdots$

If yes: the point-like excitation at ξ_1 is a **local** excitation

If no: the point-like excitation at ξ_1 is a **topological** excitation

Local and topological excitations

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$|\Psi_{\xi_1,\xi_2,\cdots}\rangle$ = the ground state of $H_0 + \delta H_{\xi_1} + \delta H_{\xi_1} + \cdots$

$|\Psi_{\xi_2,\cdots}\rangle$ = the ground state of $H_0 + \delta H_{\xi_1} + \cdots$

If yes: the point-like excitation at ξ_1 is a **local** excitation

If no: the point-like excitation at ξ_1 is a **topological** excitation

Example: Consider an 1D Ising model $H_0 = -J\sum_i \sigma^z_i\sigma^z_{i+1}$ with one of the degenerate ground states $|\Psi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$

a state w/ three point-like excitations $|\Psi_{\xi_1\xi_2\xi_3}\rangle = |\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$

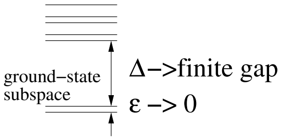
ξ_1 ξ_2 ξ_3 - The point-like excitation at ξ_1 is a spin flip created by $\sigma^x_{\xi_1}$ – a local excitation.

- The point-like excitations at ξ_2, ξ_3 are topological excitations that cannot be created by any local operators.

The pair can be created by a string operator $W_{\xi_2\xi_3} = \prod_{i=\xi_2}^{\xi_3} \sigma^x_i$.

Experimental consequence of topological excitations

- The topological topological excitations are **fractionalized** local excitations: a spin-flip can be viewed as a bound state of two wall excitations spin-flip = wall $\otimes$ wall. $|\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$
- Energy cost of spin-flip $\Delta_{\text{flip}} = 4J$
  Energy cost of domain wall $\Delta_{\text{wall}} = 2J$.
- The many-body spectrum gap on a ring $\Delta = \Delta_{\text{flip}} = 2\Delta_{\text{wall}}$. This gap can be measured by neutron scattering.



- The thermal activation gap measured by specific heat $c \sim T^\alpha e^{-\frac{\Delta_{\text{therm}}}{k_B T}}$ is $\Delta_{\text{therm}} = \Delta_{\text{wall}}$.
  The difference of the neutron gap Δ and the thermal activation gap Δ_{therm} $\to$ fractionalization.

Another example: 1D spin-dimmer state

Consider a $SO(3)$ spin rotation symmetric Hamiltonian H_0 whose ground states are spin-dimmer state formed by spin-singlets, which break the translation symmetry but not spin rotation symmetry:

$$(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)$$
$$\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow$$

- Local excitation = spin-1 excitation

$$(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)\uparrow\uparrow(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)$$

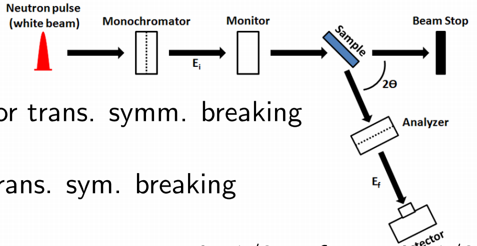
- Topo. excitation (domain wall) = spin-1/2 excitation (spinon)

$$(\uparrow\downarrow)(\uparrow\downarrow)\uparrow(\uparrow\downarrow)(\uparrow\downarrow)(\uparrow\downarrow)\uparrow(\uparrow\downarrow)(\uparrow\downarrow)$$

- Neutron scattering only creates the spin-1 excitation = two spinons. It measures the two-spinon gap (spin-1 gap). Thermal activation sees single spinon gap.

Neutron scattering spectrum

Neutron dump energy-momentum into the sample creating a few excitations.



- Without fractionalization, nor trans. symm. breaking

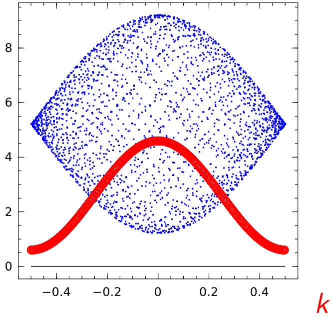
$\epsilon_{\text{spin-1}}(k) = 2.6 + 2\cos(k)$

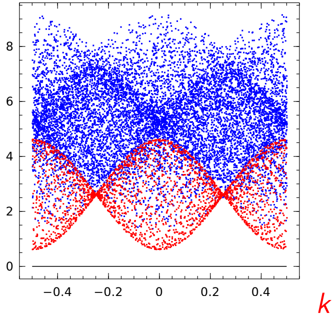
- With fractionalization and trans. sym. breaking

$\epsilon_{\text{spin-1/2}}(k) = \frac{1}{2}\epsilon(2k)_{\text{spin-1}}$

one spin-1 + two spin-1

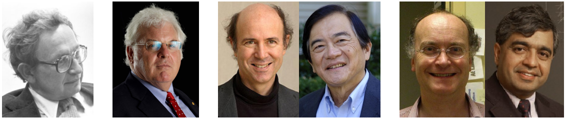
two spin-1/2 + four spin-1/2





2D Spin liquid without symmetry breaking (topo. order)

The spin-1 fractionalization into spin-1/2 spinon can happen in 2D spin liquid without translation and $SO(3)$ spin-rotation symmetry breaking:



- On square lattice:

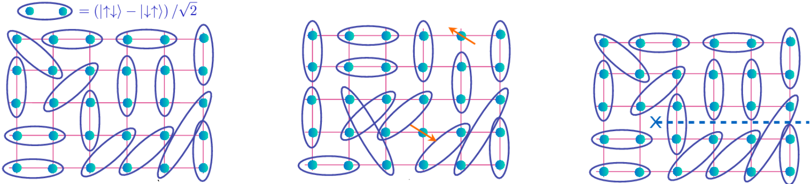
chiral spin liquid $\sum \Psi(RVB)|RVB\rangle$ → topological order

Kalmeyer-Laughlin PRL **59** 2095 (87); Wen-Wilczek-Zee PRB **39** 11413 (89)

Z_2 **spin liquid** $\sum |RVB\rangle$ (emergent low energy Z_2 gauge theory)

Read-Sachdev PRL **66** 1773 (91); Wen PRB **44** 2664 (91)

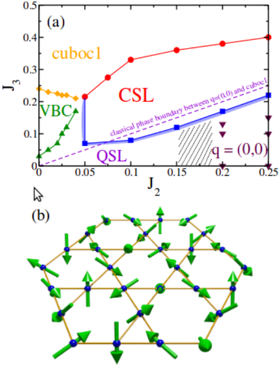
Z_2-charge (spin-1/2) = Spinon. Z_2-vortex (spin-0) = Vison.
Bound state = fermion (spin-1/2).

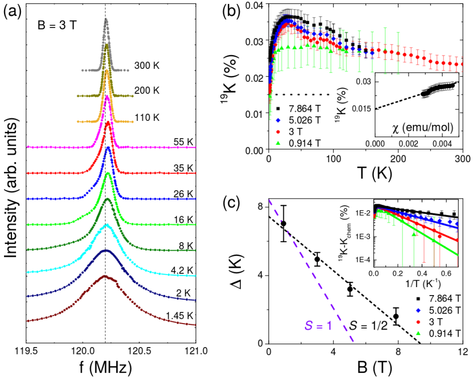


2D Spin liquid without symmetry breaking (topo. order)

- On Kagome lattice:

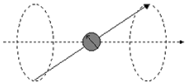
Feng etal arXiv:1702.01658 $Cu_3Zn(OH)_6FBr$

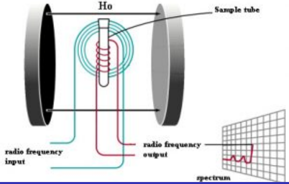




Gong-Zhu-Balents-Sheng arXiv:1412.1571

J_1-J_2-J_3 model





Duality between 1D boson/spin and 1D fermion systems

To obtain the correct critical theory for the transverse Ising model, we need to use the duality between 1D boson/spin systems and 1D fermion systems.

Duality: Two different theories that describe the same thing. Two different looking theories that are equivalent.

- If we view down-spin as vacuum and up-spin as a boson, we can view a hard-core boson system as a spin-1/2 system. Now we view a system of hard-core bosons hopping on a line/ring of L sites as a spin-1/2 system. How to write down the spin Hamiltonian to describe such a boson-hopping system?

  $\sigma^{\pm} = (\sigma^x \pm \mathrm{i}\sigma^y)/2$: σ_i^+ annihilates (σ_i^- creates) a boson at site-i, $|\downarrow\rangle = |1\rangle, |\uparrow\rangle = |0\rangle$. $H_{\text{boson-hc}} = \sum_i (-t\sigma_i^+\sigma_{i+1}^- + h.c.)$ describes a hard-core bosons hopping model.

- Similarly, we can also view a system of spin-less fermions on a line/ring of L sites as a spin-1/2 system. How to write down the spin Hamiltonian for such a fermion-hopping system?

Jordan-Wigner transformation on a 1D line of L sites

- $c_i = \sigma_i^+ \prod_{j<i} \sigma_j^z, \quad \sigma^\pm = (\sigma^x \pm \mathrm{i}\sigma^y)/2$. One can check that
$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{A, B\} \equiv AB - BA.$$
$c_i^\dagger, c_i$ create/annihilate a **fermion** at site-i, $|\downarrow\rangle = |0\rangle, |\uparrow\rangle = |1\rangle$
- Mapping between spin/boson chain and fermion chain:
$c_i^\dagger c_i = \sigma_i^- \sigma_i^+ = (-\sigma_i^z + 1)/2 = n_i$, fermion number operator
$c_i^\dagger c_{i+1} = \sigma_i^- \sigma_{i+1}^+ \sigma_i^z = \sigma_i^- \sigma_{i+1}^+, \qquad c_i c_{i+1} = \sigma_i^+ \sigma_{i+1}^+ \sigma_i^z = -\sigma_i^+ \sigma_{i+1}^+$
- **XY model = fermion model** on an open chain
$H_{\text{fermion}} = \sum_i (-t c_i^\dagger c_{i+1} + h.c.) - \mu n_i \quad \leftrightarrow$
$H_{\text{XY}} = \sum_i (-t\sigma_i^+ \sigma_{i+1}^- + h.c.) + \mu \frac{\sigma_i^z}{2} = \sum_i -\frac{t}{2}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \mu \frac{\sigma_i^z}{2}$
- A phase transition in XY model: as we tune μ through $\mu_c = \pm 2t$, the ground state energy density ϵ_μ has a singularity
$\to$ a phase transition.

How to solve the model exactly to obtain the above result?

The model H_{fermion} or H_{XY} looks not solvable since H's are not a sum of commuting terms.

Make the Hamiltonian into a sum of commuting terms

- The anti-commutation relation

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0, \qquad \{c_i, c_j^\dagger\} = \delta_{ij}$$

is invariant under the unitary transformation of the fermion operators:

$$\tilde{c}_i = U_{ij} c_j : \quad \{\tilde{c}_i, \tilde{c}_j\} = \{\tilde{c}_i^\dagger, \tilde{c}_j^\dagger\} = 0, \quad \{\tilde{c}_i, \tilde{c}_j^\dagger\} = \delta_{ij}$$

- Assume the fermions live on a ring. see the homework
Let $\psi_k = \frac{1}{\sqrt{L}} \sum_i \mathrm{e}^{\mathrm{i}\, ki} c_i$ ($k = \frac{2\pi}{L} \times$ integer)

$$H_{\text{fermion}} = \sum_i (-t c_i^\dagger c_{i+1} + h.c.) + g c_i^\dagger c_i = \sum_k \epsilon(k) \psi_k^\dagger \psi_k$$

$$\epsilon(k) = -2t \cos k - \mu, \quad [\psi_k^\dagger \psi_k, \psi_{k'}^\dagger \psi_{k'}] = 0, \quad n_k \equiv \psi_k^\dagger \psi_k = \pm 1.$$

- From the one-body dispersion, we obtain many-body energy spectrum $E = \sum_k \epsilon(k) n_k$, $K = \sum_k k n_k \bmod \frac{2\pi}{a}$, $n_k = 0, 1$.

Majorana fermions and critical point of Ising model

- $\lambda_i^x = \sigma_i^x \prod_{j<i} \sigma_j^z, \quad \lambda_i^y = \sigma_i^y \prod_{j<i} \sigma_j^z$. One can check that

  $(\lambda_i^x)^\dagger = \lambda_i^x,\ (\lambda_i^y)^\dagger = \lambda_i^y;\ \ \{\lambda_i^x, \lambda_j^x\} = \{\lambda_i^y, \lambda_j^y\} = 2\delta_{ij},\ \{\lambda_i^x, \lambda_j^y\} = 0.$

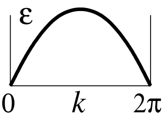
- **Ising model = Majorana-fermion** on a open chain of L sites:

  $$\lambda_i^x \lambda_i^y = \mathrm{i}\sigma_i^z, \qquad \lambda_i^y \lambda_{i+1}^x = \sigma_i^y \sigma_{i+1}^x \sigma_i^z = \mathrm{i}\sigma_i^x \sigma_{i+1}^x$$

  $$H_{\text{Ising}} = \sum_i -\sigma_i^x \sigma_{i+1}^x - h\sigma_i^z \quad \leftrightarrow \quad H_{\text{fermion}} = \sum_i \mathrm{i}\lambda_i^y \lambda_{i+1}^x + \mathrm{i}\, h \lambda_i^x \lambda_i^y$$

  Critical point (gapless point) is at $h = 1$ (not $h = 2$ from meanfield theory): $H_{\text{fermion}}^{\text{critical}} = \sum_I \mathrm{i}\eta_I \eta_{I+1}, \quad \eta_{2i+1} = \lambda_i^x, \ \ \eta_{2i} = \lambda_i^y$.

- In k-space, $\psi_k = \frac{1}{\sqrt{2}} \sum_I \frac{\mathrm{e}^{\mathrm{i}\frac{k}{2}I}}{\sqrt{2L}} \eta_I$, $\frac{k}{2} = \frac{2\pi}{2L} n \in [-\pi, \pi]$:

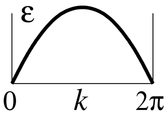
  

  $\psi_k^\dagger = \psi_{-k}, \quad \{\psi_k^\dagger, \psi_{k'}\} = \delta_{k-k'}$ (assume on a ring)

  $$H_{\text{fermion}}^{\text{critical}} = \sum_{k\in[-2\pi,2\pi]} 2\mathrm{i}\,\mathrm{e}^{\mathrm{i}\frac{1}{2}k} \psi_{-k}\psi_k = \sum_{k\in[0,2\pi]} \epsilon(k)\psi_k^\dagger \psi_k, \quad \epsilon(k) = 4|\sin\frac{k}{2}|.$$

1D Ising critical point: 1/2 mode of right (left) movers

- The Majorana fermion contain
  a right-moving mode $\epsilon = vk$ and
  a left-moving modes. $\epsilon = -vk$



- Thermal energy density (for a right moving mode):

$$\epsilon_T = \int_0^{+\infty} \frac{\mathrm{d}k}{2\pi} \frac{vk}{\mathrm{e}^{vk/k_BT}+1} = \frac{k_B^2T^2}{2\pi v} \int_0^{+\infty} \mathrm{d}x \frac{x}{\mathrm{e}^x+1} = \frac{k_B^2T^2}{v} \frac{\pi}{24}$$

  where $\int_0^{+\infty} \mathrm{d}x \frac{x}{\mathrm{e}^x+1} = \frac{\pi^2}{12}$

- Specific heat

$$c_T = \frac{\partial \epsilon_T}{\partial T} = \frac{1}{2} k_B \frac{k_BT}{v} \frac{\pi}{6}$$

  Central charge $c = 1/2$ for right (left) movers.

- On a ring and at critical point: $E = \epsilon L + \frac{2\pi v}{L}(-\frac{c}{24})$.

The neutron scattering and spectral function (Ising model)

Assume the neutron spin couples to Ising spin via $S_i^z \sigma_i^z$ (no S^z-spin flip, but scattering depends on S^z, *ie* flip $S^{x,y}$). After scattering, the neutron dump something to the system $|\Psi\rangle \to \sigma_i^z|\Psi\rangle$. What is the scattering spectrum?

$$I(E,K) = \langle\Psi|\sigma_i^z \delta(\hat H - E)\delta(\hat K - K)\sigma_i^z|\Psi\rangle$$

$$\sigma_i^z = \mathrm{i}\eta_{2i}\eta_{2i+1} = \frac{2\mathrm{i}}{L}\sum_{k_1,k_2} \mathrm{e}^{\mathrm{i}\, k_1 i}\mathrm{e}^{\mathrm{i}\, k_2(i+\frac{1}{2})}\psi_{k_1}\psi_{k_2}$$

$$\begin{aligned}
I(E,K) &= \frac{4}{L^2}\langle\Psi|\sum_{k_1,k_2} \mathrm{e}^{\mathrm{i}\, k_1 i}\mathrm{e}^{\mathrm{i}\, k_2(i+\frac{1}{2})}\psi_{k_1}\psi_{k_2}\delta(\epsilon_{k_1'}+\epsilon_{k_2'}-E) \\
&\qquad \delta(k_1'+k_2'-K)\sum_{k_1',k_2'} \mathrm{e}^{-\mathrm{i}\, k_1' i}\mathrm{e}^{-\mathrm{i}\, k_2'(i+\frac{1}{2})}\psi^\dagger_{k_2'}\psi^\dagger_{k_1'}|\Psi\rangle \\
&= \frac{4}{L^2}\sum_{k_1,k_2\in[0,2\pi]} \delta(\epsilon_{k_1}+\epsilon_{k_2}-E)\delta(k_1+k_2-K)(1-\mathrm{e}^{\mathrm{i}\,\frac{1}{2}(k_1-k_2)})
\end{aligned}$$

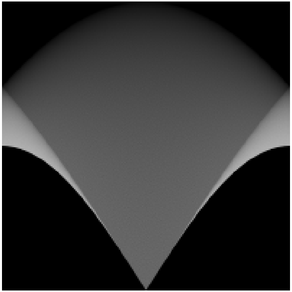
The neutron scattering and spectral function (Ising model)

$$I(E,K) = 4\int_0^{2\pi} \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{(2\pi)^2}\delta(\epsilon_{k_1}+\epsilon_{k_2}-E)\delta(k_1+k_2-K)(1-\cos\frac{k_1-k_2}{2})$$

$$I_0(E,K) = 4\int_0^{2\pi} \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{(2\pi)^2}\delta(\epsilon_{k_1}+\epsilon_{k_2}-E)\delta(k_1+k_2-K)$$

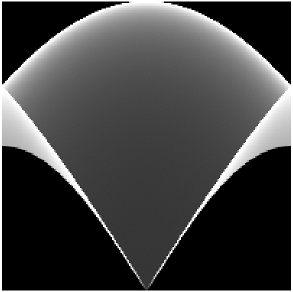
where $\epsilon_k = 4|\sin\frac{k}{2}|$.

$I(E,K)$



$-\pi$ K π

$I_0(E,K)$: two-fermion density of states



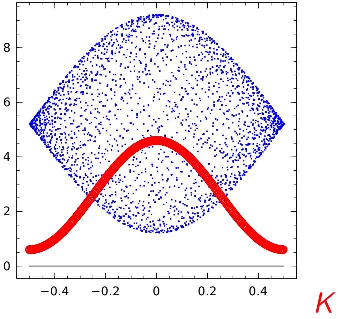
$-\pi$ K π

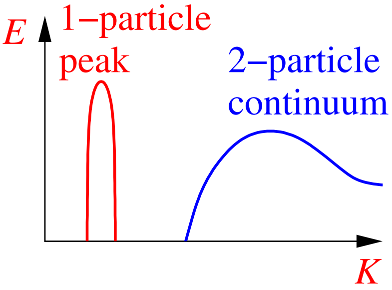
A general picture of specture function

We can understand the spectral function of an operator O_x by writing it in terms of quasiparticle creating/annihilation operators

$$O_i = C_1 a_i^\dagger + C_2 a_i^\dagger a_{i+1}^\dagger + \cdots$$
$$= C_1 \int \mathrm{d}k \; a_k^\dagger + + C_2 \int \mathrm{d}k_1 \mathrm{d}k_2 \; a_{k_1}^\dagger a_{k_2}^\dagger \mathrm{e}^{-\mathrm{i}[k_1 i + k_2(i+1)]} + \ldots$$

Assume one-particle spectrum to be $\epsilon(k) = 2.6 + 2\cos(k) \to$
Two-particle spectrum will be $E = \epsilon(k_1) + \epsilon(k_2), \; K = k_1 + k_2$





The neutron scattering and spectral function (XY model)

1D XY model (superfuild of bosons) = 1D non-interacting fermions

$H_{\mathrm{XY}} = \sum_i -\frac{t}{2}(\sigma^x_i\sigma^x_{i+1} + \sigma^y_i\sigma^y_{i+1}) - \mu\frac{\sigma^z_i}{2} \leftrightarrow H_{\mathrm{f}} = \sum_i (tc^\dagger_i c_{i+1} + h.c.) - \mu n_i$

Let us assume the neutron coupling is $S^z_i\sigma^z_i$ (*ie* neutrons see the boson density) → Spectral function of operator $\sigma^z_i = c^\dagger_i c_i$ (adding a particle-hole pair)

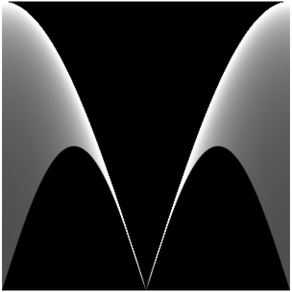
$$
\begin{aligned}
I(E,K) &= \langle\Psi|c^\dagger_i c_i \delta(\hat H - E)\delta(\hat K - K)c^\dagger_i c_i|\Psi\rangle \\
&= \frac{1}{L^2}\langle\Psi|\sum_{k_1,k_2} \mathrm{e}^{\mathrm{i}\,k_1 i}\mathrm{e}^{\mathrm{i}\,k_2 i}\psi^\dagger_{k_1}\psi_{k_2}\delta(-\epsilon_{k_1'} + \epsilon_{k_2'} - E) \\
&\qquad\qquad \delta(-k_1' + k_2' - K)\sum_{k_1',k_2'} \mathrm{e}^{-\mathrm{i}\,k_1' i}\mathrm{e}^{-\mathrm{i}\,k_2' i}\psi^\dagger_{k_2'}\psi_{k_1'}|\Psi\rangle \\
&= \int_{\epsilon_{k_1}<0,\ \epsilon_{k_2}>0} \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{(2\pi)^2}\delta(-\epsilon_{k_1} + \epsilon_{k_2} - E)\delta(-k_1 + k_2 - K)
\end{aligned}
$$

where $\epsilon_k = 2t\cos k - \mu$ and $c_i = \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{\mathrm{i}\,ki}\psi_k$

The neutron scattering and spectral function (XY model)

Spectral function of $n_i \sim \sigma_i^z$ for the superfluid/XY-model

For $\mu = 0, \ \langle \sigma_i^z \rangle = 0$



$-\pi$ K π

For $\mu = -1, \ \langle \sigma_i^z \rangle \neq 0$

$-\pi$ K π

Particle-hole spactral function

- What is the spectral function of σ_i^+ (single particle)?
  $\sigma_i^+ = c_i^\dagger \prod_{j<i}(2c_j^\dagger c_j - 1)$

The neutron scattering and spectral function (XY model)

Spectral function of $\sigma_i^+\sigma_{i+1}^+$ (adding two bosons)

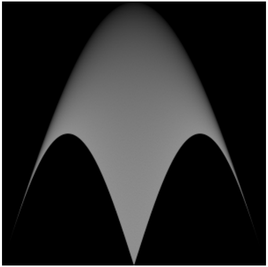
$$I(E,K) = \langle\Psi|c_{i+1}c_i\delta(\hat H - E)\delta(\hat K - K)c_i^\dagger c_{i+1}^\dagger|\Psi\rangle$$

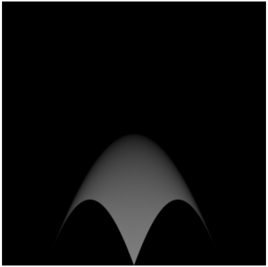
$$= \frac{1}{L^2}\langle\Psi|\sum_{k_1,k_2} \mathrm{e}^{\mathrm{i}\,k_1(i+1)}\mathrm{e}^{\mathrm{i}\,k_2 i}\psi_{k_1}\psi_{k_2}\delta(\epsilon_{k_1'}+\epsilon_{k_2'}-E)$$

$$\delta(k_1'+k_2'-K)\sum_{k_1',k_2'}\mathrm{e}^{-\mathrm{i}\,k_1'(i+1)}\mathrm{e}^{-\mathrm{i}\,k_2' i}\psi_{k_2'}^\dagger\psi_{k_1'}^\dagger|\Psi\rangle$$

$$= \int_{\substack{\epsilon_{k_1}>0\\ \epsilon_{k_2}>0}} \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{(2\pi)^2}\delta(\epsilon_{k_1}+\epsilon_{k_2}-E)\delta(k_1+k_2-K)[1-\cos(k_1-k_2)]$$

$\mu = 0$ and
$\mu = -1$
2-particle
spectral function





XY model: dynamical variational approach

We are going to use the approximated variational approach.
for XY model $H = -\sum_i J(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + h\sigma_i^z)$.
Trial wave function $|\Psi_{\phi_i}\rangle = \otimes_i |\phi_i\rangle$,
where $|\phi_i\rangle = \frac{|\uparrow\rangle + \phi_i|\downarrow\rangle}{\sqrt{1+|\phi_i|^2}}$, $\langle \sigma_i^+ \rangle = \frac{\phi_i}{1+|\phi_i|^2}$.

- Average energy

$$\bar{H} = -\sum_i \Big[2J \frac{\phi_i \phi_{i+1}^* + h.c.}{(1+|\phi_i|^2)(1+|\phi_{i+1}|^2)} + h \frac{1-|\phi_i|^2}{1+|\phi_i|^2} \Big]$$

Geometric phase term $\langle \phi_i | \frac{\mathrm{d}}{\mathrm{d}t} | \phi_i \rangle = \frac{\phi_i^* \dot{\phi}_i}{1+|\phi_i|^2} + \frac{\mathrm{d}}{\mathrm{d}t} \#$
Phase space Lagrangian in symmetry breaking phase
($\phi_i = \bar{\phi} + \varphi_i$ for $J > 0$ or $\phi_i = \bar{\phi}(-)^i + \varphi_i$ for $J < 0$)

$$L = \langle \Phi_{\phi_i} | \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} - H | \Phi_{\phi_i} \rangle = \sum_i \mathrm{i} \phi_i^* \dot{\phi}_i + 2J(\phi_i \phi_{i+1}^* + h.c.) - 2h|\phi_i|^2 - g|\phi_i|^4$$

$$= \sum_i \mathrm{i} \varphi_i^* \dot{\varphi}_i + 2J(\varphi_i \varphi_{i+1}^* + h.c.) - 2h\varphi_i \varphi_i^* - g\bar{\phi}^2 [4\varphi_i \varphi_i^* + \varphi_i^2 + (\varphi_i^*)^2]$$

with $g\bar{\phi}^2 = 2|J| - h$.

Quantum XY model

Quantization:

$$[\varphi_i, \varphi_j^\dagger] = \delta_{ij}, \ \ \varphi_i = \frac{1}{\sqrt{L}} \sum_k \mathrm{e}^{\mathrm{i}\, ki} a_k, \ \ [a_k, a_q^\dagger] = \delta_{kq}$$

$$H = \sum_i -2J(\varphi_i \varphi_{i+1}^\dagger + h.c.) + 2h\varphi_i^\dagger \varphi_i + (2|J| - h)(4\varphi_i^\dagger \varphi_i + \varphi_i\varphi_i + \varphi_i^\dagger \varphi_i^\dagger)$$

$$= \sum_k (-4J\cos k + 8|J| - 2h) a_k^\dagger a_k + (2|J| - h)(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger)$$

$$= \sum_{k\in[0,\pi]} \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} -4J\cos k + 8|J| - 2h & 2(2|J| - h) \\ 2(2|J| - h) & -4J\cos k + 8|J| - 2h \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

$$= \sum_{k\in[0,\pi]} \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} \epsilon_k & \Delta \\ \Delta & \epsilon_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

To diagonalize the above Hamiltonian, let

$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = U \begin{pmatrix} b_k \\ b_{-k}^\dagger \end{pmatrix}, \ U = \begin{pmatrix} u_k & -v_k \\ -v_k & u_k \end{pmatrix}, \ U \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where $u_k^2 - v_k^2 = 1$

Quantum XY model

$$H = \sum_{k\in[0,\pi]} \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} \epsilon_k & \Delta \\ \Delta & \epsilon_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

$$U \begin{pmatrix} \epsilon & \Delta \\ \Delta & \epsilon \end{pmatrix} U = \begin{pmatrix} (u^2+v^2)\epsilon - 2uv\Delta & (u^2+v^2)\Delta - 2uv\epsilon \\ (u^2+v^2)\Delta - 2uv\epsilon & (u^2+v^2)\epsilon - 2uv\Delta \end{pmatrix}$$
$$= \begin{pmatrix} E_k & 0 \\ 0 & E_k \end{pmatrix}, \qquad E_k = \sqrt{\epsilon^2 - \Delta^2}$$

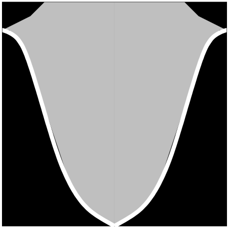
$$u^2 + v^2 = \frac{\epsilon}{E_k}, \qquad 2uv = \frac{\Delta}{E_k},$$
$$u = \sqrt{\frac{\frac{\epsilon}{E_k} + 1}{2}}, \qquad v = \sqrt{\frac{\frac{\epsilon}{E_k} - 1}{2}}$$

$$H = \sum_k b_k^\dagger \underbrace{\sqrt{(-4J\cos k + 8|J| - 2h)^2 - (4|J| - 2h)^2}}_{\sqrt{\epsilon^2-\Delta^2}=E_k,\quad \text{spin-wave dispersion}} b_k$$

The spectral function – XY model (only for $\langle\sigma^+\rangle = \bar\phi$)

- Spectral function for $\sigma^+ \sim \bar\phi + \varphi_i^\dagger$, and $(\sigma^+)^2 \sim \bar\phi^2 + 2\bar\phi\varphi_i^\dagger + (\varphi_i^\dagger)^2$

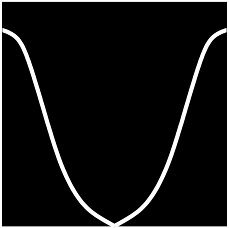
$$\varphi_i^\dagger = \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{-\mathrm{i}\,ki} a_k^\dagger$$
$$= \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{-\mathrm{i}\,ki}(u_k b_k^\dagger - v_k b_{-k})$$



$$I(E,K) \sim u_K^2 \delta(E_K - E) = \frac{\frac{\epsilon}{E_k}+1}{2}\delta(E_K - E) \to \infty|_{k\to 0}$$

- Spectral function for $n_i = \frac{\sigma_i^z - 1}{2} \sim \sigma_i^x \sim \varphi_i + \varphi_i^\dagger$

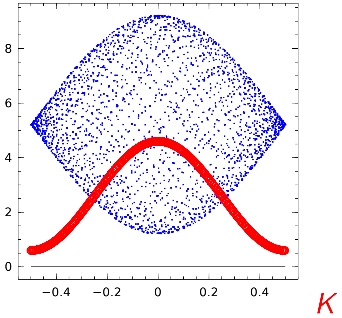
$$\varphi_i + \varphi_i^\dagger = \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{-\mathrm{i}\,ki}(a_{-k} + a_k^\dagger)$$
$$= \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{-\mathrm{i}\,ki}(u_k b_{-k} - v_k b_k^\dagger + u_k b_k^\dagger - v_k b_{-k})$$

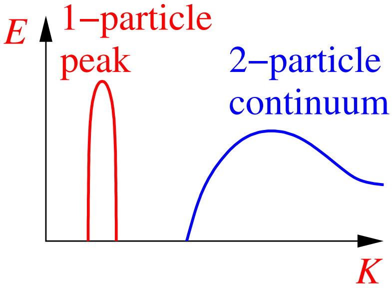


$$I(E,K) \sim (u_K - v_K)^2 \delta(E_K - E) = \frac{E_k}{\epsilon_k + \Delta}\delta(E_K - E) \to 0|_{k\to 0}$$

The spectral function – XY model (only for $\langle\sigma^+\rangle = \bar{\phi}$)

The following picture work in higher dimension since $\langle\sigma_i^+\rangle = \bar{\phi}$ (symmetry breaking) $\langle\sigma_i^+\sigma_j^+\rangle \sim \textit{const}.$ for large $|i-j|$





But does not quite work in 1 dimension (or 1+1 dimensions) since $\langle\sigma_i^+\rangle = 0$ (no symmetry breaking).

We only have a nearly symmetry breaking

$$\langle\sigma_i^+\sigma_j^+\rangle \sim \frac{1}{|i-j|^\alpha} \text{ for large } |i-j|$$

Neutron scattering spectrum for α-$RuCl_3$

Banerjee etal arXiv:1706.07003

- Spin-1/2 on honeycomb lattice with strong spin-orbital coupling.
- Spin ordered phase below 8T, spin liquid above 8T
- Magnetic field:
  (a-e) $B: 0, 2, 4, 6, 8T$
  (a-e) $T = 2K$
  (f) $T = 2K, B = 0T$