Quantum many-body systems: Symmetry breaking

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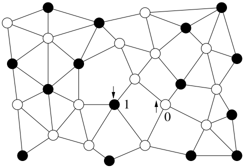
What is a many-body quantum system?



- 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 quantum state, a vector in $\mathcal{V}_{tot}$:
  $|\Psi\rangle = \sum \Psi(m_1, ..., m_N)|m_1\rangle \otimes ... \otimes |m_N\rangle$,
  basis of $\mathcal{V}_i$: $|m_i\rangle \in \mathcal{V}_i$
- A local Hamiltonian $H = \sum_{\boldsymbol{x}} H_{\boldsymbol{x}}$ and $H_{\boldsymbol{x}}$ are local hermitian operators acting on a few neighboring $\mathcal{V}_i$'s.

What is a 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:

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

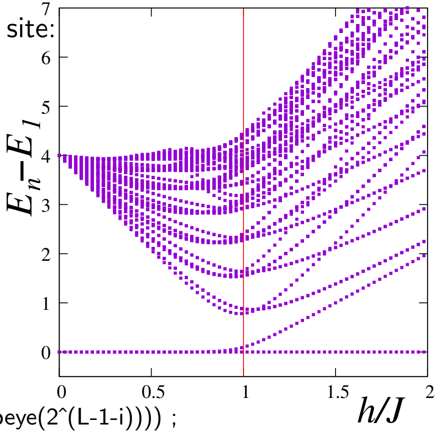
  – transverse Ising model. H is a $2^L \times 2^L$ matrix.

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
(similar code for Matlab or Julia)




```
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
```

Why near 2-fold degeneratcy?

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

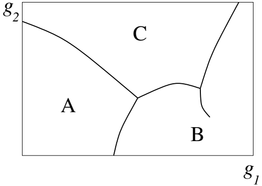
What are quantum phases and quantum phase transitions?

- Phases are defined through phase transitions.

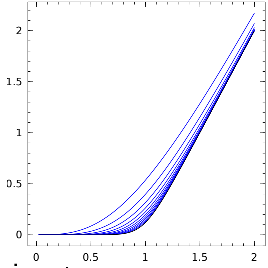
  What are phase transitions?

  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 $L = 3, \cdots, 13$



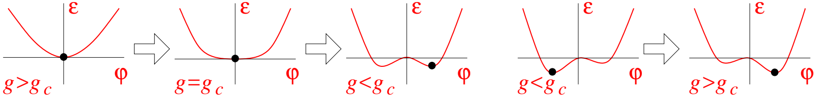
- There is no singularity for finite systems. Singularity appears only for infinite systems.
- Spontaneous symmetry breaking is a mechanism to cause a singularity in ground state energy density ϵ_g.
  $\to$ Spontaneous symmetry breaking causes phase transition.

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

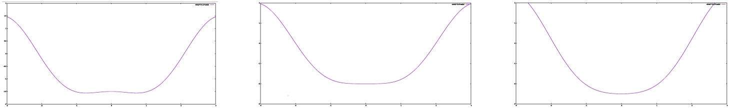
Use trial wave function $|\Psi_\phi\rangle = \otimes_i|\psi_i\rangle$, $|\psi_i\rangle = \cos\frac{\phi}{2}|\uparrow\rangle + \sin\frac{\phi}{2}|\downarrow\rangle$

to estimate the ground state energy

$\epsilon_h(\phi) = \langle\Psi_\phi|H|\Psi_\phi\rangle = -\sum\langle\psi_i|\sigma_i^x|\psi_i\rangle\langle\psi_{i+1}|\sigma_{i+1}^x|\psi_{i+1}\rangle - h\sum\langle\psi_i|\sigma_i^z|\psi_i\rangle$.

$= (2J\cos\frac{\phi}{2}\sin\frac{\phi}{2})^2 - h(\cos^2\frac{\phi}{2} - \sin^2\frac{\phi}{2}) = \sin^2\phi - h\cos\phi$

Phase transition at $h/J = 2$. ($h/J = 1.5, \quad 2.0, \quad 2.5$)



- *Why $\epsilon_h(\phi) = \epsilon_h(-\phi)$?* Z_2-Symmetry: $U = \prod_j \sigma_j^z$, $U^2 = 1$.

  Symmetry trans.: $U\sigma_i^z U^\dagger = \sigma_i^z$, $U\sigma_i^x U^\dagger = -\sigma_i^x$, $U\sigma_i^y U^\dagger = -\sigma_i^y$.

  $\to UHU^\dagger = H$. 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).

Ginzberg-Landau theory of continuous phase transition

- 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.

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**)

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: $U|\Psi_{\text{grnd}}\rangle = e^{i\theta}|\Psi_{\text{grnd}}\rangle$. 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 $\Delta \sim e^{-L/\xi}$.

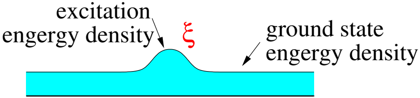
- Discrete-symmetry-breaking phase has exponentially nearly degenerate ground states, which cannot be distingushed by any symmetric local operators, but can be distingushed by symmetry-breaking local operators

Excitations above the ground state: quasiparticles

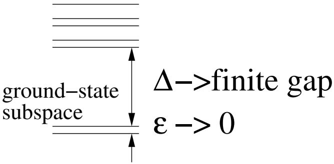
The answer is very different for gapped system and gapless systems. Here, we only consider the definition of quasiparticle for gapped systems.

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

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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 $|\Psi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$
- a state w/ three point-like excitations $|\Psi_{\xi_1\xi_2\xi_3}\rangle = |\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$

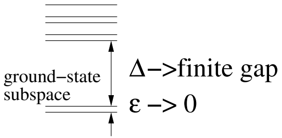
ξ_1 ξ_2 ξ_3

- 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 $c \sim T^{\alpha} \mathrm{e}^{-\frac{\Delta_{\text{therm}}}{k_B T}}$ is $\Delta_{\text{therm}} = \Delta_{\text{wall}}$.

  The difference of the neutron gap Δ and the thermal activation gap Δ_{therm} $\rightarrow$ 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

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

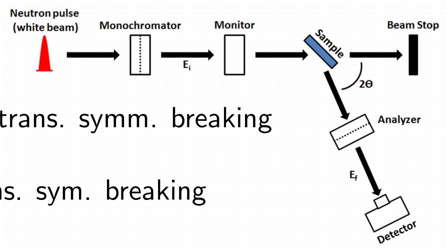
- Topo. excitation (domain wall) = spin-1/2 excitation (spinon)

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

- 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.

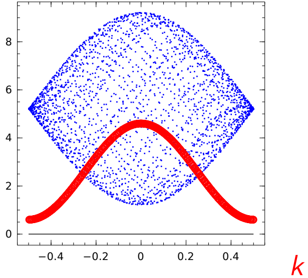
Neutron scattering spectrum

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

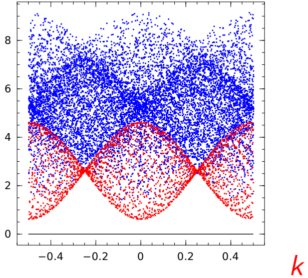


- Without fractionalization, nor trans. symm. breaking
  $\epsilon_{\text{spin-1}}(k) = 2.6 + 2\cos(k)$
- With fractionalization and trans. sym. breaking
  $\epsilon_{\text{spin-1/2}}(k) = \frac{1}{2}\epsilon(2k)_{\text{spin-1}}$

one spin-1 + two spin-1



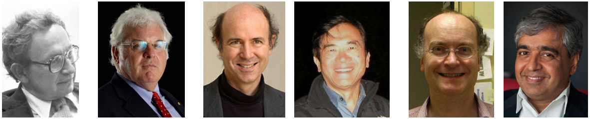
two spin-1/2 + four spin-1/2



- Two-particle spectrum: $\epsilon_{\text{two}}(k) = \epsilon_{\text{one}}(k_1) + \epsilon_{\text{one}}(k - k_1)$.

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:

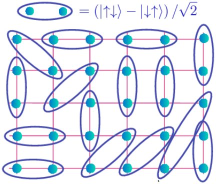
chiral spin liquid $\sum \Psi(RVB)|RVB\rangle$ → topological order

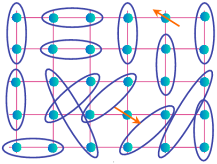
Kalmeyer-Laughlin PRL **59** 2095 (87); Wen-Wilczek-Zee PRB **39** 11413 (89)

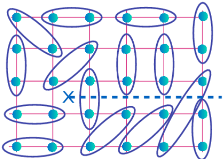
Z_2 **spin liquid** $\sum |RVB\rangle$ (emergent low energy Z_2 gauge theory)

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).



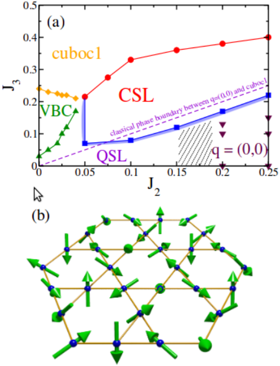


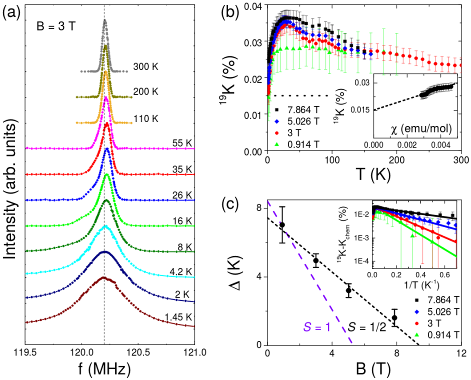


2D Spin liquid without symmetry breaking (topo. order)

- On Kagome lattice:

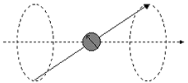
Feng etal arXiv:1702.01658 $Cu_3Zn(OH)_6FBr$

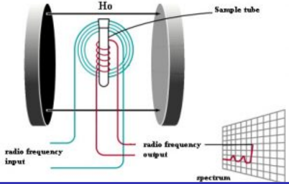




Gong-Zhu-Balents-Sheng arXiv:1412.1571

J_1-J_2-J_3 model





Neutral spin-1/2 or spin-1 excitations

Consider a 2D Mott insulator of electrons where the electron spins form a 2D gapped spin liquid state, that do not break the $SO(3)$ spin rotation symmetry. The gapped excitations may be spin-1/2 excitations or spin-1 excitations. In an external magnetic field B an excitation has the following dispersion relation

$$\epsilon_\sigma(k) = \Delta + \frac{\hbar^2 k^2}{2m} + g\mu_B B\sigma$$

where $\sigma = \pm\frac{1}{2}$ if the excitation has spin-1/2, and $\sigma = 0, \pm 1$ if the excitation has spin-1. (Note that $g\mu_B\sigma$, $\sigma = \pm\frac{1}{2}$, is magnetic moment of spin up/down electrons.) Find the low temperature spin polarization $\sum \sigma / Area$ per unit area as a function of magnetic field B and temperature for spin-1/2 and spin-1 cases. Comment on how to use those results to detect experimentally if the excitations has spin-1/2 or spin-1. (See arXiv:1702.01658 *Gapped spin-1/2 spinon excitations in a new kagome quantum spin liquid compound* $Cu_3Zn(OH)_6FBr$.)

Neutral spin-1/2 or spin-1 excitations

We note that the spin excitations are always charge neutral. For an electron system, a charge neutral excitation naively should have integer spins. So a charge neutral spin-1/2 excitation is highly unusual and corresponds to a topological excitation. The appearance of charge neutral spin-1/2 excitation implies that the 2D spin liquid has a topological order. However, in 1D, a spin dimmer phase can have such a kind of charge neutral spin-1/2 topological excitation:

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

where $(\uparrow\downarrow)$ represent a spin singlet (a dimmer).

Some problems about 1D Ising model

- Compute the energy spectra (say of lowest 10 eigenstates) for the transverse Ising model on a ring of size $L = 10$ (or bigger):

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

for $J = 1$ and $h = \frac{1}{2}, 1, 2$. We can use such numerical results for different L's to study the following two questions.

- For $J = 1, h = \frac{1}{2}$, show that the emergence of near 2-fold degeneracy become better and better as $L \to \infty$. Such an emergence of degeneracy for space with spherical topology S^d is a sign of spontaneous symmetry breaking (this can be used as a definition of spontaneous symmetry breaking). Show the splitting of the 2-fold degeneracy to have a form (in large L limit)

$$\Delta \sim \mathrm{e}^{-L^\alpha/\xi}$$

and find the values of α and ξ.

Some problems about 1D Ising model

- At the critical point $J = 1, h = 1$, show the splitting between the two lowest eigenstates to have a form (in large L limit)

$$\Delta = A_{-1}/L.$$

- Show that the ground states (or more precisely the Hamiltonians) for $J = 1, h = 2$ and for $J = 1, h = -2$ belong to different phases, despite both states do not break the Z_2 symmetry and the translation symmetry (*ie* they have have the same symmetry). In other words, the two Hamiltonians with $J = 1, h = 2$ and for $J = 1, h = -2$ cannot be deformed into each other without encounter a phase transition, if the deformation path does not break the Z_2 symmetry and the translation symmetry.

  On the other hand, if the deformation path does break the Z_2 symmetry or the translation symmetry, then the two Hamiltonians with $J = 1, h = 2$ and for $J = 1, h = -2$ can be deformed into each other without encounter a phase transition.

Some problems about 1D Ising model

(Hint: consider the $h \to \pm\infty$ limit and compute the total Z_2 quantum number for the Z_2 transformation

$$U = \prod_i \sigma_i^z$$

for $L =$ even and odd cases. Note that the eigenvalues of U are ± 1. The total Z_2 quantum number is the eigenvalues of U. If $U|\psi\rangle = |\psi\rangle$, we say $|\psi\rangle$ has a total Z_2 quantum number $+1$ (or 0 mod 2). If $U|\psi\rangle = -|\psi\rangle$, we say $|\psi\rangle$ has a total Z_2 quantum number -1 (or 1 mod 2). Does U commute with H? Does such Z_2 quantum number change as we make $|h|$ smaller and smaller?)