Content

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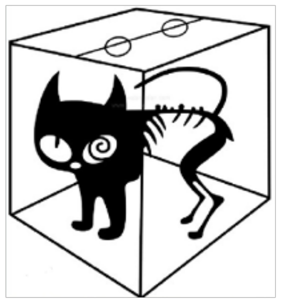
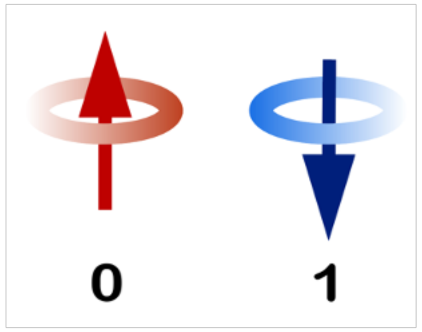
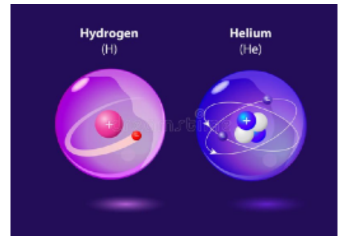
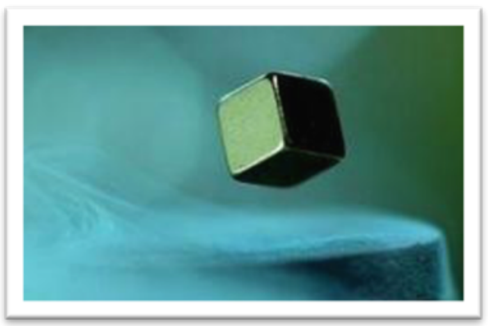
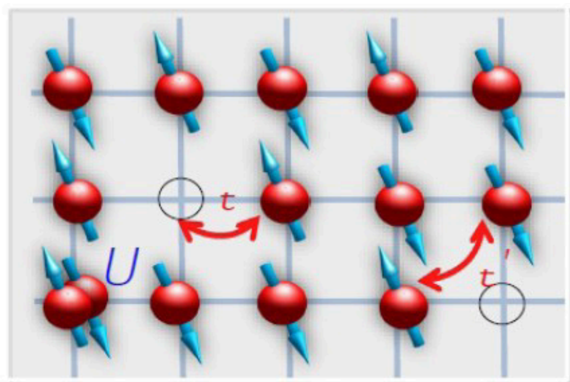
Quantum lattice model

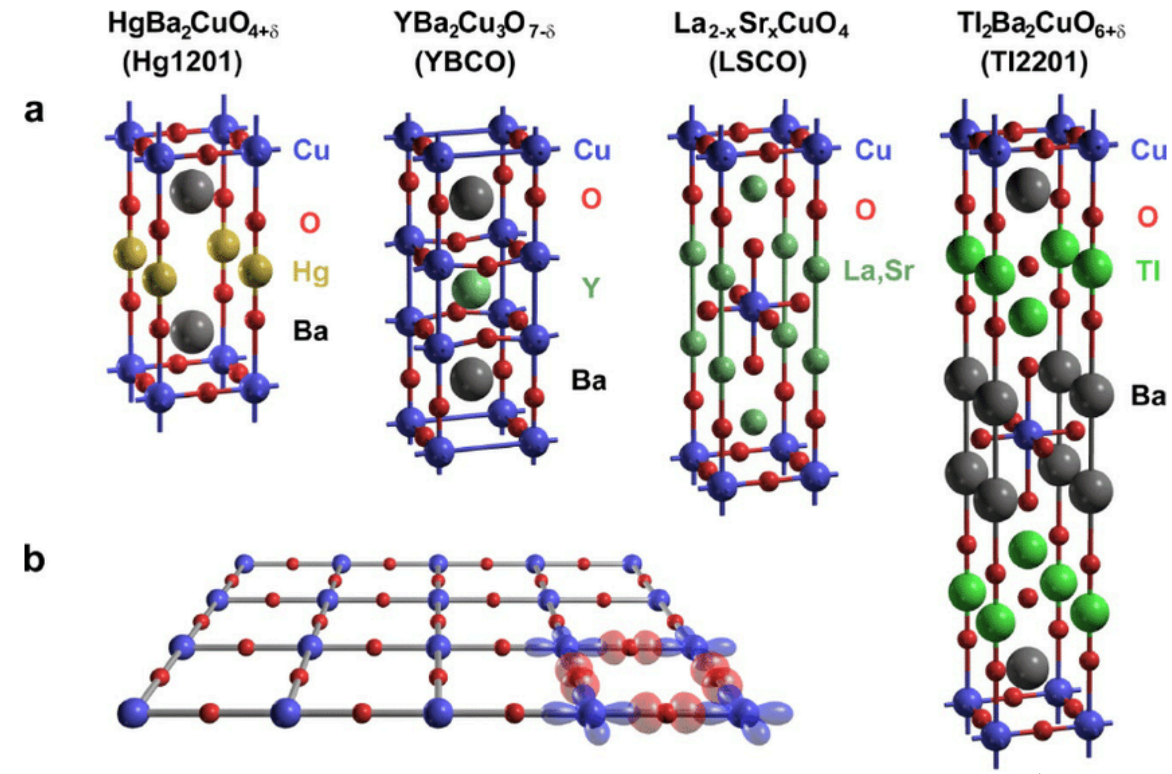


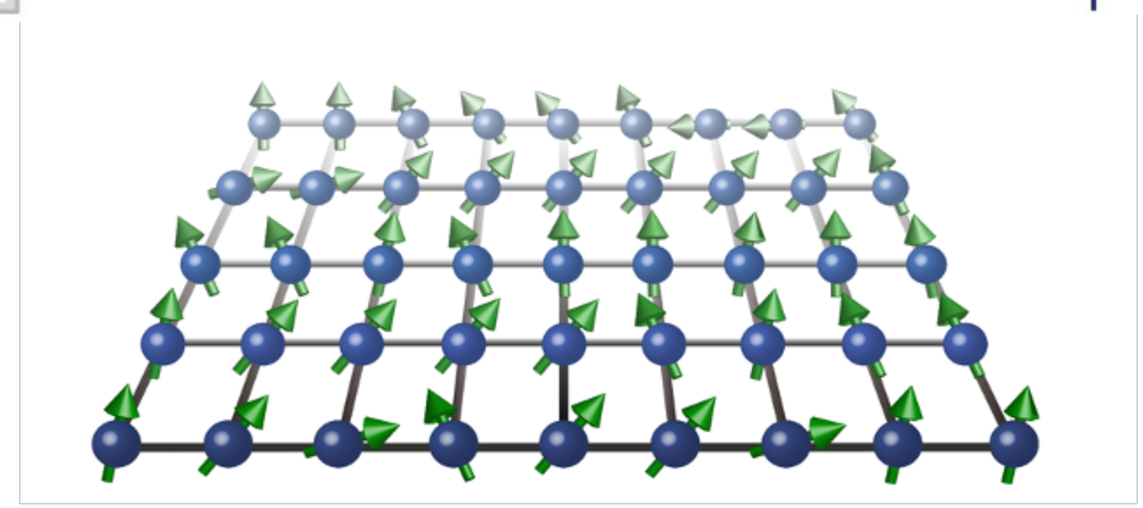


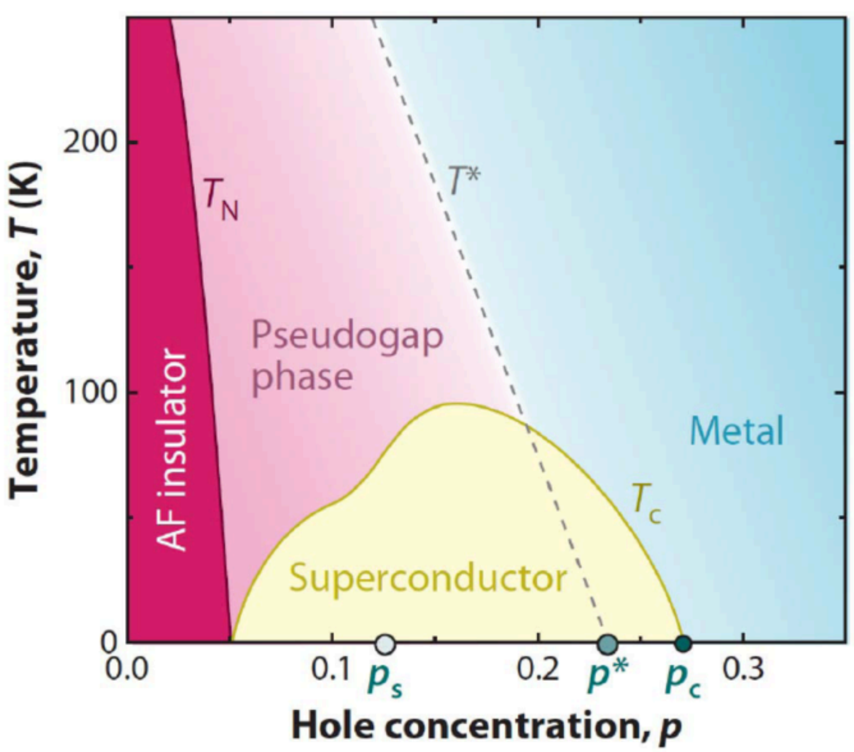












$$H = J \sum_{\langle i,j \rangle} \overrightarrow{S}_i \cdot \overrightarrow{S}_j \qquad \overrightarrow{S}_i = \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} \qquad [S_i^\alpha, S_j^\beta] = i\hbar \epsilon_{\alpha\beta\gamma} S_i^\gamma \delta_{ij}$$

Basis of the Hilbert space

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$|S_i^z = +1/2\rangle_i = |\uparrow\rangle_i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i \qquad |S_i^z = -1/2\rangle_i = |\downarrow\rangle_i = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i$$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_i^z = \frac{1}{2}\sigma_i^z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

$$S_i^z|\uparrow\rangle_i = +\frac{1}{2}|\uparrow\rangle_i$$

$$S_i^z|\downarrow\rangle_i = -\frac{1}{2}|\downarrow\rangle_i$$

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_i^+ = S_i^x + iS_i^y = \frac{1}{2}\sigma_i^x + i\frac{1}{2}\sigma_i^y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$S_i^+|\downarrow\rangle_i = |\uparrow\rangle_i$$

$$S_i^+|\uparrow\rangle_i = 0$$

$$S_i^- = S_i^x - iS_i^y = \frac{1}{2}\sigma_i^x - i\frac{1}{2}\sigma_i^y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$S_i^-|\uparrow\rangle_i = |\downarrow\rangle_i$$

$$S_i^-|\downarrow\rangle_i = 0$$

$$\{|S_1^z, S_2^z, \cdots, S_N^z\rangle\} = \left\{ \begin{array}{c} |\uparrow,\uparrow,\cdots,\uparrow,\uparrow\rangle \\ |\uparrow,\uparrow,\cdots,\uparrow,\downarrow\rangle \\ |\uparrow,\uparrow,\cdots,\downarrow,\uparrow\rangle \\ \vdots \\ |\uparrow,\downarrow,\cdots,\downarrow,\downarrow\rangle \\ |\downarrow,\downarrow,\cdots,\downarrow,\downarrow\rangle \end{array} \right\} \quad 2^N$$

Hamiltonian matrix

$$H = J\sum_{\langle i,j\rangle} \overrightarrow{S}_i \cdot \overrightarrow{S}_j = J\sum_{\langle i,j\rangle} (\frac{1}{2}(S_i^+S_j^- + S_i^-S_j^+) + S_i^zS_j^z)$$

$$H|\uparrow\uparrow\rangle = \frac{J}{4}|\uparrow\uparrow\rangle$$

$$H|\downarrow\downarrow\rangle = \frac{J}{4}|\downarrow\downarrow\rangle$$

$$H|\uparrow\downarrow\rangle = J(\frac{1}{2}(S_1^+S_2^- + S_1^-S_2^+) + S_1^zS_2^z)|\uparrow\downarrow\rangle = \frac{J}{2}|\downarrow\uparrow\rangle - \frac{J}{4}|\uparrow\downarrow\rangle$$

$$H|\downarrow\uparrow\rangle = J(\frac{1}{2}(S_1^+S_2^- + S_1^-S_2^+) + S_1^zS_2^z)|\downarrow\uparrow\rangle = \frac{J}{2}|\uparrow\downarrow\rangle - \frac{J}{4}|\downarrow\uparrow\rangle$$

$$\langle\uparrow\uparrow|H|\uparrow\uparrow\rangle = \frac{J}{4}$$

$$\langle\downarrow\downarrow|H|\downarrow\downarrow\rangle = \frac{J}{4}$$

$$\langle\uparrow\downarrow|H|\uparrow\downarrow\rangle = -\frac{J}{4}$$

$$\langle\downarrow\uparrow|H|\uparrow\downarrow\rangle = \frac{J}{2}$$

$$\langle\uparrow\downarrow|H|\downarrow\uparrow\rangle = \frac{J}{2}$$

$$\langle\downarrow\uparrow|H|\downarrow\uparrow\rangle = -\frac{J}{4}$$

$$H = J\begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$ in the basis $$\begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

Block-diagonalization $S^z_{tot} = \sum_i S^z_i$ $[H, S^z_{tot}] = 0$ different blocks are not connected by H

$$S^z_{tot} = +1 : |\uparrow\uparrow\rangle, E = \frac{J}{4}$$

$$S^z_{tot} = -1 : |\downarrow\downarrow\rangle, E = \frac{J}{4}$$

$$S^z_{tot} = 0 : \{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\} \quad H_0 = J\begin{pmatrix} -\frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{4} \end{pmatrix}$$

$$|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \qquad H_0|S\rangle = -\frac{3}{4}J|S\rangle$$

$$|T\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \qquad H_0|T\rangle = \frac{1}{4}J|T\rangle$$

Triplet $\{\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ $E = \frac{1}{4}J$

J (gap)

Singlet $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ $E = -\frac{3}{4}J$

Hilbert space size

Dimensionality of the Hilbert space $d = dim(H) = 2^N$

Computation complexity for diagonalising $d \times d$ matrix $O(d^3) = O(2^{3N})$

$N = 10 \quad dim = 1{,}024 \sim 10^3$

$N = 20 \quad dim = 1{,}048{,}576 \sim 10^6$

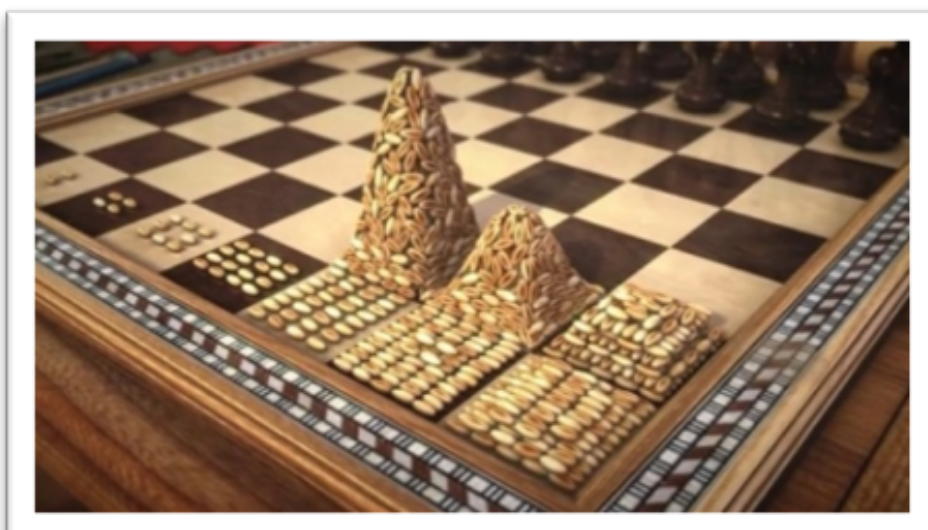
$N = 30 \quad dim = 1{,}073{,}741{,}824 \sim 10^9$

$N = 40 \quad dim = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

$N = 50 \quad dim = 1{,}125{,}899{,}906{,}842{,}624 \sim 10^{15}$

↕ right now

📍 Lead to the "exponential wall"



Wheat grains on chessboard — Sessa, ancient Indian Minister

$2^{64} - 1$ = 18,446,744,073,709,551,615 grains of wheat, weighing about 1,199,000,000,000 tons.
About 1,645 times the global production of wheat.

Solving exponentially complex problem in polynomial time

State Representation

$|S_1^z, \cdots, S_N^z\rangle$ $\quad 2^N$ states, use the bit representation $\quad H_{ij} = \langle i | H | j \rangle \quad i, j = 0,1,\cdots,2^N - 1$

$|0\rangle = |\downarrow, \downarrow, \cdots, \downarrow, \downarrow, \downarrow\rangle \quad (00\cdots000)$

$|1\rangle = |\downarrow, \downarrow, \cdots, \downarrow, \downarrow, \uparrow\rangle \quad (00\cdots001)$

$|2\rangle = |\downarrow, \downarrow, \cdots, \downarrow, \uparrow, \downarrow\rangle \quad (00\cdots010)$

$|3\rangle = |\downarrow, \downarrow, \cdots, \downarrow, \uparrow, \uparrow\rangle \quad (00\cdots011)$

Exclusive or: true if arguments differ

XOR operation

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle i,j \rangle} \left(\frac{1}{2}\underline{(S_i^+ S_j^- + S_i^- S_j^+)} + S_i^z S_j^z\right)$$

Construct the Hamiltonian matrix by examining and flipping the bits.

do $a = 0,\ 2^N - 1$

do $i = 0,\ N - 1$

$j =$ **mod**$(i + 1,\ N)$

if $(a[i] == a[j])$ **then**

$H(a,a) = H(a,a) + \frac{1}{4}$

else

$H(a,a) = H(a,a) - \frac{1}{4}$

$b =$ **XOR**$(a, i, j) \quad H(a,b) = H(a,b) + \frac{1}{2}$

end if

end do

end do

Use numpy.linalg.eig in Python.

Measurement

Total magnetisation $m_z = \sum_{i=1}^{N} S_i^z$ U is the matrix whose columns are eigenvectors of H

$U(i,n) = vec(i,n)$ i:th component of the eigenvector n

$$|n\rangle_{eigen} = \sum_{i=1}^{2^N} \phi_i |i\rangle \qquad \langle n|m_z|n\rangle = \sum_{i,j=1}^{2^N} \phi_i \phi_j \langle j|m_z|i\rangle = \sum_i^{2^N} \phi_i^2 \langle i|m_z|i\rangle = \sum_i^{2^N} \phi_i^2 m_z(i)$$

Expectation value of operator A in the n-th eigenstate $\langle n|A|n\rangle = [U^\dagger A U]_{nn}$

m_z commute with H, share the same eigenstates $|n\rangle$ $S_{aa}^z = \frac{1}{2}(n_\uparrow - n_\downarrow)$ $n_\downarrow = N - n_\uparrow$

Discuss the ground state wave function of Heisenberg chain and 2d square lattice

Hamiltonian matrix is block-diagonalised

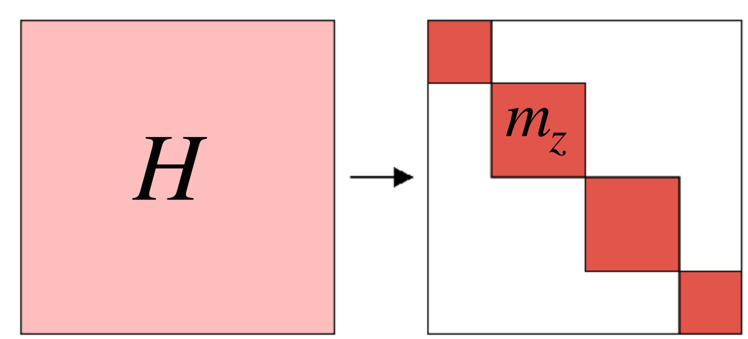
$$\frac{N!}{(N/2)!(N/2)!}$$

$N = 40 \quad dim = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

In the $m_z = 0$ sector, dimension of the subspace $\frac{40!}{20!20!} \approx 138 \times 10^9$

Use symmetries to further split the blocks:

- Blocks correspond to fixed values of m_z
- No H matrix elements between states of different m_z
- Blocks can be diagonalised individually



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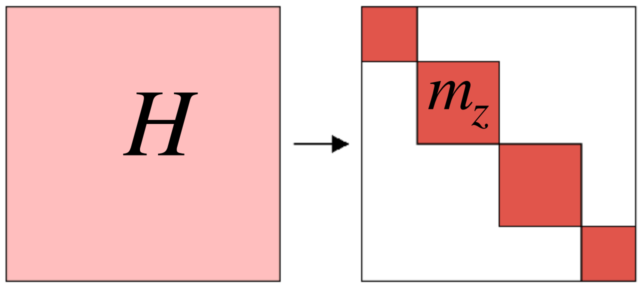


$N = 4, n_\uparrow = 2 \qquad M = \frac{4!}{2!2!} = 6$

$s_1 = 3\ (0011)$
$s_2 = 5\ (0101)$
$s_3 = 6\ (0110)$
$s_4 = 9\ (1001)$
$s_5 = 10\ (1010)$
$s_6 = 12\ (1100)$

Store the state-integers in list with $n_\uparrow$ $s_a, a = 1,2,\cdots,M$

do $s = 0,\ 2^N - 1$

  if $(\sum_i s[i] = n_\uparrow)$ **then** $a = a + 1;\ s_a = s$

  end if

end do

$M = a$

each block is a $M \times M$ matrix

Hamiltonian construction

do $a = 0,\ M - 1$

  do $i = 0,\ N - 1$

    $j =$ **mod**$(i + 1,\ N)$

    if $(s_a[i] == s_a[j])$ **then**

      $H(a,a) = H(a,a) + \frac{1}{4}$

    else

      $H(a,a) = H(a,a) - \frac{1}{4}$

      $b =$ **XOR**(a, i, j)

      findstate (s, b) $H(a,b) = H(a,b) + \frac{1}{2}$

    end if

  end do

end do

Find the location b as a state in the list s_a ← **findstate** (s, b)

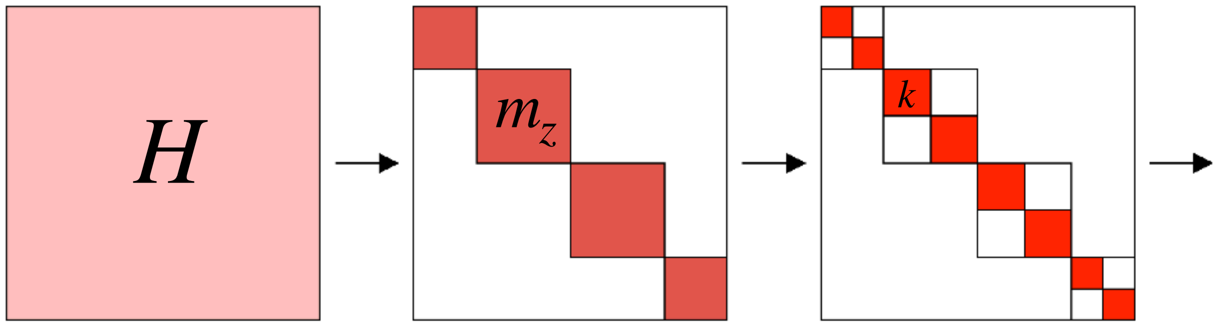
12 site PBC

Full diag: 2m25s   Measurement mz: 2m25s

Block diag: 4s !!

Hamiltonian matrix is block-diagonalised

Using momentum as an example (for translationally invariant systems)

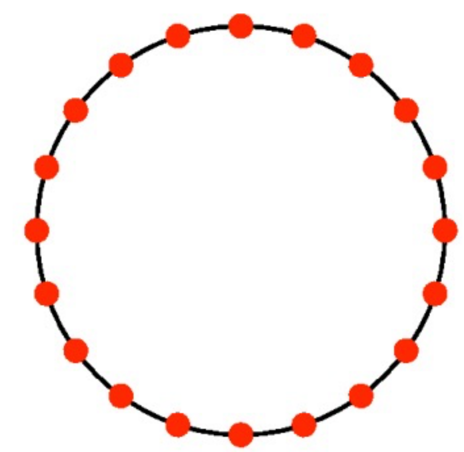


Other symmetries (conserved quantum numbers):

- further split the blocks
- construct basis states that obey the symmetries

$T|n\rangle = e^{ik}|n\rangle \qquad k = m\frac{2\pi}{N},\ m = 0,1,\cdots,N-1$ translate the state by one lattice spacing

In spin basis $\quad T|s_1^z, s_2^z, \cdots, s_N^z\rangle = |s_N^z, s_1^z, \cdots, s_{N-1}^z\rangle \qquad [T,H] = 0$



Use eigenstates of T with given k as basis in each block

a momentum state can be constructed from representative state as

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}}\sum_{r=0}^{N-1} e^{-ikr}T^r|a\rangle, \quad |a\rangle = |s_1^z, s_2^z, \cdots, s_N^z\rangle$$

construct ordered list of **representatives**

If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1,2,\cdots,N-1\}$$

Representative is the one with smallest integer

$$\underline{(0011)} \rightarrow (0110), (1100), (1001)$$

$$\underline{(0101)} \rightarrow (1010)$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle, \quad |a\rangle = |s_1^z, s_2^z, \cdots, s_N^z\rangle \qquad k = m\frac{2\pi}{N}, m = 0,1,\cdots, N-1$$

$T^R|a\rangle = |a\rangle$ for some $R < N$

$$kR = n2\pi \quad m = n\frac{N}{R} \rightarrow \quad \mathrm{mod}\ (m, N/R) = 0$$

Normalization of a state with periodicity R_a $\quad \langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times (\frac{N}{R_a})^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$

Find all allowed **representatives** and their **periodicities**

$(a_1, a_2, a_3, \cdots, a_M) \qquad\qquad R_a$

do $s = 0,\ 2^N - 1$

checkstate(s, R) ⟶

- **R = periodicity** if integer **s** is a new **representative**
- **R = -1** if
  - the magnetization is not the one considered
  - some translation of |s> gives an integer < s
  - |s> is not compatible with the momentum

if $(R \geq 0)$ **then** $a = a + 1;\ s_a = s; R_a = R$

end if

end do

$M = a$

each block is a $M \times M$ matrix

Translations of the **representative**; cyclic permutation

r	T^r	
0	27	0 0 0 1 1 0 1 1
1	54	0 0 1 1 0 1 1 0
2	108	0 1 1 0 1 1 0 0
3	216	1 1 0 1 1 0 0 0
4	177	1 0 1 1 0 0 0 1
5	99	0 1 1 0 0 0 1 1
6	198	1 1 0 0 0 1 1 0
7	141	1 0 0 0 1 1 0 1

checkstate(s, R)

$R = -1$

if $(\sum_i s[i] \neq n_\uparrow)$ **return** → check the magnetisation

$t = s$

do $i = 1,\ N$

  $t =$ **cyclebits**(t, N) → Cyclic permutations of integer t

  if $(t < s)$ **then**

    return

  else if $(t = s)$ **then**

    if (**mod**$(k,\ N/i) \neq 0$) **return**

    $R = i$; **return**

  end if

end do

check momentum compatibility:
m is the integer index of momentum k

momentum $= k\dfrac{2\pi}{N},\ k = 0,1,\cdots,N-1$

check if the translated state has lower integer representation
The representative is the smallest integer among all translations

$$H = \sum_{j=0}^{N} \underbrace{S_j^z S_{j+1}^z}_{H_0} + \underbrace{\frac{1}{2}(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+)}_{H_j}$$

momentum state

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle, \quad |a\rangle = |s_1^z, s_2^z, \cdots, s_N^z\rangle$$

act with H on a momentum state

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

$$\frac{1}{2}|b_j\rangle = T^{l_j} H_j |a\rangle$$

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \sum_{j=0}^{N} e^{-ikr} T^r H_j |a\rangle$$

$$= \sum_{j=0}^{N} \frac{h_a^j}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^{(r-l_i)} |b_j\rangle = \sum_{j=0}^{N} h_a^j e^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}} \underbrace{\frac{1}{\sqrt{N_{b_j}}} \sum_{r=0}^{N-1} e^{-ikr} T^r |b_j\rangle}_{|b_j(k)\rangle}$$

Finding the representative r of a state-integer s $\quad |r\rangle = T^l |s\rangle$

Lowest integer among all translations

representative (s, r, l)

$r = s;\ t = s;\ l = 0$

do $i = 1,\ N - 1$

  $t =$ **cyclebits**(t, N)

  if $(t < r)$ **then** $r = t;\ l = i$ **end if**

end do

Matrix elements

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=0}^{N} S_j^z S_{j+1}^z$$

$$\langle b_j(k)|H_j|a(k)\rangle = e^{-ikl_j} \frac{1}{2} \sqrt{\frac{N_{b_j}}{N_a}} = e^{-ikl_j} \frac{1}{2} \sqrt{\frac{R_a}{R_{b_j}}}$$

$$k = m\frac{2\pi}{N},\ m = 0,1,\cdots,N-1 \qquad N_a = \frac{N^2}{R_a}$$

Hamiltonian construction

do $a = 0, M - 1$

do $i = 0, N - 1$

$j =$ **mod**$(i + 1, N)$

if $(s_a[i] == s_a[j])$ **then**

$$H(a, a) = H(a, a) + \frac{1}{4}$$

else

$$H(a, a) = H(a, a) - \frac{1}{4}$$

$s =$ **flip**(s_a, i, j)

representative (s, r, l)

findstate (r, b)

if $(b \geq 0)$ **then**

$$H(a, b) = H(a, b) + \frac{1}{2}\sqrt{\frac{R_a}{R_b}}e^{-i2\pi kl/N}$$

end if

end if

end do

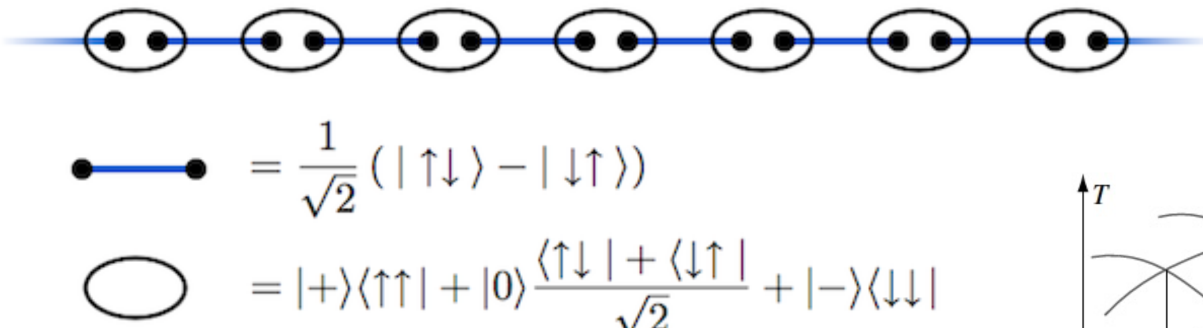
end do

Full diag: impossible

Block diag Mz: impossible

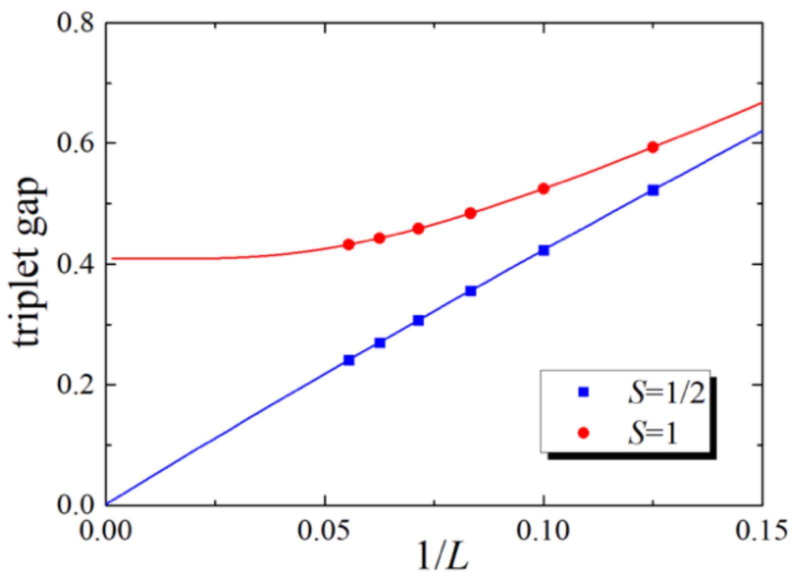
16 site PBC

Block diag k: 19 m 42 s !!!

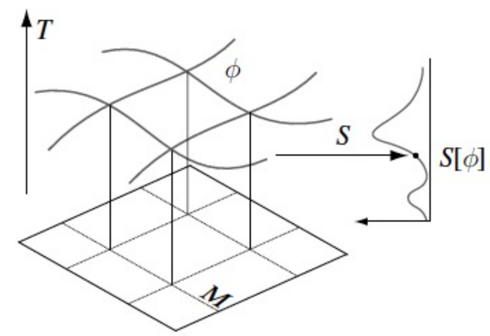


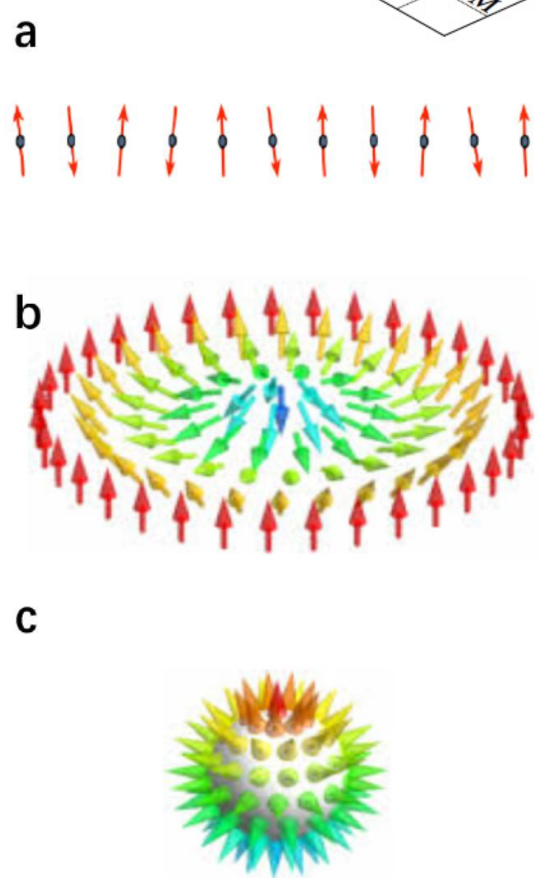
$$= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$



From Prof. Han-Qing Wu of SYSU





$$H = J\sum_{\langle i,j\rangle} S_i \cdot S_j$$

$$Z(g) = \int \mathscr{D}\vec{n}(x,t)\ e^{-S_{NLS}(\vec{n}) + S_{top}(\vec{n})}$$

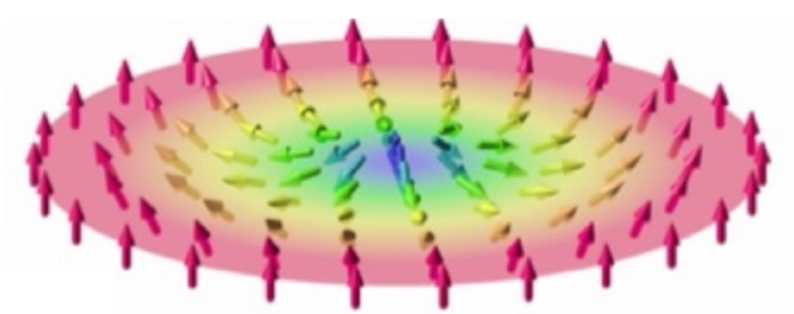
$$S_{NLS} = \frac{1}{2g}\int dtdx\left(\frac{1}{v}\left(\frac{\partial \vec{n}}{\partial t}\right)^2 - v\left(\frac{\partial \vec{n}}{\partial x}\right)^2\right)$$

$$g = 2/S \qquad \vec{n} = \phi \qquad \frac{\partial \phi}{\partial t} = \pm v\frac{\partial \phi}{\partial x}$$

$S = 1/2, 1, 3/2, \cdots$ Small spin, dynamic mass generation, gap

$$S_{top} = i\theta\frac{1}{4\pi}\int dtdx\,\vec{n}\cdot\left(\frac{\partial \vec{n}}{\partial x} \times \frac{\partial \vec{n}}{\partial t}\right)$$

$\theta = 2\pi S$ winding number = 1 for a skyrmion



Skyrmions are topological defects

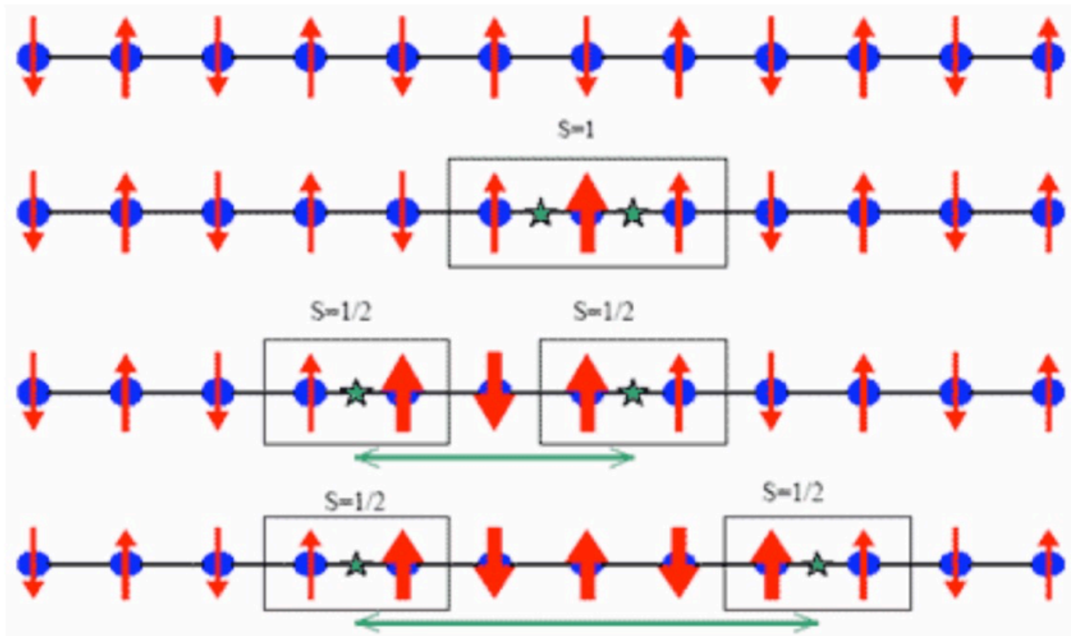
$S = 1, \theta = 2\pi \quad e^{-S_{top}} = 1$ does not contribute

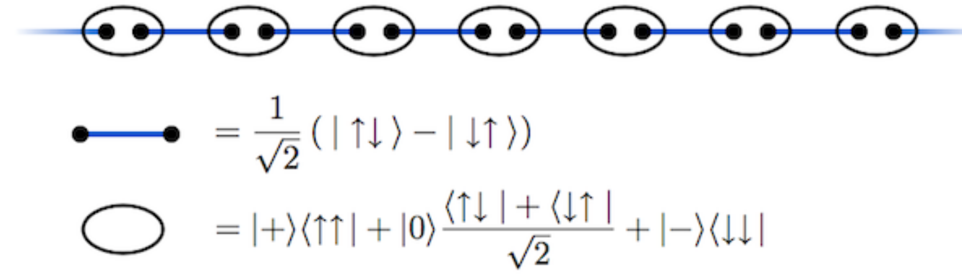
$S = 1/2, \theta = \pi \quad e^{-S_{top}} = (-1)^{\#skyrion}$

cancels the gap

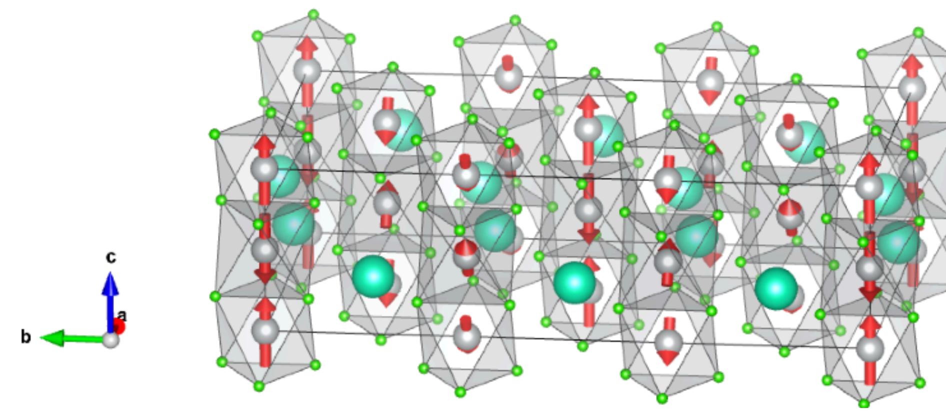
Chap.9 in Condensed Matter Field Theory, Altland & Simons

Excitations in Heisenberg chain

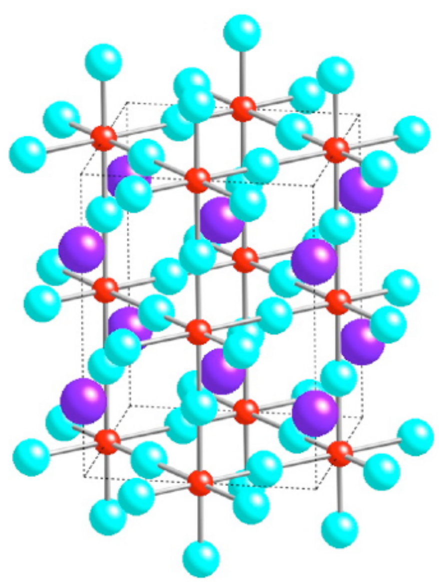


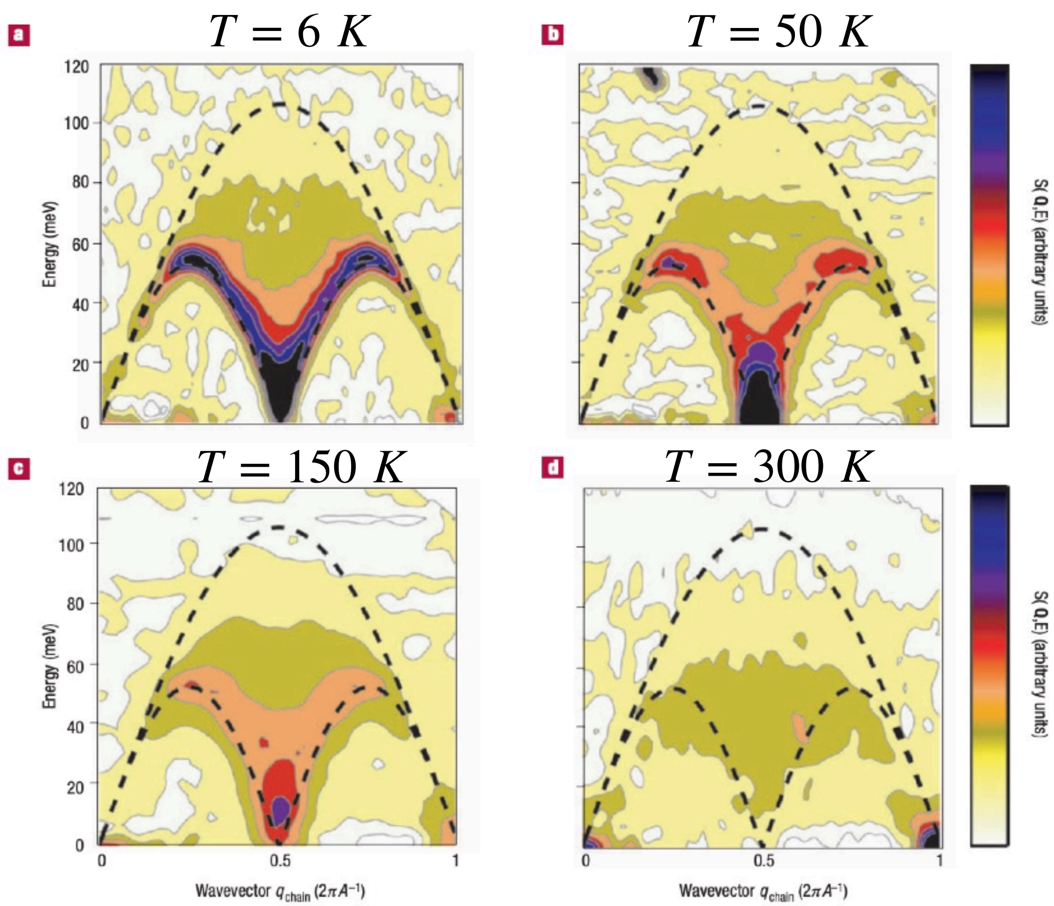


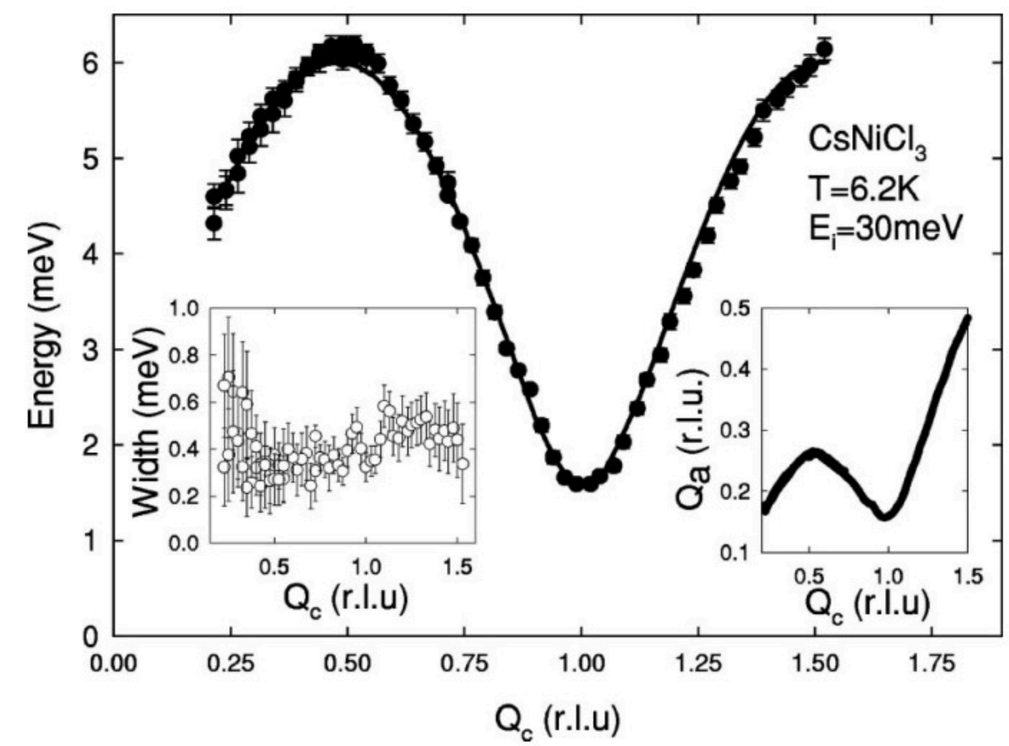
$CsNiCl_3$



$KCuF_3$

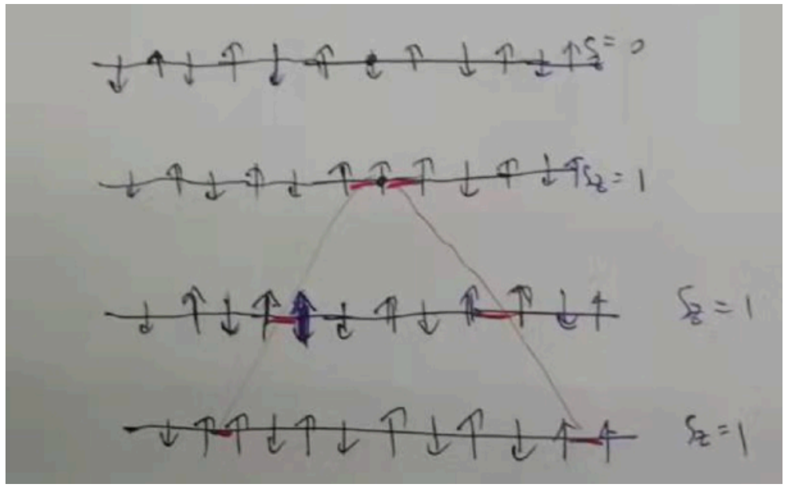


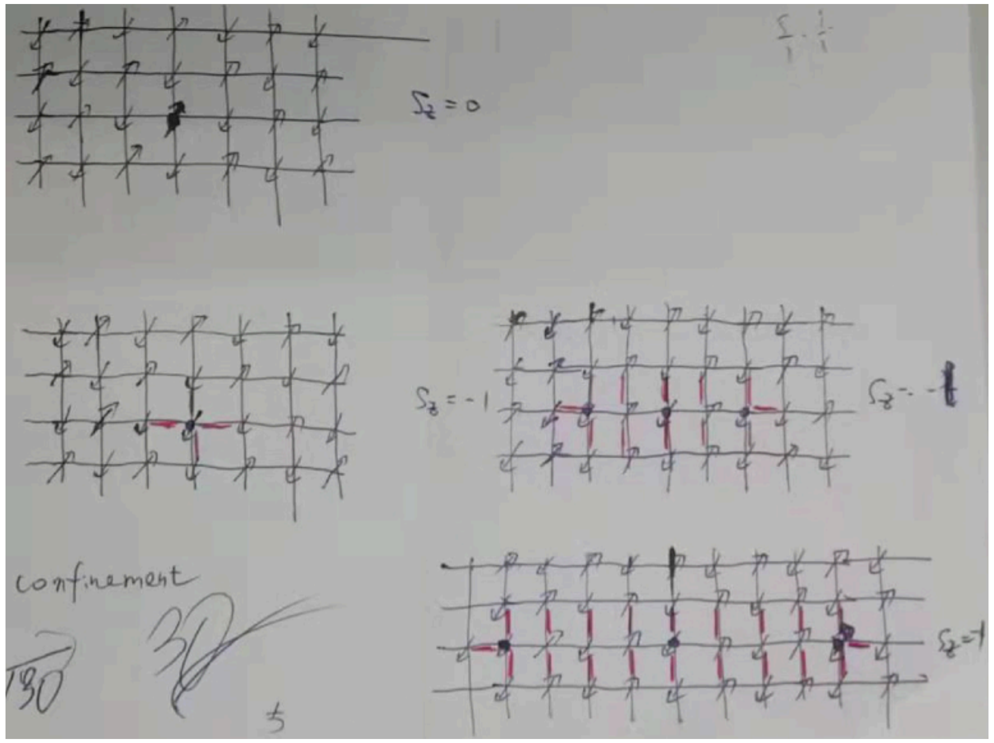


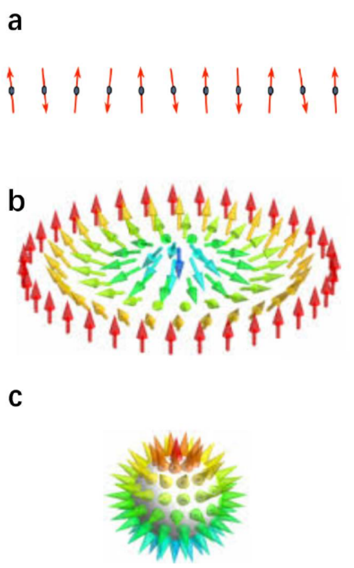


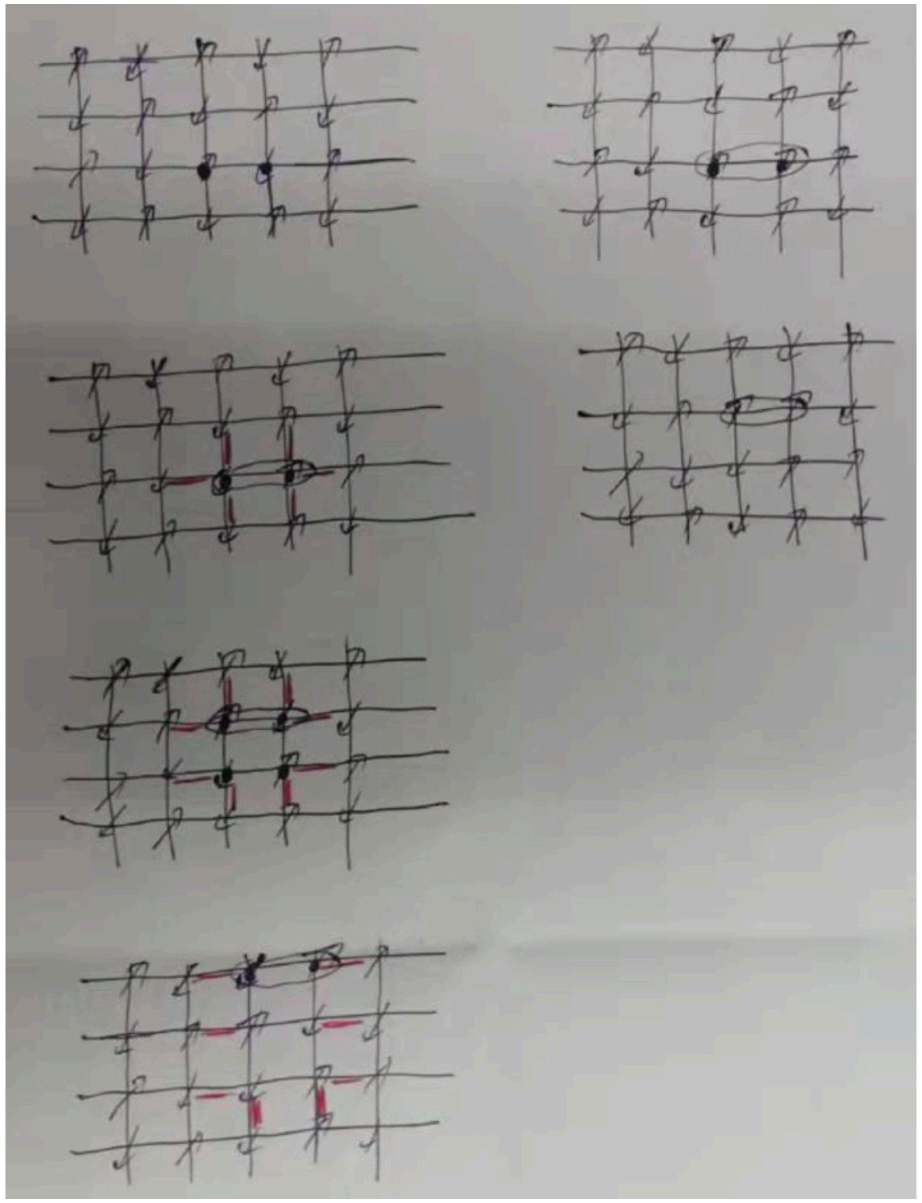
Lake, Tennant, Frost and Nagler, Nature Materials 4, 329 (2005)

Kenzelmann, Cowley, Buyers, Tun, Coldea, Enderle, Phys. Rev. B 66, 024407 (2002) https://www.nobelprize.org/uploads/2018/06/advanced-physicsprize2016.pdf









The wormhole effect on the path integral of reduced density matrix — Unlock the mystery of energy spectrum and entanglement spectrum