

Flavor wave model homework problems

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A. In this part, we will develop a method to solve the ground state without diagonalizing the Hamiltonian.

(1) Assume a particle can be described by spin only, with $S = 1$. and the Hamiltonian is

$$H = S_z.$$

Write down the matrix form for H , the eigenstates of H and their energies. We will write down the ground state to be $|a_0\rangle$.

Comment: In this note, we use the commutation relation for spin operators: $[S_x, S_y] = iS_z$ instead of $[S_x, S_y] = i\hbar S_z$. Which means for spin $1/2$, $S_z = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix}$ instead of $S_z = \begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}$.

(2) Assume a initial state to be $|\psi_0\rangle = \frac{1}{\sqrt{3}}(|S_z = -1\rangle + |S_z = 0\rangle + |S_z = 1\rangle)$. Let $\varepsilon = 10^{-2}$. Calculate

$$|\phi_1\rangle = (1 - \varepsilon H) |\psi_0\rangle$$

$$|\psi_1\rangle = \frac{|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle}$$

Look at the $|\psi_1\rangle$, and show that there are more weights of ground state in $|\psi_1\rangle$ than $|\psi_0\rangle$.

(3) Define

$$|\phi_{n+1}\rangle = (1 - \varepsilon H) |\psi_n\rangle$$

$$|\psi_{n+1}\rangle = \frac{|\phi_{n+1}\rangle}{\langle\phi_{n+1}|\phi_{n+1}\rangle}.$$

Draw (i) $|\langle a_0|\psi_n\rangle|^2$ as a function of n . and (ii) $\langle\psi_n|H|\psi_n\rangle$ as a function of n . Also try with different positive values of ε and see how the value will change the speed of converging.

(4) repeat (2) and (3) with $|\psi_0\rangle = |S_z = 0\rangle$. (Some weird thing could happen, depending on the computer.)

(5) repeat (4) but in each step, add a random small distortion to the wavefunction. Observe how the algorithm converges. Remember to Normalize the wavefunction after distortion.

(6) For a general Hamiltonian

$$H = \sum_{i=0}^{d-1} E_i |a_i\rangle \langle a_i|$$

with the eigenenergies $E_0 < E_1 \leq E_2 \leq \dots \leq E_{d-1}$, prove that $\forall |\psi_0\rangle$ that $\langle a_0|\psi_0\rangle \neq 0$, $\exists \varepsilon > 0$, the series $\{|\psi_n\rangle\}$ generated in (2) satisfies

$$\lim_{n \rightarrow \infty} |\langle a_0|\psi_n\rangle|^2 = 1.$$

Hint: Consider an ε that $0 < \varepsilon < 1/|E_{d-1}|$ and find a q that $0 < q < 1$ and $\left(1 - \sqrt{|\langle a_0|\psi_{n+1}\rangle|^2}\right) < q \left(1 - \sqrt{|\langle a_0|\psi_n\rangle|^2}\right)$.

Comment: From this part, to make sure the algorithm works, a small fluctuation should be added in each step to get a nonzero $\langle a_0|\psi_0\rangle$.

(7) Now we know that this algorithm always converges. Let's figure out how to make it fast. Consider a Hamiltonian in (6) with conditions $d > 2$ and $E_0 < E_1 < E_{d-1}$. Define:

$$|\phi_{n+1}\rangle = (-H + z) |\psi_n\rangle$$

$$|\psi_{n+1}\rangle = \frac{|\phi_{n+1}\rangle}{\langle\phi_{n+1}|\phi_{n+1}\rangle}.$$

where z is a real number and define $x_n = 1 - |\langle a_0|\psi_n\rangle|$. Prove that, when $x_0 < 1$, (i) $\forall z > \frac{-E_0 - E_{d-1}}{2}$, $\exists q$, $0 < q < 1$ and

$$\lim_{n \rightarrow \infty} \frac{x_{n+1}}{x_n} = q,$$

and (ii) q is minimized when

$$z = -\frac{1}{2}(E_1 + E_{d-1})$$

B. This part is to use the method in A to solve the ground state with mean-field approximation.

Consider 2 identical interacting atoms in an external magnetic field and they both have spin-orbital coupling. The Hamiltonian is

$$H = H_1 + H_2 + H_{12}$$

where H_1 and H_2 are the Hamiltonian of two isolated atoms and H_{12} describes the interaction between the atoms. This will be calculated with mean field approximation later.

(1) First we will write down H_1 and H_2 . Assume these two atoms are same and both have quantum numbers $S = 1/2$ and $L = 1$. The Hamiltonian is a sum of spin-orbital coupling and also coupling to the external magnetic field \mathbf{B} .

$$H_1 = \lambda \mathbf{S} \cdot \mathbf{L} + \mu_B(2\mathbf{S} + \mathbf{L}) \cdot \mathbf{B}$$

To write down the matrix form, we need work in the proper space. The space is a product of spin space and orbital space, which means the dimension should be the product of dimension of the spin space and the dimension of the orbital space $(2S+1)(2L+1) = 6$. Because when any spin operator is projected into the orbital space, it should be identity, we can write down the operators in this way:

$$S_z = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1/2 \end{bmatrix}$$

$$L_z = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

now you can write down the single atom Hamiltonian

$$H_1 = \lambda \mathbf{S} \cdot \mathbf{L} + \mu_B(2\mathbf{S} + \mathbf{L}) \cdot \mathbf{B} = \lambda(S_x L_x + S_y L_y + S_z L_z) + \mu_B(B_x(2S_x + L_x) + B_y(2S_y + L_y) + B_z(2S_z + L_z))$$

and look at how the eigenvalues change as a function of λ and \mathbf{B} .

(2) Assume the interaction between two atoms is

$$H_{12} = J \mathbf{S}_1 \cdot \mathbf{S}_2$$

To solve the ground state, we should work in a larger space of dimension $6 \times 6 = 36$, but this matrix is assumed to be too large and we will apply mean-field approximation. In mean field approximation, we will ignore the entanglement between the atoms, which means the ground state can be written as a product of two atoms

$$|\psi_{1,2}\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$$

and total Hamiltonian on atom 1 is

$$h_1 = H_1 + J \mathbf{S} \cdot \langle \psi_2 | \mathbf{S} | \psi_2 \rangle = J(S_x \langle \psi_2 | S_x | \psi_2 \rangle + S_y \langle \psi_2 | S_y | \psi_2 \rangle + S_z \langle \psi_2 | S_z | \psi_2 \rangle)$$

and also the total Hamiltonian on atom 2 is

$$h_2 = H_2 + J \mathbf{S} \cdot \langle \psi_1 | \mathbf{S} | \psi_1 \rangle = J(S_x \langle \psi_1 | S_x | \psi_1 \rangle + S_y \langle \psi_1 | S_y | \psi_1 \rangle + S_z \langle \psi_1 | S_z | \psi_1 \rangle)$$

Notice that h_1 is a function of $|\psi_2\rangle$. Now you can use the method in part A on two atoms to solve the ground state. You can plot the magnetic moment as a function of λ , J and \mathbf{B} .

(4) Let consider the same atom with $L = 1$ and $S = 1/2$ in a chain with ferromagnetic coupling between nearest neighbours. This gives a terrifying Hamiltonian:

$$H = \sum_i \lambda \mathbf{S}_i \cdot \mathbf{L}_i + \mu_B(2\mathbf{S}_i + \mathbf{L}_i) \cdot \mathbf{B} - J \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

where \mathbf{S}_i is the spin operator of the i -th atom on the chain. λ is an arbitrary real number and J is positive. First we write down the effective Hamiltonian on each atom with a wave function $|\psi\rangle$

$$\begin{aligned}
h &= \lambda \mathbf{S} \cdot \mathbf{L} + \mu_B (2\mathbf{S} + \mathbf{L}) \cdot \mathbf{B} - 2J\mathbf{S} \cdot \langle \psi | \mathbf{S} | \psi \rangle \\
&= \lambda (S_x L_x + S_y L_y + S_z L_z) + \mu_B (B_x (2S_x + L_x) + B_y (2S_y + L_y) + B_z (2S_z + L_z)) \\
&\quad - 2JS_x \langle \psi | S_x | \psi \rangle - 2JS_y \langle \psi | S_y | \psi \rangle - 2JS_z \langle \psi | S_z | \psi \rangle
\end{aligned}$$

where all the matrices are $(2S+1)(2L+1) = 6$ dimensional matrices. Now lets assign numbers $\lambda = 1 \text{ meV}$ and $J = 1 \text{ meV}$ with constant $\mu_B = 0.05788 \text{ meV/T}$, you should be able to get the ground state. Try start from a external field $\mathbf{B} = 40 \text{ T } \hat{z}$ and decrease the field to 0 slowly. Calculate the magnetic dipole per atom $m_z = -\langle \psi | 2S_z + L_z | \psi \rangle$ and plot the magnetic dipole as a function of field. You should see the saturated first at a strong field, which gives $m_z = 2$. As field decreases, you should see m_z starts decreasing at a certain field and it doesn't go to 0 when the field approaches 0 and it jumps when the field changes sign. This makes sense because this is a ferromagnetic system and there is only single domain.

(5) Now we will look at a antiferromagnetic system. The difference is that there are 2 atoms per unit cell. We will label the atoms as $(i, 1)$ and $(i, 2)$. With a positive number J , the Hamiltonian is

$$H = \sum_i \lambda (\mathbf{S}_{i,1} \cdot \mathbf{L}_{i,1} + \mathbf{S}_{i,2} \cdot \mathbf{L}_{i,2}) + \mu_B (2\mathbf{S}_{i,1} + \mathbf{L}_{i,1} + 2\mathbf{S}_{i,2} + \mathbf{L}_{i,2}) \cdot \mathbf{B} + \frac{J}{2} (\mathbf{S}_{i-1,2} \cdot \mathbf{S}_{i,1} + 2\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + \mathbf{S}_{i,2} \cdot \mathbf{S}_{i+1,1})$$

We will apply the assumption: $|\psi_{i,1}\rangle = |\psi_1\rangle$ and $|\psi_{i,2}\rangle = |\psi_2\rangle$ and now the mean field on atom 1 will be:

$$\begin{aligned}
h_1 &= \lambda \mathbf{S} \cdot \mathbf{L} + \mu_B (2\mathbf{S} + \mathbf{L}) \cdot \mathbf{B} + 2J\mathbf{S} \cdot \langle \psi_2 | \mathbf{S} | \psi_2 \rangle \\
&= \lambda (S_x L_x + S_y L_y + S_z L_z) + \mu_B (B_x (2S_x + L_x) + B_y (2S_y + L_y) + B_z (2S_z + L_z)) \\
&\quad + 2JS_x \langle \psi_2 | S_x | \psi_2 \rangle + 2JS_y \langle \psi_2 | S_y | \psi_2 \rangle + 2JS_z \langle \psi_2 | S_z | \psi_2 \rangle
\end{aligned}$$

and switch 1 and 2 to get the mean field for atom 2:

$$\begin{aligned}
h_2 &= \lambda (S_x L_x + S_y L_y + S_z L_z) + \mu_B (B_x (2S_x + L_x) + B_y (2S_y + L_y) + B_z (2S_z + L_z)) \\
&\quad + 2JS_x \langle \psi_1 | S_x | \psi_1 \rangle + 2JS_y \langle \psi_1 | S_y | \psi_1 \rangle + 2JS_z \langle \psi_1 | S_z | \psi_1 \rangle
\end{aligned}$$

Now start a strong magnetic field and calculate the magnetic dipole as a function of field. Notice that the algorithm fails at a weak field.

C. This part is about flavour model. We will solve the dispersion of magnons and other extra modes. Lets start from theory calculations and then apply the algorithm on ferromagnetic chain, antiferromagnetic chain, 2D ferromagnetic chain, and some actual materials. There are three practice examples and we will be using them for the whole C part.

(a). 1D ferromagnetic chain with Heisenberg interaction between nearest neighbours, all the atoms only have spin degree of freedom. The Hamiltonian is

$$H = \sum_i g\mu_B \mathbf{B} \cdot \mathbf{S}_i - J\mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

g is the Lande g-factor. J is positive. The Hamiltonian can be rewritten as

$$H = \sum_i g\mu_B (B^x S_i^x + B^y S_i^y + B^z S_i^z) - J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z)$$

(b). 1D antiferromagnetic chain with Heisenberg interaction between nearest neighbours, all the atoms only have spin degree of freedom. The Hamiltonian is

$$\begin{aligned}
H &= \sum_i g\mu_B \mathbf{B} \cdot (\mathbf{S}_{i,1} + \mathbf{S}_{i,2}) + J(\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + \mathbf{S}_{i,1} \cdot \mathbf{S}_{i-1,2}) \\
&= \sum_i g\mu_B \mathbf{B} \cdot (\mathbf{S}_{i,1} + \mathbf{S}_{i,2}) + J(S_{i,1}^x S_{i,2}^x + S_{i,1}^y S_{i,2}^y + S_{i,1}^z S_{i,2}^z + S_{i,1}^x S_{i-1,2}^x + S_{i,1}^y S_{i-1,2}^y + S_{i,1}^z S_{i-1,2}^z)
\end{aligned}$$

(c). 2D triangular ferromagnetic system with a ring-exchange and a easy plane. Since it is a 2D system, we need two integers to label unit cells. S needs to be larger than $1/2$. Let's assume $S = 1$, The Hamiltonian is

$$H = \sum_{i,j} g\mu_B \mathbf{B} \cdot \mathbf{S}_{i,j} - \delta(S_i^z)^2 - J_1 \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} - J_2 \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} - r S_{i,j}^+ S_{i+1,j}^+ S_{i,j+1}^+ S_{i+1,j+1}^+ - r^* S_{i,j}^- S_{i+1,j}^- S_{i,j+1}^- S_{i+1,j+1}^-$$

where r is an arbitrary complex number. This is the number that controls the ring exchange.

(1). In this part we will show the algorithm for an arbitrary system. We assume the system has some unit cells which can

be labeled as the position of each cell $\{\mathbf{r}\}$, each unit cell has N same atoms, which all have d dimensions. The total hamiltonian should be written as

$$H = \sum_{\mathbf{r}} \sum_{p=1}^N H_{\mathbf{r},p} + H_{\text{interaction}}$$

and constained by symmetry, all the $H_{\mathbf{r},p}$ ahould be same for all \mathbf{r} . The interaction part will be a sum of a list, each list of the term will have this form: $\sum_{\mathbf{r}} J_{(\mathbf{0},p_1),(\mathbf{r}_2,p_2)\dots(\mathbf{r}_s,p_s)} \mathbf{X}_{\mathbf{r},p_1}^1 \mathbf{X}_{\mathbf{r}+\mathbf{r}_2,p_2}^2 \dots \mathbf{X}_{\mathbf{r}+\mathbf{r}_s,p_s}^s$. For the three examples, we have 3, 6, and 8 terms. After these examples, we will assume the ground state is already solved and the i -th atom in all unit cells have the same wave function:

$$|\psi_{\mathbf{r},p}\rangle = |\psi_p\rangle$$

and the local mean field hamiltain is known and diagonalized:

$$h_p = \sum_{m=0}^{d-1} E_{p,m} |\psi_{p,m}\rangle \langle \psi_{p,m}|$$

where $E_{p,0} < E_{p,1} \leq \dots \leq E_{p,d-1}$, and $|\psi_{p,0}\rangle = |\psi_p\rangle$ Now, for any operator \hat{X} acting on the i -th atom, we will introduce a expansion, define number:

$$X_{p,mn} = \langle \psi_{p,m} | \hat{X} | \psi_{p,n} \rangle$$

and the \hat{X} operator acting on p -th atom of the \mathbf{r} unit cell will have a expansion:

$$\hat{X} \approx X_{p,00} + \sum_{m=1}^{d-1} \left(\hat{b}_{\mathbf{r}pm}^\dagger X_{p,m0} + X_{p,0m} \hat{b}_{\mathbf{r}pm} \right) - X_{p,00} \sum_{m=1}^{d-1} \hat{b}_{\mathbf{r}pm}^\dagger \hat{b}_{\mathbf{r}im} + \sum_{m=1}^{d-1} \sum_{n=1}^{d-1} \hat{b}_{\mathbf{r}pm}^\dagger X_{p,mn} \hat{b}_{\mathbf{r}pn}$$

where the b and b^\dagger operators follow the commutation relations:

$$\begin{aligned} [\hat{b}_{\mathbf{r}pm}, \hat{b}_{\mathbf{r}'qn}] &= [\hat{b}_{\mathbf{r}pm}^\dagger, \hat{b}_{\mathbf{r}'qn}^\dagger] = 0 \\ [\hat{b}_{\mathbf{r}pm}, \hat{b}_{\mathbf{r}'qn}^\dagger] &= \delta_{\mathbf{r}\mathbf{r}'} \delta_{pq} \delta_{mn} \end{aligned}$$

Now for each term in the interaction list, you can apply this expansion and get a bunch of terms. Only the second order terms will be kept. You should get a hamiltonian in this form:

$$H = \sum_{\mathbf{r}, \mathbf{r}'} \mathbf{X}_{\mathbf{r}}^\dagger \mathbf{H}_{\mathbf{r}\mathbf{r}'} \mathbf{X}_{\mathbf{r}'}$$

where $\mathbf{X}_{\mathbf{r}}$ is a column verctors of dimension $2N(d-1)$,

$$\mathbf{X}_{\mathbf{r}} = \left(b_{\mathbf{r},11}, b_{\mathbf{r},12}, \dots, b_{\mathbf{r},1(d-1)}, b_{\mathbf{r},21}, \dots, b_{\mathbf{r},N(d-1)}, b_{\mathbf{r},1i}^\dagger, b_{\mathbf{r},12}^\dagger, \dots, b_{\mathbf{r},1(d-1)}^\dagger, b_{\mathbf{r},21}^\dagger, \dots, b_{\mathbf{r},N(d-1)}^\dagger \right)^\top$$

and $\mathbf{H}_{\mathbf{r},\mathbf{r}'}$ is a $2N(d-1) \times 2N(d-1)$ matrix.

For example, in example (a), Let's put in numbers $S = 1$, $g = 2$ and $J = 1 \text{ meV}$ and $\mathbf{B} = 0.01 \text{ T } \hat{z}$. We can write down the mean field(in meV):

$$\begin{aligned} h &= g\mu_B B^z S^z - 2JS^z \langle \psi | S_z | \psi \rangle \\ &= 2 \times 0.05788 \times 0.01 \times \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} - 2 \times 1 \times \left(\begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \langle \psi | S_y | \psi \rangle \right. \\ &\quad \left. + \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix} \langle \psi | S_z | \psi \rangle + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \langle \psi | S_z | \psi \rangle \right) \end{aligned}$$

Using the method in part (B), we can find the ground state $|\psi\rangle$ and the mean field h :

$$\begin{aligned} |\psi\rangle &= \begin{bmatrix} 0.500000 \\ 0.707107 \\ 0.500000 \end{bmatrix} \\ h &= \begin{bmatrix} 0 & -1.41503 & 0 \\ -1.41503 & 0 & -1.41503 \\ 0 & -1.41503 & 0 \end{bmatrix} \end{aligned}$$

now we can diagonalize the Hamiltonian:

$$E_0 = -2.001158, E_1 = 0.00000, E_2 = 2.001158$$

$$|\psi_0\rangle = \begin{bmatrix} 0.500000 \\ 0.707107 \\ 0.500000 \end{bmatrix}, |\psi_1\rangle = \begin{bmatrix} -0.707107 \\ 0.000000 \\ 0.707107 \end{bmatrix}, |\psi_2\rangle = \begin{bmatrix} 0.500000 \\ -0.707107 \\ 0.500000 \end{bmatrix}$$

with these numbers, we can get the transformed matrices for S^x , S^y , S^z :

$$S_{mn}^x = \begin{bmatrix} 1.000000 & 0.000000 & 0.000000 \\ 0.000000 & 0.000000 & 0.000000 \\ 0.000000 & 0.000000 & -1.000000 \end{bmatrix}$$

$$S_{mn}^y = \begin{bmatrix} 0.000000 & -0.707107i & 0.000000 \\ 0.707107i & 0.000000 & -0.707107i \\ 0.000000 & 0.707107i & 0.000000 \end{bmatrix}$$

$$S_{mn}^z = \begin{bmatrix} 0.000000 & -0.707107 & 0.000000 \\ -0.707107 & 0.000000 & -0.707107 \\ 0.000000 & -0.707107 & 0.000000 \end{bmatrix}$$

Now the operators can be written in a series(since there is only one atom per unit cell, we will remove the p index, only write as b_{im}):

$$S_i^x \approx 1.000000 + 1.000000 b_{i1} b_{i1}^\dagger + 2.000000 b_{i2} b_{i2}^\dagger$$

$$S_i^y \approx -0.707107i b_{i1}^\dagger + 0.707107i b_{i1} - 0.707107i b_{i1}^\dagger b_{i2} + 0.707107i b_{i2}^\dagger b_{i1}$$

$$S_i^z \approx -0.707107 b_{i1}^\dagger - 0.707107 b_{i1} - 0.707107 b_{i1}^\dagger b_{i2} - 0.707107 b_{i2}^\dagger b_{i1}$$

Comment: Notice even in this form, all spin operators keep Hermitian.

Now For the three interactions $S_i^x S_{i+1}^x$, $S_i^y S_{i+1}^y$, $S_i^z S_{i+1}^z$, we will show (only the quadratic terms)

$$S_i^x S_{i+1}^x \approx 1.000000 (b_{i1}^\dagger b_{i1} + b_{(i+1)1}^\dagger b_{(i+1)1}) + 2.000000 (b_{i2}^\dagger b_{i2} + b_{(i+1)2}^\dagger b_{(i+1)2})$$

$$= \begin{bmatrix} b_{i1}^\dagger & b_{i2}^\dagger & b_{i1} & b_{i2} \end{bmatrix} \begin{bmatrix} 1.000000 & 0 & 0 & 0 \\ 0 & 2.000000 & 0 & 0 \\ 0 & 0 & 1.000000 & 0 \\ 0 & 0 & 0 & 2.000000 \end{bmatrix} \begin{bmatrix} b_{(i+1)1} \\ b_{(i+1)2} \\ b_{(i+1)1}^\dagger \\ b_{(i+1)2}^\dagger \end{bmatrix}$$

There are constants, because $b_{(i+1)1} b_{(i+1)1}^\dagger = b_{(i+1)1}^\dagger b_{(i+1)1} + 1$, but it is not written.

$$S_i^z S_{i+1}^z \approx 0.500000 (b_{i1}^\dagger b_{(i+1)1}^\dagger + b_{i1} b_{(i+1)1} + b_{i1} b_{(i+1)1}^\dagger + b_{i1}^\dagger b_{(i+1)1})$$

$$= \begin{bmatrix} b_{i1}^\dagger & b_{i2}^\dagger & b_{i1} & b_{i2} \end{bmatrix} \begin{bmatrix} 0.500000 & 0 & 0.500000 & 0 \\ 0 & 0 & 0 & 0 \\ 0.500000 & 0 & 0.500000 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{(i+1)1} \\ b_{(i+1)2} \\ b_{(i+1)1}^\dagger \\ b_{(i+1)2}^\dagger \end{bmatrix}$$

After the Hamiltonian is written, we will do Fourier transforms. Define:

$$\hat{b}_{\mathbf{k}pm} = \frac{1}{\sqrt{A}} \sum_{\mathbf{r}} \hat{b}_{\mathbf{r}pm} e^{-i\mathbf{k}\cdot\mathbf{r}}$$

$$\hat{b}_{\mathbf{k}pm}^\dagger = \frac{1}{\sqrt{A}} \sum_{\mathbf{r}} \hat{b}_{\mathbf{r}pm}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}}$$

where A is the normalizing factor which gives the commutation relation $[\hat{b}_{\mathbf{k}pm}, \hat{b}_{\mathbf{k}'qn}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{pq} \delta_{mn}$. Now the Hamiltonian can be written in the momentum space and an algorithm proposed by Colpa could properly diagonalize this Hamiltonian. In the algorithm, the Hamiltonian is written as $\sum_{\mathbf{k}} \mathbf{X}_{\mathbf{k}}^\dagger \mathbf{H}_{\mathbf{k}} \mathbf{X}_{\mathbf{k}}$ where $\mathbf{X}_{\mathbf{k}} = (b_{\mathbf{k}11}, \dots, b_{\mathbf{k}1(d-1)}, \dots, b_{\mathbf{k}n(d-1)}, b_{(-\mathbf{k})11}^\dagger, \dots, b_{(-\mathbf{k})n(d-1)}^\dagger)^\top$. It is very easy to get the energies. Define a matrix:

$$\mathbf{g} = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{bmatrix},$$

where $\mathbf{1}$ means a identity matrix of dimension $n(d-1)$ and $\mathbf{0}$ means a zero matrix. To get the energies, solve the eigenvalues of matrix $\mathbf{H.g}$. There will be $n(d-1)$ positive numbers and the other negative ones on the positive numbers times -1 . The $n(d-1)$ numbers are the energies of excitations. After this, Plotting the numbers as with different k will give you the dispersion. There is another way to get the energies and get information of the transformation. The first step is to do Cholesky decomposition $\mathbf{H} = \mathbf{K}^\dagger \mathbf{K}$. This requires that \mathbf{H} must be positive definite, otherwise is not decomposivable. If you do not get this, it means that you made a mistake. (needs to be finished)

In example (a). We will first show the the Fourier transformation for $S_j^x S_{j+1}^x$ (since i is used for imaginary number, we will change the index or unit cell to j):

$$S_j^x S_{j+1}^x \approx 1.000000 \left(b_{j1}^\dagger b_{j1} + b_{(j+1)1}^\dagger b_{(j+1)1} \right) + 2.000000 \left(b_{j2}^\dagger b_{j2} + b_{(j+1)2}^\dagger b_{(j+1)2} \right)$$

We have

$$b_{km} = \frac{1}{\sqrt{A}} \sum_j b_{jm} e^{-i(kj)}$$

$$b_{km}^\dagger = \frac{1}{\sqrt{A}} \sum_j b_{jm}^\dagger e^{+i(kj)}$$

and the inverse transforms:

$$b_{jm} = \frac{1}{\sqrt{A}} \sum_k b_{km} e^{i(kj)}$$

$$b_{jm}^\dagger = \frac{1}{\sqrt{A}} \sum_k b_{km}^\dagger e^{-i(kj)}$$

for $m = 1, 2$. and we have:

$$\begin{aligned} & \sum_j b_{j1}^\dagger b_{j1} \\ &= \frac{1}{A} \sum_j \sum_k \sum_{k'} b_{k1}^\dagger e^{-ikj} b_{k'1}^\dagger e^{+ik'j} \\ &= \frac{1}{A} \sum_{kk'} b_{k1}^\dagger b_{k'1} \sum_j e^{i(k'-k)j} \\ &= \frac{1}{A} \sum_{kk'} b_{k1}^\dagger b_{k'1} A \delta_{k,k'} \\ &= \sum_k b_{k1}^\dagger b_{k1} \end{aligned}$$

Now the $S_j^x S_{j+1}^x$ term is going to be

$$\begin{aligned} & \sum_j 1.000000 \left(b_{j1}^\dagger b_{j1} + b_{(j+1)1}^\dagger b_{(j+1)1} \right) + 2.000000 \left(b_{j2}^\dagger b_{j2} + b_{(j+1)2}^\dagger b_{(j+1)2} \right) \\ &= \sum_k 2.000000 b_{k1}^\dagger b_{k1} + 4.000000 b_{k2}^\dagger b_{k2} \\ &= 0.500000 \begin{bmatrix} b_{k1}^\dagger & b_{k2}^\dagger & b_{(-k)1} & b_{(-k)2} \end{bmatrix} \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix} \end{aligned}$$

and the $S_j^z S_{j+1}^z$ term will be

$$\begin{aligned}
& 0.500000 \sum_j \left(b_{j1}^\dagger b_{(j+1)1}^\dagger + b_{j1} b_{(j+1)1} + b_{j1} b_{(j+1)1}^\dagger + b_{j1}^\dagger b_{(j+1)1} \right) \\
&= \frac{0.500000}{A} \sum_j \sum_k \sum_{k'} \left(b_{k1}^\dagger b_{k'1}^\dagger e^{-ikj} e^{-ik'(j+1)} + b_{k1} b_{k'1} e^{ikj} e^{ik'(j+1)} + b_{k1} b_{k'1}^\dagger e^{ikj} e^{-ik'(j+1)} + b_{k1}^\dagger b_{k'1} e^{-ikj} e^{ik'(j+1)} \right) \\
&= \frac{0.500000}{A} \sum_k \sum_{k'} \left(b_{k1}^\dagger b_{k'1}^\dagger e^{-ik'} \sum_j e^{-i(k+k')j} + b_{k1} b_{k'1} e^{ik'} \sum_j e^{i(k+k')j} + b_{k1} b_{k'1}^\dagger e^{-ik'} \sum_j e^{i(k-k')j} + b_{k1}^\dagger b_{k'1} e^{ik'} \sum_j e^{-i(k+k')j} \right) \\
&= 0.500000 \sum_k \sum_{k'} \left(b_{k1}^\dagger b_{k'1}^\dagger e^{-ik'} \delta_{-k,k'} + b_{k1} b_{k'1} e^{ik'} \delta_{-k,k'} + b_{k1} b_{k'1}^\dagger e^{-ik'} \delta_{k,k'} + b_{k1}^\dagger b_{k'1} e^{ik'} \delta_{k,k'} \right) \\
&= 0.500000 \sum_k \sum_{k'} \left(b_{k1}^\dagger b_{(-k)1}^\dagger e^{ik} + b_{k1} b_{(-k)1} e^{-ik} + b_{k1} b_{k1}^\dagger e^{-ik} + b_{k1}^\dagger b_{k1} e^{ik} \right) \\
&= 0.500000 \begin{bmatrix} b_{k1}^\dagger & b_{k2}^\dagger & b_{(-k)1} & b_{(-k)2} \end{bmatrix} \begin{bmatrix} e^{ik} & 0 & e^{-ik} & 0 \\ 0 & 0 & 0 & 0 \\ e^{ik} & 0 & e^{-ik} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix}
\end{aligned}$$
