

Flavor wave model homework problems

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The purpose of this file is to understand and develop your own program of the flavor wave model. There has been linear spin wave theory (LSWT) and it was proved successfully on many materials. The dispersion and cross section for inelastic neutron scattering can be correctly predicted by linear spin wave theory. However, there are some properties that can not be predicted by LSWT. First, the actual spin quantum number does not affect the theory a lot. The actual S number will only be multiplied to the interactions. This means that all difference spin systems are identical to $S = 1/2$ system. This directly leads to a result that the number of modes is equal to the number of spins per unit cell. This works for most of the actual materials. In these materials, all the magnon modes are close to each other energetically and they are far away from all possible excitations who have much higher energy than the magnons. However in some materials, such as FeI_2 [1, 2], Sr_2IrO_4 [3], CoO [4], CoTiO_3 [5], there are some modes, who are not magnons predicted by linear spin wave theory, above the magnon modes and (1) they are not far away from the magnons modes (2) they are momentum dependent. In magnetic materials, they are usually called Spin-Orbital(SO) excitons. One way to explain the dispersion of those higher modes is to build a separate model because they don't exist in LSWT. For this reason, a flavor wave model is proposed. In this model, each ion is treated as a vector in a larger space. The consequence is that there will be more excitations. The low-energy magnons and high-energy SO excitons can be considered simultaneously in one model.

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 an 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 $|\psi\rangle$

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

where all the matrices are $(2S+1)(2L+1) = 6$ dimensional matrices. Now let's 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:

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

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

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

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. Let's 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

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

(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 constrained by symmetry, all the $H_{\mathbf{r},p}$ should 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 hamiltonian 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 an 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 an 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:

$$[\hat{b}_{\mathbf{r}pm}, \hat{b}_{\mathbf{r}'qn}] = [\hat{b}_{\mathbf{r}pm}^\dagger, \hat{b}_{\mathbf{r}'qn}^\dagger] = 0$$

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

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 vector 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 $J = 1$ meV and $\mathbf{B} = -0.08639 \text{ T } \hat{x}$. We can write down the mean field (in meV):

$$\begin{aligned} h &= g\mu_B B^z S^z - 2JS^z \langle \psi | S_z | \psi \rangle \\ &= 2 \times 0.05788 \times 0.08639 \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} - 2 \times 1 \times \left(\begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \langle \psi | S_x | \psi \rangle \right. \\ &\quad \left. + \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix} \langle \psi | S_y | \psi \rangle + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \langle \psi | S_z | \psi \rangle \right) \end{aligned}$$

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

$$|\psi\rangle = \begin{bmatrix} 1.00 \\ 0.00 \\ 0.00 \end{bmatrix}$$

$$h = \begin{bmatrix} -2.02 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2.02 \end{bmatrix}$$

now we can diagonalize the Hamiltonian:

$$E_0 = -2.02, E_1 = 0.00000, E_2 = 2.02$$

$$|\psi_0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, |\psi_1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, |\psi_2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

with these numbers, we can get the transformed matrices for S^x , S^y , S^z (because this is a easy problem, I will be using the exact answers. In real materials, only numerical values are available):

$$S_{mn}^x = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$S_{mn}^y = \begin{bmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{bmatrix}$$

$$S_{mn}^z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Now the operators can be written in a series However, we will rewrite the Hamiltonian so that it looks more symmetric:

$$H = \sum_i g\mu_B (B^x S^x + B^y S^y + B^z S^z) - \frac{J}{2} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z + S_{i-1}^x S_i^x + S_{i-1}^y S_i^y + S_{i-1}^z S_i^z)$$

Since there is only one atom per unit cell, we will remove the p index, only write as b_{im} :

$$S_i^x \approx \frac{1}{\sqrt{2}} b_{i1}^\dagger + \frac{1}{\sqrt{2}} b_{i1} + \frac{1}{\sqrt{2}} b_{i1}^\dagger b_{i2} + \frac{1}{\sqrt{2}} b_{i2}^\dagger b_{i1}$$

$$S_i^y \approx \frac{i}{\sqrt{2}} b_{i1}^\dagger - \frac{i}{\sqrt{2}} b_{i1} - \frac{i}{\sqrt{2}} b_{i1}^\dagger b_{i2} + \frac{i}{\sqrt{2}} b_{i2}^\dagger b_{i1}$$

$$S_i^z \approx 1 - b_{i1} b_{i1}^\dagger - 2b_{i2} b_{i2}^\dagger$$

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)

$$\begin{aligned} S_i^x S_{i+1}^x &\approx \frac{1}{2} \left(b_{i1}^\dagger b_{(i+1)1}^\dagger + b_{i1} b_{(i+1)1} + b_{i1} b_{(i+1)1}^\dagger + b_{i1}^\dagger b_{(i+1)1} \right) \\ &= \begin{bmatrix} b_{i1}^\dagger & b_{i2}^\dagger & b_{i1} & b_{i2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{(i+1)1} \\ b_{(i+1)2} \\ b_{(i+1)1}^\dagger \\ b_{(i+1)2}^\dagger \end{bmatrix} \end{aligned}$$

$$\begin{aligned} S_i^y S_{i+1}^y &\approx \frac{1}{2} \left(-b_{i1}^\dagger b_{(i+1)1}^\dagger - b_{i1} b_{(i+1)1} + b_{i1} b_{(i+1)1}^\dagger + b_{i1}^\dagger b_{(i+1)1} \right) \\ &= \begin{bmatrix} b_{i1}^\dagger & b_{i2}^\dagger & b_{i1} & b_{i2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{(i+1)1} \\ b_{(i+1)2} \\ b_{(i+1)1}^\dagger \\ b_{(i+1)2}^\dagger \end{bmatrix} \end{aligned}$$

$$S_i^z S_{i+1}^z \approx - \left(b_{i1}^\dagger b_{i1} + b_{(i+1)1}^\dagger b_{(i+1)1} \right) - 2 \left(b_{i2}^\dagger b_{i2} + b_{(i+1)2}^\dagger b_{(i+1)2} \right)$$

And

$$S_{i-1}^x S_i^x \approx \frac{1}{2} \left(b_{(i-1)1}^\dagger b_{i1}^\dagger + b_{(i-1)1} b_{i1} + b_{(i-1)1} b_{i1}^\dagger + b_{(i-1)1}^\dagger b_{i1} \right)$$

$$S_{i-1}^y S_i^y \approx \frac{1}{2} \left(-b_{(i-1)1}^\dagger b_{i1}^\dagger - b_{(i-1)1} b_{i1} + b_{(i-1)1} b_{i1}^\dagger + b_{(i-1)1}^\dagger b_{i1} \right)$$

$$S_{i-1}^z S_i^z \approx - \left(b_{(i-1)1}^\dagger b_{(i-1)1} + b_{i1}^\dagger b_{i1} \right) - 2 \left(b_{(i-1)2}^\dagger b_{(i-1)2} + b_{i2}^\dagger b_{i2} \right)$$

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. Notice how the $S_i^z S_{i+1}^z$ term is different from othes.

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

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

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

and inverse Fourier transforms:

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

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

where A is the nomalizing 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.

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

$$b_{km} = \frac{1}{\sqrt{A}} \sum_j b_{jm} e^{-ikj}$$

$$b_{km}^\dagger = \frac{1}{\sqrt{A}} \sum_j b_{jm}^\dagger e^{+ikj}$$

and the inverse transforms:

$$b_{jm} = \frac{1}{\sqrt{A}} \sum_k b_{km} e^{ikj}$$

$$b_{jm}^\dagger = \frac{1}{\sqrt{A}} \sum_k b_{km}^\dagger e^{-ikj}$$

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 $S_j^z S_{j+1}^z$ term is going to be

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

Notice that term doesn't change with momentum k . Just substitute k by $-k$, we can get

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

And the $S_j^x S_{j+1}^x$ term:

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

and the $S_j^y S_{j+1}^y$ term:

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

With the same method, you can also get the transformed term of $S_{(j-1)}^x S_j^x$ and $S_{(j-1)}^y S_j^y$:

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

And

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

The single atom Hamiltonian

$$h_0 = g\mu_B B^z S^z = \begin{bmatrix} -0.02 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0.02 \end{bmatrix}$$

and the bosonic operator form is:

$$h_j \approx -0.02 + 0.02 b_{j1}^\dagger b_{j1} + 0.04 b_{j2}^\dagger b_{j2}$$

And transform this into the momentum space:

$$\begin{aligned}
& \sum_j h_j \\
&= \sum_j -0.02 + 0.02 b_{j1}^\dagger b_{j1} + 0.04 b_{j2}^\dagger b_{j2} \\
&= \sum_k 0.02 b_{k1}^\dagger b_{k1} + 0.04 b_{k2}^\dagger b_{k2} \quad (\text{constant ignored}) \\
&= \sum_k \begin{bmatrix} b_{k1}^\dagger & b_{k2}^\dagger & b_{(-k)1} & b_{(-k)2} \end{bmatrix} \begin{bmatrix} 0.02 & 0 & 0 & 0 \\ 0 & 0.04 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix}
\end{aligned}$$

In fact we are going to write twice of this term, which means we have:

$$\sum_j h_j = \sum_k \begin{bmatrix} b_{k1}^\dagger & b_{k2}^\dagger & b_{(-k)1} & b_{(-k)2} \end{bmatrix} \begin{bmatrix} 0.02 & 0 & 0 & 0 \\ 0 & 0.04 & 0 & 0 \\ 0 & 0 & 0.02 & 0 \\ 0 & 0 & 0 & 0.04 \end{bmatrix} \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix}$$

Now summing up all the terms, and remember that there is a coefficient $-\frac{J}{2} = -\frac{1}{2}$ in front of the six terms. We can get the Hamiltonian in the momentum space:

$$\begin{aligned}
H &= \sum_k \begin{bmatrix} b_{k1}^\dagger \\ b_{k2}^\dagger \\ b_{(-k)1} \\ b_{(-k)2} \end{bmatrix}^T \left(\underbrace{\begin{bmatrix} 0.02 & 0 & 0 & 0 \\ 0 & 0.04 & 0 & 0 \\ 0 & 0 & 0.02 & 0 \\ 0 & 0 & 0 & 0.04 \end{bmatrix}}_{h_j} \underbrace{-\frac{1}{2} \begin{bmatrix} -2 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{-\frac{J}{2} S_j^z S_{j+1}^z} \underbrace{-\frac{1}{4} \begin{bmatrix} e^{ik} & 0 & e^{ik} & 0 \\ 0 & 0 & 0 & 0 \\ e^{ik} & 0 & e^{-ik} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{-\frac{J}{2} S_j^x S_{j+1}^x} \underbrace{-\frac{1}{4} \begin{bmatrix} e^{ik} & 0 & -e^{ik} & 0 \\ 0 & 0 & 0 & 0 \\ -e^{ik} & 0 & e^{-ik} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{-\frac{J}{2} S_j^y S_{j+1}^y} \right. \\
&\quad \left. \underbrace{-\frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -4 \end{bmatrix}}_{-\frac{J}{2} S_j^z S_{j-1}^z} \underbrace{-\frac{1}{4} \begin{bmatrix} e^{-ik} & 0 & e^{ik} & 0 \\ 0 & 0 & 0 & 0 \\ e^{ik} & 0 & e^{ik} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{-\frac{J}{2} S_j^x S_{j-1}^x} \underbrace{-\frac{1}{4} \begin{bmatrix} e^{-ik} & 0 & -e^{ik} & 0 \\ 0 & 0 & 0 & 0 \\ -e^{ik} & 0 & e^{ik} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{-\frac{J}{2} S_j^y S_{j-1}^y} \right) \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix} \\
&= \sum_k \begin{bmatrix} b_{k1}^\dagger \\ b_{k2}^\dagger \\ b_{(-k)1} \\ b_{(-k)2} \end{bmatrix}^T \begin{bmatrix} 1.02 - \cos k & 0 & 0 & 0 \\ 0 & 2.04 & 0 & 0 \\ 0 & 0 & 1.02 - \cos k & 0 \\ 0 & 0 & 0 & 2.04 \end{bmatrix} \begin{bmatrix} b_{k1} \\ b_{k2} \\ b_{(-k)1}^\dagger \\ b_{(-k)2}^\dagger \end{bmatrix}
\end{aligned}$$

Now you get a form in $H = \sum_{\mathbf{k}} \mathbf{X}_{\mathbf{k}}^\dagger \mathbf{H}_{\mathbf{k}} \mathbf{X}_{\mathbf{k}}$ and we need to diagonalize the $\mathbf{H}_{\mathbf{k}}$ matrix. There is 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 $\mathbf{X}_{\mathbf{k}} = (b_{k1}, \dots, b_{k1(d-1)}, \dots, b_{kn(d-1)})$ and $\mathbf{H}_{\mathbf{k}}$ is a Hermitian matrix. 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 an identity matrix of dimension $n(d-1)$ and $\mathbf{0}$ means a zero matrix. To get the energies, solve the eigenvalues of matrix $\mathbf{H}\mathbf{g}$. 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.

In example (a),

$$\mathbf{H}_k = \begin{bmatrix} 1.02 - \cos k & 0 & 0 & 0 \\ 0 & 2.04 & 0 & 0 \\ 0 & 0 & 1.02 - \cos k & 0 \\ 0 & 0 & 0 & 2.04 \end{bmatrix}$$

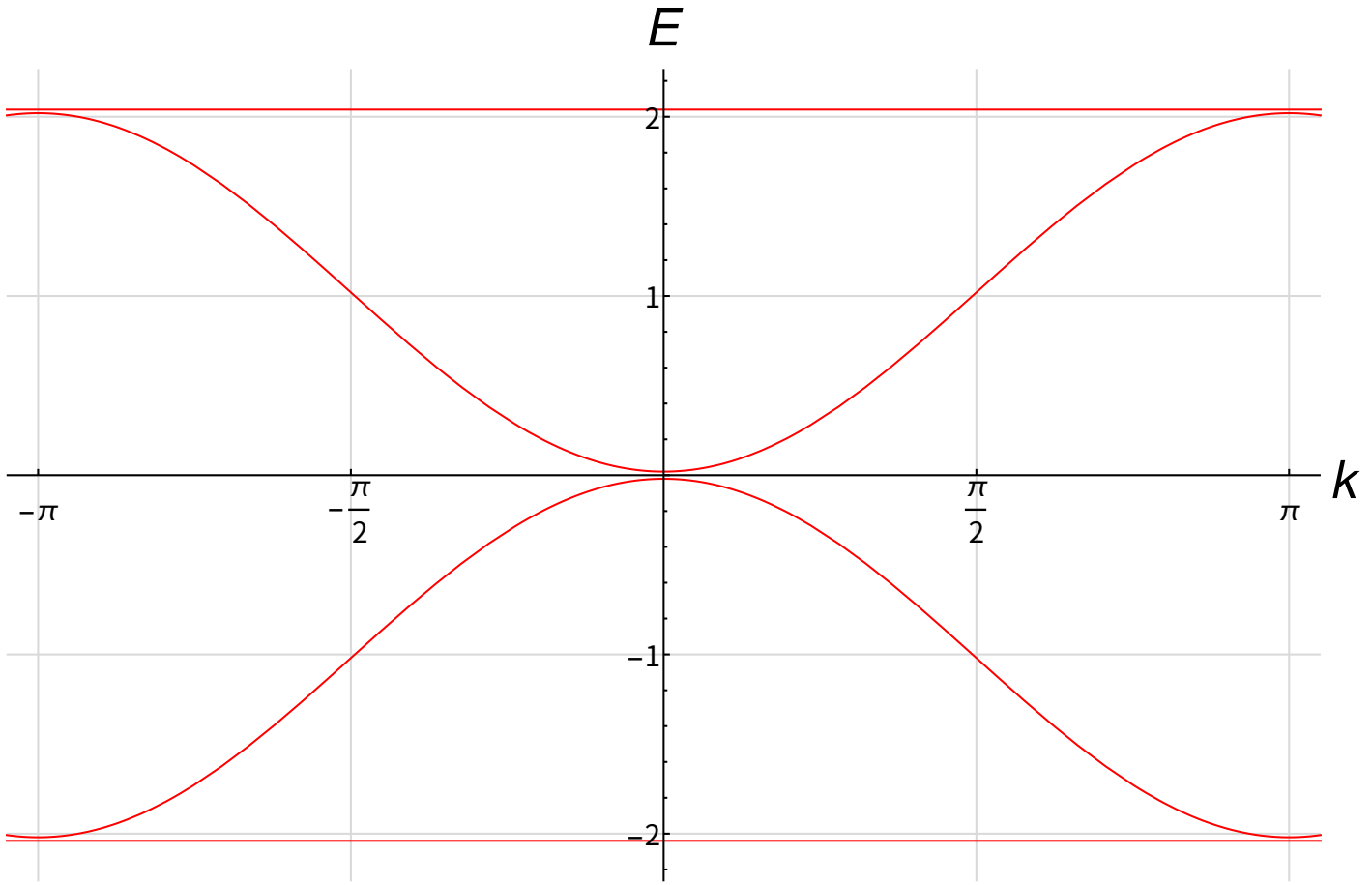


Figure 1: **Dispersion of a 1D ferromagnetic chain.** $S = 1$ and there is a small magnetic field.

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

so that

$$\mathbf{H}\mathbf{g} = \begin{bmatrix} 1.02 - \cos k & 0 & 0 & 0 \\ 0 & 2.04 & 0 & 0 \\ 0 & 0 & -(1.02 - \cos k) & 0 \\ 0 & 0 & 0 & -2.04 \end{bmatrix}$$

This is already diagonalized. So the spectrum is figured out. You can plot it and you should get a figure like [3] Fig. 1

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