Flavor wave model homework problems

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

(1) Assume a particle can be discribed 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: $[S_x, S_y] = 2\mathrm{i}S_z$ in stead of $[S_x, S_y] = \mathrm{i}\hbar S_z$. Which means for spin 1/2, $S_z = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix}$.

(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 differenct 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 $E_0 < E_1 \leqslant E_2 \leqslant \ldots \leqslant E_{d-1}$, prove that $\forall\,|\psi_0\rangle$ that $\langle a_0|\psi_0\rangle \neq 0$, $\exists\varepsilon > 0$, the series $\{|\psi_n\rangle\}$ generatred in (2) satisfies

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

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 fluctuaction should be added in each step to get a nonzero $\langle a_0|\psi_0\rangle$.

(7) Now we know that this algorithrm always converges. Let's figure out how to make it fast. Consider a Hamiltonian in (5) 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 (i) $\forall z > \frac{-E_0 - E_{d-1}}{2}$, $\exists q$, $0 < q < 1$ and

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

and (ii) q is minimized when

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

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 $\boldsymbol{B}$.

$$H_1 = \lambda \boldsymbol{S} \cdot \boldsymbol{L} + \mu_{\mathrm{B}}(2\boldsymbol{S} + \boldsymbol{L}) \cdot \boldsymbol{B}$$

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

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

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

(2) Assume the interaction between two atoms is

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

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

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

and also the total Hamiltonian on atom 2 is

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

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 groud state. You can plot the magnetic moment as a function of λ, J and $\boldsymbol{B}$.

(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:

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

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

$$
\begin{aligned}
h &= \lambda \boldsymbol{S}\cdot\boldsymbol{L} + \mu_{\mathrm{B}}(2\boldsymbol{S}+\boldsymbol{L})\cdot\boldsymbol{B} - 2J\boldsymbol{S}\cdot\langle\psi|\,\boldsymbol{S}\,|\psi\rangle \\
&= \lambda\left(S_xL_x + S_yL_y + S_zL_z\right) + \mu_{\mathrm{B}}\left(B_x(2S_x+L_x) + B_y(2S_y+L_y) + B_z(2S_z+L_z)\right) \\
&\qquad - 2JS_x\langle\psi|\,S_x\,|\psi\rangle - 2JS_y\langle\psi|\,S_y\,|\psi\rangle - 2JS_z\langle\psi|\,S_z\,|\psi\rangle
\end{aligned}
$$

where all the matrices are $(2S+1)(2L+1) = 6$ dimensional matrices. Now lets assign numbers $\lambda = 1\,\mathrm{meV}$ and $J = 1\,\mathrm{meV}$ wich constant $\mu_{\mathrm{B}} = 0.057\,88\,\mathrm{meV/T}$, you should be able to get the ground state. Try start from a external field $\boldsymbol{B} = 40\,\mathrm{T}\ \hat{z}$ 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 doen't go to 0 when the field aprroches 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

$$
H = \sum_i \lambda\left(\boldsymbol{S}_{i,1}\cdot\boldsymbol{L}_{i,1} + \boldsymbol{S}_{i,2}\cdot\boldsymbol{L}_{i,2}\right) + \mu_{\mathrm{B}}(2\boldsymbol{S}_{i,1} + \boldsymbol{L}_{i,1} + 2\boldsymbol{S}_{i,2} + \boldsymbol{L}_{i,2})\cdot\boldsymbol{B} + \frac{J}{2}\left(\boldsymbol{S}_{i-1,2}\cdot\boldsymbol{S}_{i,1} + 2\boldsymbol{S}_{i,1}\cdot\boldsymbol{S}_{i,2} + \boldsymbol{S}_{i,2}\cdot\boldsymbol{S}_{i+1,1}\right)
$$

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:

$$
\begin{aligned}
h_1 &= \lambda \boldsymbol{S}\cdot\boldsymbol{L} + \mu_{\mathrm{B}}(2\boldsymbol{S}+\boldsymbol{L})\cdot\boldsymbol{B} + 2J\boldsymbol{S}\cdot\langle\psi_2|\,\boldsymbol{S}\,|\psi_2\rangle \\
&= \lambda\left(S_xL_x + S_yL_y + S_zL_z\right) + \mu_{\mathrm{B}}\left(B_x(2S_x+L_x) + B_y(2S_y+L_y) + B_z(2S_z+L_z)\right) \\
&\qquad + 2JS_x\langle\psi_2|\,S_x\,|\psi_2\rangle + 2JS_y\langle\psi_2|\,S_y\,|\psi_2\rangle + 2JS_z\langle\psi_2|\,S_z\,|\psi_2\rangle
\end{aligned}
$$

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

$$
\begin{aligned}
h_2 &= \lambda\left(S_xL_x + S_yL_y + S_zL_z\right) + \mu_{\mathrm{B}}\left(B_x(2S_x+L_x) + B_y(2S_y+L_y) + B_z(2S_z+L_z)\right) \\
&\qquad + 2JS_x\langle\psi_1|\,S_x\,|\psi_1\rangle + 2JS_y\langle\psi_1|\,S_y\,|\psi_1\rangle + 2JS_z\langle\psi_1|\,S_z\,|\psi_1\rangle
\end{aligned}
$$

Now start a strong magnetic field and calculate the magnetic dipole as a function of field. Notice that the algotighm 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.

(1). In this part we will derive for an arbitrary system. We assume the system has some unit cells which can be labeled as the position of each cell $\{\boldsymbol{r}\}$, each unit cell has n same atoms, which all have D dimensions. The total hamiltonian should be written as

$$
H = \sum_{\boldsymbol{r},i} H_{\boldsymbol{r},i} + H_{\mathrm{interaction}}
$$

and constained by symmetry, all the $H_{\boldsymbol{r},i}$ ahouls be same for all $\boldsymbol{r}$. The interaction part will be a sum of a list, each list of the term will have this form: $J_{(\boldsymbol{r}_1,i_1),(\boldsymbol{r}_2,i_2)\cdots(\boldsymbol{r}_s,i_s)}\boldsymbol{X}^1_{\boldsymbol{r}_1,i_1}\boldsymbol{X}^2_{\boldsymbol{r}_2,i_2}\cdots\boldsymbol{X}^s_{\boldsymbol{r}_s,i_s}$. To illatrate this, lets look at some examples:

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

$$
H = \sum_i g\mu_{\mathrm{B}}\boldsymbol{B}\cdot\boldsymbol{S_i} - J\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}
$$

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

$$
H = \sum_i g\mu_{\mathrm{B}}(B^xS^x + B^yS^y + B^zS^z) - J(S_i^xS_{i+1}^x + S_i^yS_{i+1}^y + S_i^zS_{i+1}^z)
$$

Now there are three terms in the interaction.

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

$$
H = \sum_i g\mu_{\mathrm{B}}\boldsymbol{B}\cdot(\boldsymbol{S}_{i,1} + \boldsymbol{S}_{i,2})
$$

We will assume the ground state is already solved and the i-th atom in all unit cells have the same wave function:

$$
|\psi_{\boldsymbol{r},i}\rangle = |\psi_i\rangle
$$

and