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 $|a_0\rangle$

(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) 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 $\langle a_0|\psi_0\rangle$.

(6) 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

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

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 $\boldsymbol{B}$.

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

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 $\boldsymbol{B}$.

(3) Now let apply this aprroximation to a magnetic system. Consider a 2D square lattice.