

Homework Of Superconductivity and Magnetism

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1 Superconductivity

- Considering the 2-D potential have the form:

$$U(r) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases} \quad (1)$$

Find the shallow energy level when $U_0 \ll \hbar^2/ma^2$ for the case $M_z = 0$, where M_z is the projection of the orbital moment on the z-axis.

In the polar coordinate, the kinetic have the form:

$$K(r, \theta)\psi(r, \theta) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \psi(r, \theta)}{\partial r} \right) + \frac{1}{r} \frac{\partial^2 \psi(r, \theta)}{\partial \theta^2} \quad (2)$$

Since $M_z = 0$, we have the ansatz:

$$\psi(r, \theta) = \frac{1}{\sqrt{4\pi}} R(r) \quad (3)$$

Therefore, the second term of (2) vanished. The stationary Schrödinger equation have the form:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{\partial R}{\partial r} + \frac{\partial^2 R}{\partial r^2} \right) + V(r)R = ER$$

Or in the form of Bessel equation:

$$r^2 \frac{\partial^2 R}{\partial r^2} + r \frac{\partial R}{\partial r} + \frac{2m(E - V)}{\hbar^2} R = 0 \quad (4)$$

Inside the circle, we have the equation:

$$r^2 \frac{\partial^2 R}{\partial r^2} + r \frac{\partial R}{\partial r} + \frac{2m(E + U_0)}{\hbar^2} R = 0 \quad (5)$$

Which have the general solution:

$$R(r) = C_1 J_0 \left(\sqrt{\frac{2m(E + U_0)}{\hbar^2}} r \right) + C_2 Y_0 \left(\sqrt{\frac{2m(E + U_0)}{\hbar^2}} r \right) \quad (6)$$

But since the radius have to be continuous at $r = 0$, where $Y_0(r)$ is not, therefore: $C_2 = 0$. Hence

$$R(r) = C_1 J_0 \left(\sqrt{\frac{2m(E + U_0)}{\hbar^2}} r \right) \quad (7)$$

Outside the circle, we have:

$$r^2 \frac{\partial^2 R}{\partial r^2} + r \frac{\partial R}{\partial r} - \frac{2m|E|}{\hbar^2} R = 0 \quad (8)$$

Which yields the modified Bessel functions as the solution:

$$R(r) = C_3 I_0 \left(\sqrt{\frac{2m|E|}{\hbar^2}} r \right) + C_4 K_0 \left(\sqrt{\frac{2m|E|}{\hbar^2}} r \right) \quad (9)$$

The constrain condition now is $R(r)$ have to vanished at $r \rightarrow \infty$, which $I_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}r\right)$ is not, therefore:

$$R(r) = C_2 K_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}r\right) \quad (10)$$

At $r = a$, the function have to be continuous:

$$C_2 = C_1 \frac{J_0\left(\sqrt{\frac{2m(E+U_0)}{\hbar^2}}a\right)}{K_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}a\right)} \quad (11)$$

And also their derivative, we using the properties of Bessel function:

$$\frac{d}{dx} J_0(x) = -J_1(x); \quad \frac{d}{dx} K_0(x) = -K_1(x) \quad (12)$$

to get:

$$\sqrt{\frac{E+U_0}{|E|}} C_1 J_1\left(\sqrt{\frac{2m(E+U_0)}{\hbar^2}}a\right) = C_2 K_1\left(\sqrt{\frac{2m|E|}{\hbar^2}}r\right) \quad (13)$$

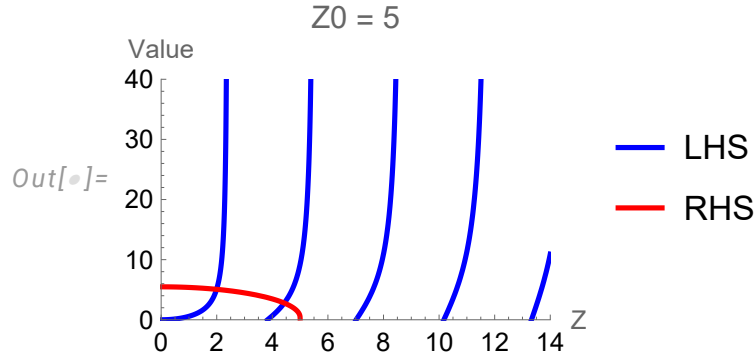
Or:

$$\sqrt{\frac{E+U_0}{|E|}} = \frac{K_1\left(\sqrt{\frac{2m|E|}{\hbar^2}}a\right)}{J_1\left(\sqrt{\frac{2m(E+U_0)}{\hbar^2}}a\right)} \frac{J_0\left(\sqrt{\frac{2m(E+U_0)}{\hbar^2}}a\right)}{K_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}a\right)} \quad (14)$$

set $Z = \sqrt{2m(E+U_0)}a/\hbar$, $Z_0 = \sqrt{2mU_0}a/\hbar$, equation become:

$$\begin{aligned} \frac{Z}{\sqrt{Z^2 - Z_0^2}} &= \frac{K_1(\sqrt{Z_0^2 - Z^2})}{J_1(Z)} \frac{J_0(Z)}{K_0(\sqrt{Z_0^2 - Z^2})} \\ Z \frac{J_1(Z)}{J_0(Z)} &= \sqrt{Z^2 - Z_0^2} \frac{K_1(\sqrt{Z_0^2 - Z^2})}{K_0(\sqrt{Z_0^2 - Z^2})} \end{aligned} \quad (15)$$

Plot these two, we have: According to the LHS, we seeing that however the U_0 small, always exist a solution Z for



both side to match. At very shallow case: $U_0 \ll \frac{\hbar^2}{2ma^2}$ or $Z \ll 1$, we need to approximate the

2 Magnetism

Consider Hamiltonian:

$$\mathcal{H}_{int.} = -\vec{M} \cdot \vec{H} \quad (16)$$

Choosing the axis to be along the magnetic field \vec{H} .

- Using semi-classical:

$$Z = 2\pi \int_0^\pi e^{\beta m H \cos(\theta)} \sin \theta d\theta = \frac{2\pi}{\beta m H} 2 \sinh(\beta m H) \quad (17)$$

Calculate: $\langle \vec{M} \cdot \vec{a} \rangle$, $\vec{a} = (a_x, a_y, a_z)$. We have:

$$\langle \vec{M} \cdot \vec{a} \rangle = \langle a_x M_x + a_y M_y + a_z M_z \rangle = a_x \langle M_x \rangle + a_y \langle M_y \rangle + a_z \langle M_z \rangle \quad (18)$$

$$\langle M_x \rangle \propto m \int \cos(\phi) \sin(\theta) e^{\beta m H \cos \theta} \sin(\theta) d\phi d\theta = 0 \quad (19)$$

$$\langle M_y \rangle \propto m \int \sin(\phi) \sin(\theta) e^{\beta m H \cos \theta} \sin(\theta) d\phi d\theta = 0 \quad (20)$$

$$\begin{aligned} \langle M_z \rangle &= \frac{m}{Z} \int_0^{2\pi} \int_0^\pi \cos \theta e^{\beta m H \cos(\theta)} \sin \theta d\theta d\phi = \frac{2\pi m}{Z} \partial_{\beta m H} \int_0^\pi e^{\beta m H \cos \theta} \sin \theta d\theta \\ &= m \left(\coth \beta m H - \frac{1}{\beta m H} \right) = mL(\beta m H), \end{aligned} \quad (21)$$

in which $L(x)$ is Langevin function. Therefore:

$$\langle \vec{M} \cdot \vec{a} \rangle = a_z mL(\beta m H) \quad (22)$$

Consider: $\langle M_z^2 \rangle - (\langle M_z \rangle)^2$.

$$\begin{aligned} \langle M_z^2 \rangle &= \frac{m^2}{Z} \frac{\partial^2 Z}{\partial (\beta m H)^2} = m^2 \frac{\beta m H}{\sinh \beta m H} \left(\frac{\sinh(\beta m H)}{\beta m H} - 2 \cosh(\beta m H) \frac{1}{(\beta m H)^2} + \frac{2 \sinh(\beta m H)}{(\beta m H)^3} \right) \\ &= m^2 \left(1 - 2 \coth(\beta m H) \frac{1}{\beta m H} + \frac{2}{(\beta m H)^2} \right) \\ (\langle M_z \rangle)^2 &= m^2 \left(1 + \frac{1}{\sinh(\beta m H)^2} - \frac{2 \coth \beta m H}{\beta m H} + \frac{1}{(\beta m H)^2} \right) \end{aligned} \quad (23)$$

$$\langle M_z^2 \rangle - (\langle M_z \rangle)^2 = m^2 \left(\frac{1}{(\beta m H)^2} - \frac{1}{\sinh(\beta m H)^2} \right) \quad (24)$$

At $T \rightarrow 0, \beta \rightarrow \infty$:

$$\langle M_z^2 \rangle - (\langle M_z \rangle)^2 \rightarrow 0; \langle M_z \rangle = m \left(\coth(\beta m H) - \frac{1}{\beta m H} \right) \rightarrow m \quad (25)$$

In this case, all spin aligned with the external field, give no fluctuation in the distribution of the $\langle M_z \rangle$. At $T \rightarrow \infty, \beta \rightarrow 0$:

$$\langle M_z^2 \rangle - (\langle M_z \rangle)^2 \rightarrow \frac{m^2}{3}; \langle M_z \rangle = m \left(\coth(\beta m H) - \frac{1}{\beta m H} \right) \rightarrow 0 \quad (26)$$

In this case, the spin align in both side with the same number. And the fluctuation difference than 0, proportional to m^2 .

• Using quantum theory, know that $\vec{L} = 0, S = 1/2, \vec{M} = 2\mu_B \vec{S}$:

$$Z = \sum_{m_z=-1/2}^{1/2} e^{\beta 2\mu_B H m_z} = 2 \cosh(\beta \mu_B H) \quad (27)$$

Which in turn give:

$$\langle S_z \rangle = \frac{1}{Z} \sum_{m_z=-1/2}^{1/2} m_z e^{\beta 2\mu_B H m_z} = \frac{1}{2} \tanh(\beta \mu_B H) \quad (28)$$

$$\langle S_z^2 \rangle = \frac{1}{Z} \sum_{m_z=-1/2}^{1/2} m_z^2 e^{\beta 2\mu_B H m_z} = \frac{1}{4} \quad (29)$$

$$\langle S_z^2 \rangle - \langle S_z \rangle^2 = \frac{1}{4} (1 - \tanh^2(\beta \mu_B H)) = \frac{1}{4 \cosh(\beta \mu_B H)} \quad (30)$$

At $T \rightarrow 0, \beta \rightarrow \infty$:

$$\langle S_z^2 \rangle - \langle S_z \rangle^2 \rightarrow 0, \langle S_z \rangle \rightarrow \frac{1}{2} \quad (31)$$

Like the classical results, all the spin align with the external field and no fluctuation with the distribution of S_z , all aligned.

At $T \rightarrow \infty, \beta \rightarrow 0$:

$$\langle S_z^2 \rangle - \langle S_z \rangle^2 \rightarrow \frac{1}{4}, \langle S_z \rangle \rightarrow 0 \quad (32)$$

All the spin equally divided into up and down, make the mean S_z to 0, their distribution make the variation of the spin to be half of the magnitude 1/2, indicate the distribution.

• Considering the dynamic of magnetization:

$$\frac{d\vec{M}}{dt} = -\gamma[\vec{M} \times \vec{H}] \quad (33)$$

With $\vec{H} = H_0\hat{z} + H_1e^{-\kappa t}\hat{x}$, we have the set of equation:

$$d_t M_x = -\gamma M_y H_0 \quad (34)$$

$$d_t M_y = \gamma M_x H_0 - \gamma M_z H_1 e^{-\kappa t} \quad (35)$$

$$d_t M_z = \gamma M_y H_1 e^{-\kappa t} \quad (36)$$

Since we have the condition $H_1 \ll H_0$, we can approximate the final equation to $d_t M_z = 0 \rightarrow M_z = m_0$, the m_0 also be the total magnitude of the system due to the initial condition $M_x(0) = M_y(0) = 0$. The set of equations become:

$$d_t M_x = -\gamma H_0 M_y \quad (37)$$

$$d_t M_y = \gamma M_x H_0 - \gamma m_0 H_1 e^{-\kappa t} \quad (38)$$

Take derivative the first equation and substituting the second one into it to find:

$$d_t^2 M_x + (\gamma H_0)^2 M_x = \gamma m_0 H_1 e^{-\kappa t} \quad (39)$$

Homogeneous solution yields:

$$M_{xh} = C_1 \cos(\gamma H_0 t) + C_2 \sin(\gamma H_0 t) \quad (40)$$

Particular solution can be achieved using the ansatz:

$$M_{xp} = A e^{-\kappa t} \quad (41)$$

Substituting it to get the constant A :

$$M_{xp}(t) = \frac{m_0 \gamma H_1 e^{-\kappa t}}{(\gamma H_0)^2 + \kappa^2} \quad (42)$$

The general solution is:

$$M_x(t) = C_2 \sin(\gamma H_0 t) + \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} e^{-\kappa t} + C_1 \cos(\gamma H_0 t) \quad (43)$$

At $t = 0$:

$$M_x(0) = 0 \rightarrow C_1 = -\frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} \quad (44)$$

Also at $t = 0$:

$$M_y(t) = d_t M_x(t) = C_2 \gamma H_0 \cos(\gamma H_0 t) - \kappa \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} e^{-\kappa t} - C_1 \gamma H_0 \sin(\gamma H_0 t) \quad (45)$$

$$M_y(0) = 0 \rightarrow C_2 = \kappa m_0 \frac{H_1}{H_0} \frac{1}{(\gamma H_0)^2 + \kappa^2} \quad (46)$$

So, the solution is:

$$M_x(t) = \kappa m_0 \frac{H_1}{H_0} \frac{\sin(\gamma H_0 t)}{(\gamma H_0)^2 + \kappa^2} + \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} \left(e^{-\kappa t} + \cos(\gamma H_0 t) \right) \quad (47)$$

• Adding the hopping interaction with the form¹:

$$-J_{mn} = \begin{cases} J_1, & \text{for the nearest neighbors,} \\ J_2, & \text{for the next nearest neighbors,} \\ 0, & \text{otherwise,} \end{cases} \quad (48)$$

¹I put the minus sign, indicate this calculation is for the ferromagnet

Full Hamiltonian have the form:

$$\mathcal{H} = -2\mu_B \sum_i \vec{S}_i \vec{H} - \frac{1}{2} \sum_{i,j} J_{i,j} \vec{S}_i \vec{S}_j \quad (49)$$

Since the $\vec{H} = H e_z$, the effective field have to be aligned with the external field instead of any other direction.

$$\langle \vec{S}_i \vec{S}_j \rangle \rightarrow 2\vec{S}_i \langle \vec{S}_j \rangle - \langle \vec{S}_i \rangle^2 \quad (50)$$

with: $\langle \vec{S}_j \rangle = \vec{m} \parallel \vec{H}$ as our discuss, we have the mean-field Hamiltonian:

$$\mathcal{H}_{MF} = \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - (H 2\mu_B + m J_1 Z_1 + m J_2 Z_2) \sum_i S_i^z \quad (51)$$

$$= \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - h_{eff} \sum_i S_i^z \quad (52)$$

Using this Hamiltonian, we can shift it to neglect the constant term and find the expected value of $\vec{m} = \langle S_z \rangle$, which is nothing more than the Brillouin function for the case $J = 1/2$:

$$m = \frac{1}{2} \tanh(\beta \mu_B h_{eff.})$$

Approximate up to the first order $\tanh(x) \approx x$:

$$m = \frac{1}{2} \beta \mu_B h_{eff} \xrightarrow{H \rightarrow 0} \frac{1}{2} \beta \mu_B m (J_1 Z_1 + J_2 Z_2) \quad (53)$$

To get:

$$k_B T_C = \frac{\mu_B m}{2} (J_1 Z_1 + J_2 Z_2) \quad (54)$$

For simple cubic lattice: $Z_1 = 6, Z_2 = 12$, we have:

$$k_B T_C = \mu_B m (3J_1 + 6J_2) \quad (55)$$

In both extreme case $J_i \ll J_j$, we easily obtain:

$$k_B T_C = \begin{cases} 3J_1 \mu_B m, & (J_1 \ll J_2) \\ 6J_2 \mu_B m, & (J_2 \ll J_1) \end{cases} \quad (56)$$