Homework Of Superconductivity and Magnetism

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1 Superconductivity

- Considering the 2-D potential have the form:

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

Find the shallow energy level when $U_0 \ll h^2/ma^2$ 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:

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

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

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

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:

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

Inside the circle, we have the equation:

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

Which have the general solution:

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

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

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

Outside the circle, we have:

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

Which yields the modified Bessel functions as the solution:

$$R(r) = C_3 I_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}r\right) + C_2 K_0\left(\sqrt{\frac{2m|E|}{\hbar^2}}r\right) \tag{9}$$

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

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

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

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

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

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

to get:

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

Or:

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

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

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

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

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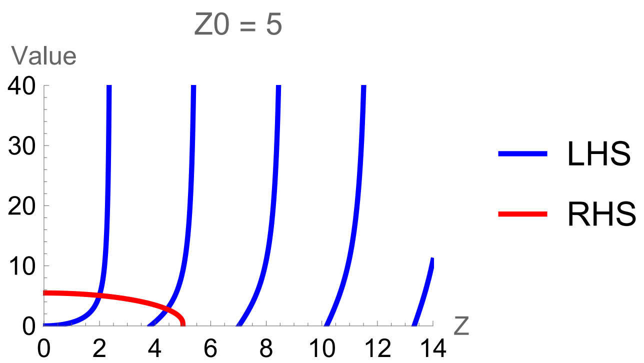

both side to match. At very shallow case: $U_0 \ll \frac{\hbar^2}{2ma^2}$ or $Z \ll 1$, we need to approximate the

2 Magnetism

Consider Hamiltonian:

$$\mathcal{H}_{int.} = -\vec{M} \cdot \vec{H} \tag{16}$$

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

- Using semi-classical:

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

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

$$\left\langle \vec{M}\cdot\vec{a}\right\rangle = \langle a_xM_x + a_yM_y + a_zM_z\rangle = a_x\langle M_x\rangle + a_y\langle M_y\rangle + a_z\langle M_z\rangle \tag{18}$$

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

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

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

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

$$\left\langle \vec{M}\cdot\vec{a}\right\rangle = a_z mL(\beta mH) \tag{22}$$

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

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

$$(\langle M_z\rangle)^2 = m^2\left(1 + \frac{1}{\sinh(\beta mH)^2} - \frac{2\coth\beta mH}{\beta mH} + \frac{1}{(\beta mH)^2}\right) \tag{23}$$

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

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

$$\left\langle M_z^2\right\rangle - (\langle M_z\rangle)^2 \to 0; \langle M_z\rangle = m\left(\coth(\beta mH) - \frac{1}{\beta mH}\right) \to m \tag{25}$$

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

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

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 $\vec{L}=0, S=1/2, \vec{M}=2\mu_B\vec{S}$:

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

Which in turn give:

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

$$\left\langle S_z^2\right\rangle =\frac{1}{Z}\sum_{m_z=-1/2}^{1/2} m_z^2 e^{\beta 2\mu_B H m_z} = \frac{1}{4} \tag{29}$$

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

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

$$\left\langle S_z^2\right\rangle - \langle S_z\rangle^2 \to 0, \langle S_z\rangle \to \frac{1}{2} \tag{31}$$

Like the classical results, all the spin align with the external field and no fluctuation with the distribution of S_z, all aligned.
At $T \to \infty, \beta \to 0$:

$$\langle S_z^2 \rangle - \langle S_z \rangle^2 \to \frac{1}{4}, \langle S_z \rangle \to 0 \tag{32}$$

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:

$$\frac{\mathrm{d}\vec{M}}{\mathrm{d}t} = -\gamma[\vec{M} \times \vec{H}] \tag{33}$$

With $\vec{H} = H_0\hat{z} + H_1 e^{-\kappa t}\hat{x}$, we have the set of equation:

$$d_t M_x = - \gamma M_y H_0 \tag{34}$$
$$d_t M_y = \gamma M_x H_0 - \gamma M_z H_1 e^{-\kappa t} \tag{35}$$
$$d_t M_z = \gamma M_y H_1 e^{-\kappa t} \tag{36}$$

Since we have the condition $H_1 \ll H_0$, we can approximate the final equation to $d_t M_z = 0 \to M_z = m_0$, 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:

$$d_t M_x = -\gamma H_0 M_y \tag{37}$$
$$d_t M_y = \gamma M_x H_0 - \gamma m_0 H_1 e^{-\kappa t} \tag{38}$$

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

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

Homogeneous solution yields:

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

Particular solution can be achieved using the ansatz:

$$M_{xp} = A e^{-\kappa t} \tag{41}$$

Substituting it to get the constant A:

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

The general solution is:

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

At $t = 0$:

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

Also at $t = 0$:

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

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

So, the solution is:

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

• Adding the hopping interaction with the form[1]:

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

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

Full Hamiltonian have the form:

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

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

$$\left\langle \vec{S}_i \vec{S}_j \right\rangle \rightarrow 2\vec{S}_i \left\langle \vec{S}_j \right\rangle - \left\langle \vec{S}_i \right\rangle^2 \tag{50}$$

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

$$\begin{aligned}\mathcal{H}_{MF} =& \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - (H 2\mu_B + m J_1 Z_1 + m J_2 Z_2) \sum_i S_i^z & (51)\\ =& \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - h_{eff} \sum_i S_i^z & (52)\end{aligned}$$

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 $tanh(x) \approx x$:

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

To get:

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

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

$$k_B T_C = \mu_B m (3J_1 + 6J_2) \tag{55}$$

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

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