Homework Of Superconductivity and Magnetism

Vo Chau Duc Phuong [1]

[1]The Abdus Salam International Center for Theoretical Physics
April 2025

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:

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

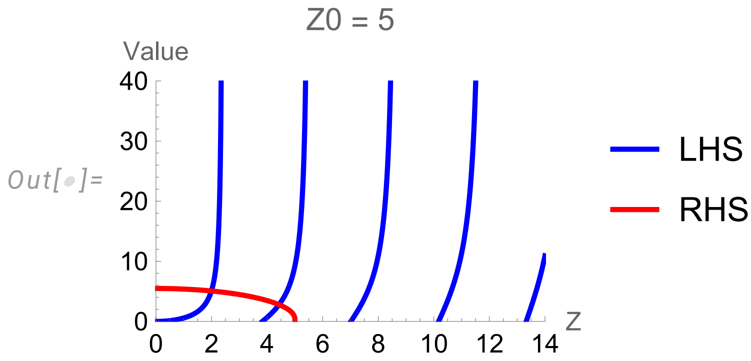
Or:

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

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

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

Plot these two, we have: According to the LHS, we seeing that however the Z_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 $Z \ll 1$ (maximum of RHS is Z_0), we need to approximate the Bessel function $J_\nu(z), K_\nu(z)$ for $z \to 0$:

$$J_\nu(z) \to \frac{(1/2z)^\nu}{\Gamma(\nu+1)}, K_0(z) \to -\ln(z), \quad K_\nu(z) \to \frac{1}{2}\Gamma(\nu)\left(\frac{1}{2}z\right)^{-\nu} \tag{16}$$

$$\frac{Z}{2}\frac{\Gamma(1)}{\Gamma(2)}Z = \sqrt{Z_0^2 - Z^2}\frac{1}{2}\Gamma(1)\left(\frac{2}{\sqrt{Z_0^2 - Z^2}}\right)\frac{1}{-\ln\left(\sqrt{Z_0^2 - Z^2}\right)}$$

$$\frac{Z^2}{2} = \frac{1}{-\ln\left(\sqrt{Z_0^2 - Z^2}\right)}$$

$$\frac{2m(E+U_0)a^2}{\hbar^2} = -\frac{1}{\ln(2mEa^2/\hbar^2)} \to E \approx \frac{\hbar^2}{2ma^2} e^{-\frac{\hbar^2}{2mU_0a^2}} = \Delta_0 e^{-\frac{\Delta_0}{U_0}}, \quad \Delta_0 = \frac{\hbar^2}{2ma^2} \tag{17}$$

• Grain Superconducting
Considering a superconducting grain with a size $d \ll \xi(T)$, using the Lanndau-Grinzburg theory of phase transition, we have the free energy as the functional of the macroscopic wave-function:

$$\Phi[\Psi] = \Phi_0 + \Phi_{Fl}[\Phi] = \Phi_0 + \int d\vec{r}\left[a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{2m}\left|\left(\frac{\hbar}{i}\nabla - 2e/c\vec{A}\right)\Psi\right|^2 + \frac{\vec{B}^2}{8\pi}\right] \tag{18}$$

The size of the grain is very small in compare with the coherence length $\xi = \frac{\hbar^2}{4m|a|}$, therefore it is reasonable to neglect the third term (also canceling the last term since we are working in the absence of the magnetic field $(B = \vec{0})$). The Ginzburg–Landau equations reduced into:

$$a\psi + \frac{b}{2}\psi|\psi|^2 = 0 \tag{19}$$

give the solution:

$$|\Psi|^2 = -\frac{a}{b} \tag{20}$$

Therefore, the contribution of the coordination-independence part is:

$$Z_{Fl} = \int d^2\Psi e^{-\frac{a|\Psi|^2 + \frac{b}{2}|\Psi|^4}{T}} = \pi e^{\frac{a^2}{2bT}} \int_0^{-a/b} d|\Psi|^2 e^{-\frac{b}{2T}(|\Psi|^2+\frac{a}{b})^2} = \pi e^{\frac{a^2}{2bT}} \sqrt{\frac{\pi T}{2b}}\left(1 - \mathrm{erf}\left(\frac{a}{\sqrt{2bT}}\right)\right) \tag{21}$$

Rewrite in term of $x = \frac{a}{\sqrt{2bT}} = \frac{\alpha}{\sqrt{2b}}\frac{(T-T_C)}{\sqrt{T}}$:

$$Z = \sqrt{\frac{\pi^3}{2b}}\sqrt{T}e^{x^2}(1 - \mathrm{erf}(x)) \tag{22}$$

Free energy will be:

$$F = -T\ln Z = -T\ln\left(\sqrt{\frac{\pi^3}{2b}}\sqrt{T}e^{x^2}(1 - \mathrm{erf}(x))\right) \tag{23}$$

From the Maxwell relation, we have the entropy:

$$S = -\frac{\mathrm{d}F}{\mathrm{d}T} = \ln(Z) + T\frac{\partial Z}{\partial T}\frac{1}{Z} = \frac{1}{2} - \frac{2\alpha\sqrt{T_c}}{\sqrt{2b}\sqrt{\pi}} + \ln\left(\sqrt{\frac{\pi^3}{2b}}\sqrt{T_C}\right) \tag{24}$$

And the specific heat:

$$C_V = -T\frac{\mathrm{d}^2F}{\mathrm{d}T^2} = \frac{1}{2} + \frac{1}{b\pi}\left(a^2(\pi-2)T_C - a\sqrt{2\pi b T_c}\right) \tag{25}$$

2 Magnetism

Consider Hamiltonian:

$$\mathcal{H}_{int.} = -\vec{M}\cdot\vec{H} \tag{26}$$

Choosing the axis to be along the magnetic field $\vec{H}$.
• Using semi-classical:

$$Z = 2\pi\int_0^\pi e^{\beta mH\cos(\theta)}\sin\theta d\theta = \frac{2\pi}{\beta mH}2\sinh(\beta mH) \tag{27}$$

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

$$\left\langle\vec{M}\cdot\vec{a}\right\rangle = \langle a_xM_x + a_yM_y + a_zM_z\rangle = a_x\langle M_x\rangle + a_y\langle M_y\rangle + a_z\langle M_z\rangle \tag{28}$$

$$\langle M_x\rangle \propto m\int\cos(\phi)\sin(\theta)e^{\beta mH\cos\theta}\sin(\theta)d\phi d\theta = 0 \tag{29}$$

$$\langle M_y\rangle \propto m\int\sin(\phi)\sin(\theta)e^{\beta mH\cos\theta}\sin(\theta)d\phi d\theta = 0 \tag{30}$$

$$\begin{aligned}\langle M_z\rangle =& \frac{m}{Z}\int_0^{2\pi}\int_0^\pi cos\theta e^{\beta mH\cos(\theta)}\sin\theta d\theta d\phi = \frac{2\pi m}{Z}\partial_{\beta mH}\int_0^\pi e^{\beta mH\cos\theta}\sin\theta d\theta \\ =& m\left(\coth\beta mH - \frac{1}{\beta mH}\right) = mL(\beta mH),\end{aligned} \tag{31}$$

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

$$\left\langle \vec{M} \cdot \vec{a} \right\rangle = a_z m L(\beta m H) \tag{32}$$

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

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

$$(\langle M_z \rangle)^2 = m^2\left(1 + \frac{1}{\sinh(\beta m H)^2} - \frac{2\coth \beta m H}{\beta m H} + \frac{1}{(\beta m H)^2}\right) \tag{33}$$

$$\left\langle M_z^2 \right\rangle - (\langle M_z \rangle)^2 = m^2\left(\frac{1}{(\beta m H)^2} - \frac{1}{\sinh(\beta m H)^2}\right) \tag{34}$$

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

$$\left\langle M_z^2 \right\rangle - (\langle M_z \rangle)^2 \to 0; \langle M_z \rangle = m\left(\coth(\beta m H) - \frac{1}{\beta m H}\right) \to m \tag{35}$$

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

$$\left\langle M_z^2 \right\rangle - (\langle M_z \rangle)^2 \to \frac{m^2}{3}; \langle M_z \rangle = m\left(\coth(\beta m H) - \frac{1}{\beta m H}\right) \to 0 \tag{36}$$

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

$$Z = \sum_{m_z=-1/2}^{1/2} e^{\beta 2\mu_B H m_z} = 2\cosh(\beta \mu_B H) \tag{37}$$

Which in turn give:

$$\langle S_z \rangle = \frac{1}{Z}\sum_{m_z=-1/2}^{1/2} m_z e^{\beta 2\mu_B H m_z} = \frac{1}{2}\tanh(\beta \mu_B H) \tag{38}$$

$$\left\langle S_z^2 \right\rangle = \frac{1}{Z}\sum_{m_z=-1/2}^{1/2} m_z^2 e^{\beta 2\mu_B H m_z} = \frac{1}{4} \tag{39}$$

$$\left\langle S_z^2 \right\rangle - \langle S_z \rangle^2 = \frac{1}{4}(1 - \tanh^2(\beta \mu_B H)) = \frac{1}{4\cosh(\beta \mu_B H)} \tag{40}$$

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

$$\left\langle S_z^2 \right\rangle - \langle S_z \rangle^2 \to 0, \langle S_z \rangle \to \frac{1}{2} \tag{41}$$

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

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

$$\left\langle S_z^2 \right\rangle - \langle S_z \rangle^2 \to \frac{1}{4}, \langle S_z \rangle \to 0 \tag{42}$$

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:

$$\frac{\mathrm{d}\vec{M}}{\mathrm{d}t} = -\gamma[\vec{M} \times \vec{H}] \tag{43}$$

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

$$d_t M_x = -\gamma M_y H_0 \tag{44}$$

$$d_t M_y = \gamma M_x H_0 - \gamma M_z H_1 e^{-\kappa t} \tag{45}$$

$$d_t M_z = \gamma M_y H_1 e^{-\kappa t} \tag{46}$$

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:

$$d_t M_x = -\gamma H_0 M_y \tag{47}$$
$$d_t M_y = \gamma M_x H_0 - \gamma m_0 H_1 e^{-\kappa t} \tag{48}$$

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

$$d_t^2 M_x + (\gamma H_0)^2 M_x = \gamma m_0 H_1 e^{-\kappa t} \tag{49}$$

Homogeneous solution yields:

$$M_{xh} = C_1 cos(\gamma H_0 t) + C_2 sin(\gamma H_0 t) \tag{50}$$

Particular solution can be achieved using the ansatz:

$$M_{xp} = A e^{-\kappa t} \tag{51}$$

Substituting it to get the constant A:

$$M_{xp}(t) = \frac{m_0 \gamma H_1 e^{-\kappa t}}{(\gamma H_0)^2 + \kappa^2} \tag{52}$$

The general solution is:

$$M_x(t) = C_2 \sin(\gamma H_0 t) + \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} e^{-\kappa t} + C_1 \cos(\gamma H_0 t) \tag{53}$$

At $t = 0$:

$$M_x(0) = 0 \rightarrow C_1 = -\frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} \tag{54}$$

Also at $t = 0$:

$$M_y(t) = d_t M_x(t) = C_2 \gamma H_0 cos(\gamma H_0 t) - \kappa \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} e^{-\kappa t} - C_1 \gamma H_0 sin(\gamma H_0 t) \tag{55}$$
$$M_y(0) = 0 \rightarrow C_2 = \kappa m_0 \frac{H_1}{H_0} \frac{1}{(\gamma H_0)^2 + \kappa^2} \tag{56}$$

So, the solution is:

$$M_x(t) = \kappa m_0 \frac{H_1}{H_0} \frac{sin(\gamma H_0 t)}{(\gamma H_0)^2 + \kappa^2} + \frac{m_0 \gamma H_1}{(\gamma H_0)^2 + \kappa^2} \left(e^{-\kappa t} + cos(\gamma H_0 t) \right) \tag{57}$$

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

$$-J_{mn} = \begin{cases} J_1, & \text{for the nearest neighbors,} \\ J_2, & \text{for the next nearest neighbors,} \\ 0, & \text{otherwise,} \end{cases} \tag{58}$$

Full Hamiltonian have the form:

$$\mathcal{H} = -2\mu_B \sum_i \vec{S}_i \vec{H} - \frac{1}{2} \sum_{i,j} J_{i,j} \vec{S}_i \vec{S}_j \tag{59}$$

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

$$\left\langle \vec{S}_i \vec{S}_j \right\rangle \rightarrow 2\vec{S}_i \left\langle \vec{S}_j \right\rangle - \left\langle \vec{S}_i \right\rangle^2 \tag{60}$$

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

$$\mathcal{H}_{MF} = \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - (H 2\mu_B + m J_1 Z_1 + m J_2 Z_2) \sum_i S_i^z \tag{61}$$
$$= \frac{J_1 N Z_1 m^2}{2} + \frac{J_2 N m^2 Z_2}{2} - h_{eff} \sum_i S_i^z \tag{62}$$

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

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 $tanh(x) \approx x$:

$$m = \frac{1}{2}\beta\mu_B h_{eff} \xrightarrow[H\to 0]{} \frac{1}{2}\beta\mu_B m(J_1 Z_1 + J_2 Z_2) \tag{63}$$

To get:

$$k_B T_C = \frac{\mu_B m}{2}(J_1 Z_1 + J_2 Z_2) \tag{64}$$

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

$$k_B T_C = \mu_B m(3J_1 + 6J_2) \tag{65}$$

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

$$k_B T_C = \begin{cases} 3J_1\mu_B m, & (J_1 \ll J_2) \\ 6J_2\mu_B m, & (J_2 \ll J_1) \end{cases} \tag{66}$$