University of Kentucky
Department of Physics and Astronomy

PHY 525. Introduction to Solid State Physics II

Final Examination.

Date: Dec 12, 2001
Time: 8:00-10:00
Answer all questions.

1. (25 points)
Consider a two dimensional square lattice of lattice parameter a. Each site provides two conducting electrons.
(a) Determine k_F in terms of a. Under free electron model, at what value of k_y will the Fermi sphere cross the boundary at $x=\pi/a$?
(b) The electrons are actually only nearly free and a gap of $2U=0.1E_F$ opens up at the Brillouin zone boundary. At what value of k_y will the Fermi surface in the first Brillouin zone cross the boundary at $x=\pi/a$? How about the second Brillouin zone?
You can express your answers in unit of π/a.

Solutions:

(a) $2\times\dfrac{\pi k_F^{\ 2}}{\left(\dfrac{2\pi}{L}\right)^2}=N \quad \Rightarrow \dfrac{k_F^{\ 2}}{2\pi}=\dfrac{N}{L^2}=\dfrac{2}{a^2}$

$$\Rightarrow k_F^{\ 2}=\frac{4\pi}{a^2}$$

$$\Rightarrow k_F=\frac{\sqrt{4\pi}}{a}=\underline{\underline{\frac{3.54}{a}=1.128\frac{\pi}{a}}}$$

The sphere will cross the zone boundary at a value of k_y so that $\left(\dfrac{\pi}{a}\right)^2+k_y^{\ 2}=k_F^{\ 2}=\left(1.128\dfrac{\pi}{a}\right)^2$

$$\Rightarrow k_y^{\ 2}=0.2732\left(\frac{\pi}{a}\right)^2$$

$$\Rightarrow k_y=\underline{\underline{0.523\frac{\pi}{a}}}$$

(b) The Fermi energy is $\dfrac{\hbar^2 k_F^{\ 2}}{2m}=\dfrac{\hbar^2}{2m}\left(1.128\dfrac{\pi}{a}\right)^2$

If the Fermi surface in the first Brillouin zone cross the zone boundary at k_y

$$\therefore \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2+k_y^{\ 2}\right]=\frac{\hbar^2 k_F^{\ 2}}{2m}+U=\left(1+\frac{0.1}{2}\right)\frac{\hbar^2 k_F^{\ 2}}{2m}=1.05\frac{\hbar^2 k_F^{\ 2}}{2m}=1.05\times\frac{\hbar^2}{2m}\left(1.128\frac{\pi}{a}\right)^2$$

$$\Rightarrow \left(\frac{\pi}{a}\right)^2+k_y^{\ 2}=1.05\times\left(1.128\frac{\pi}{a}\right)^2=1.336\left(\frac{\pi}{a}\right)^2$$

$$\Rightarrow k_y^{\ 2}=0.336\left(\frac{\pi}{a}\right)^2 \quad \Rightarrow k_y=\underline{\underline{0.580\frac{\pi}{a}}}$$

If the Fermi surface in the second Brillouin zone cross the zone boundary at k_y

$$\therefore \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2+k_y^{\ 2}\right]=\frac{\hbar^2 k_F^{\ 2}}{2m}-U=\left(1-\frac{0.1}{2}\right)\frac{\hbar^2 k_F^{\ 2}}{2m}=0.95\frac{\hbar^2 k_F^{\ 2}}{2m}=0.95\times\frac{\hbar^2}{2m}\left(1.128\frac{\pi}{a}\right)^2$$

$$\Rightarrow \left(\frac{\pi}{a}\right)^2+k_y^{\ 2}=0.95\times\left(1.128\frac{\pi}{a}\right)^2=1.2088\left(\frac{\pi}{a}\right)^2$$

$$\Rightarrow k_y^{\ 2}=0.2088\left(\frac{\pi}{a}\right)^2 \quad \Rightarrow k_y=\underline{\underline{0.457\frac{\pi}{a}}}$$

2. (25 points)

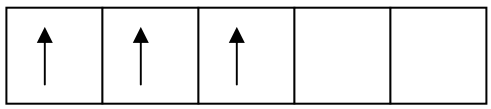
(a) Apply the Hund rules to find the ground state of an ion that has an outer shell of $3d^3$. Write your answer in atomic notation.

(b) Let the magnetic moment of the above ion be μ. Find the magnetization as a function of magnetic field and temperature for a system formed by these ions with a concentration of n.

(c) Find the magnetization in the limit of $\mu B \ll k_B T$.

Solutions:

(a)



L_z: 2 1 0 -1 -2

S = 3/2

L = 3

J=|L-S| =3/2

The ground state is $^4F_{3/2}$.

(b)

If $S = 1, S_z = -1, 0, \text{ or } +1$. In a magnetic field B, the energy level of these three states are :

$$U = -\vec{\mu} \cdot \vec{B} = S_z g \mu_B B = \begin{cases} U_{+3/2} = -\frac{3}{2}\mu B \\ U_{+1/2} = -\frac{1}{2}\mu B \\ U_{-1/2} = \frac{1}{2}\mu B \\ U_{-3/2} = \frac{3}{2}\mu B \end{cases}$$

The relative population will be :

$$\frac{N_{+1/2}}{N} = \frac{N_{+1/2}}{N_{+3/2} + N_{+1/2} + N_{-1/2} + N_{-3/2}} = \frac{\exp(-\mu B / 2k_B T)}{N}$$
$$= \frac{\exp(-\mu B / 2k_B T)}{N}$$

Similarly,

$$\frac{N_{+3/2}}{N} = \frac{\exp(-3\mu B / 2k_B T)}{N}$$
$$\frac{N_{-1/2}}{N} = \frac{\exp(\mu B / 2k_B T)}{N}$$
$$\frac{N_{-3/2}}{N} = \frac{\exp(3\mu B / 2k_B T)}{N}$$

$$\therefore M = \frac{(\frac{3}{2}N_{-3/2} + \frac{1}{2}N_{-1/2} - \frac{1}{2}N_{1/2} - \frac{3}{2}N_{-3/2})\mu}{V}$$
$$= \left[\frac{3}{2}\frac{\exp(3\mu B / 2k_B T)}{N} + \frac{1}{2}\frac{\exp(\mu B / 2k_B T)}{N} - \frac{1}{2}\frac{\exp(-\mu B / k_B T)}{N} - \frac{3}{2}\frac{\exp(-3\mu B / 2k_B T)}{N}\right]\frac{N\mu}{V}$$
$$= \left[\frac{\frac{3}{2}\left(\exp(3\mu B / 2k_B T) - \exp(-3\mu B / 2k_B T)\right) + \frac{1}{2}\left(\exp(\mu B / 2k_B T) - \exp(-\mu B / 2k_B T)\right)}{\exp(3\mu B / 2k_B T) + \exp(\mu B / 2k_B T) + \exp(-3\mu B / 2k_B T) + \exp(-\mu B / 2k_B T)}\right] n\mu$$
$$= \underline{\underline{\left[\frac{3\sinh(3\mu B / 2k_B T) + \sinh(\mu B / 2k_B T)}{2\cosh(3\mu B / 2k_B T) + 2\cosh(\mu B / 2k_B T)}\right] n\mu}}$$

(c)

In the limit $\mu B >> k_B T$, $\sinh(\mu B / k_B T) \to \frac{\mu B}{k_B T}$, and $\cosh(\mu B / k_B T) \to 1$

$$\therefore\ M \to \frac{3\frac{3\mu B}{2k_B T} + \frac{\mu B}{2k_B T}}{2+2} n\mu = \underline{\underline{\frac{5n\mu^2}{4k_B T}}} B$$

3. (25 points)

For an fcc lattice of magnetic spins it is impossible to find an antiferromagnetic arrangement in which all the nearest neighbors of any spin are antiparallel to it. The best that can be achieved, for example by having spins in alternate (2 0 0) planes ↑ and ↓, is eight antiparallel and four parallel neighbors. (Miller indices are referred to the conventional cubic unit cell).

(a) Develop a Néel theory appropriate to the case of two sublattices when only nearest neighbor exchange interactions are important; the effective field acting on an ion on the A sublattice would then be $B_A=B_a-\mu M_B-\varepsilon M_A$ with a similar expression for B_B. Show that the high temperature susceptibility is of the form $\chi=C/(T+\theta)$, where θ is related to the Néel temperature T_N by

$$\frac{\theta}{T_N}=\frac{\mu+\varepsilon}{\mu-\varepsilon} \quad .$$

(b) If the same type of stoms occupy the two sublattices. Assume a particular site in sublattice A has n_p parallel nearest neighbors in the same sublattice and n_a antiparallel nearest neighbors in sublattice B. How will ε and μ depends on n_a and n_p? Show that $\theta/ T_N=3$ for the fcc structure mentioned above.

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Solutions:

(a)

$$\begin{cases} B_A = B_a - \mu M_B - \varepsilon M_A \\ B_B = B_a - \mu M_A - \varepsilon M_B \end{cases}$$

$$\Rightarrow \begin{cases} \dfrac{M_A T}{C} = B_a - \mu M_B - \varepsilon M_A \\ \dfrac{M_B T}{C} = B_a - \mu M_A - \varepsilon M_B \end{cases} \qquad \left(\text{Curie law} \Rightarrow \chi = \frac{C}{T} \;\; ; B = \frac{M}{\chi}\right)$$

$$\Rightarrow \begin{cases} \left(\dfrac{T}{C} + \varepsilon\right) M_A + \mu M_B = B_a \\ \mu M_A + \left(\dfrac{T}{C} + \varepsilon\right) = B_a \end{cases} \qquad ---(1)$$

$$\Rightarrow \begin{cases} \left(\dfrac{T}{C} + \varepsilon\right) M_A + \mu M_B = B_a \\ \mu M_A + \left(\dfrac{T}{C} + \varepsilon\right) M_B = B_a \end{cases}$$

$$\Rightarrow \left(\frac{T}{C} + \varepsilon\right)^2 M_A - \mu^2 M_A = \left[\left(\frac{T}{C} + \varepsilon\right) - \mu\right] B_a$$

$$\Rightarrow \quad M_A = \frac{\left(\frac{T}{C} + \varepsilon\right) - \mu}{\left(\frac{T}{C} + \varepsilon\right)^2 - \mu^2} B_A = \frac{1}{\left(\frac{T}{C} + \varepsilon\right) + \mu} B_A$$

M_A and M_B can be exchanged in the original simultaneous equatios, $\therefore$ we expect the same solution for M_B:

$$M_B = \frac{1}{\left(\frac{T}{C} + \varepsilon\right) + \mu} B_A$$

$$\therefore \quad M_A + M_B = \frac{2}{\left(\frac{T}{C} + \varepsilon\right) + \mu} B_A$$

$$\chi = \frac{M_A + M_B}{B_a} \quad \Rightarrow \chi = \frac{2}{\left(\frac{T}{C} + \varepsilon\right) + \mu} = \frac{2C}{T + C(\varepsilon + \mu)}$$

χ diverges at $T = -\theta \quad \Rightarrow \quad (-\theta) + C(\varepsilon + \mu) = 0$

$$\Rightarrow \theta = C(\varepsilon + \mu) \qquad ---(2)$$

To evaluate C in terms of T_N, we note that at $T = T_N, B_a$ can be neglected.

$$\therefore \quad (1) \quad \Rightarrow \begin{cases} \left(\frac{T}{C} + \varepsilon\right) M_A + \mu M_B = 0 \\ \mu M_A + \left(\varepsilon + \frac{T}{C}\right) M_B = 0 \end{cases}$$

$$\text{Non-trivial solution at } T_N \Rightarrow \begin{vmatrix} \left(\frac{T_N}{C} + \varepsilon\right) & \mu \\ \mu & \left(\frac{T_N}{C} + \varepsilon\right) \end{vmatrix} = 0$$

$$\Rightarrow \left(\frac{T_N}{C} + \varepsilon\right) = \mu$$

$$\Rightarrow T_N = C(\mu - \varepsilon)$$

$$\Rightarrow C = \frac{T_N}{\mu - \varepsilon} \qquad ---(3)$$

Substitute (3) into (2):

$$\theta = \frac{T_N}{\mu - \varepsilon}(\mu + \varepsilon) \quad \Rightarrow \quad \underline{\underline{\frac{\theta}{T_N} = \frac{\mu + \varepsilon}{\mu - \varepsilon}}}$$

(b)

If the same type of atoms occupy both sublattice, than the coupling must be proportional to the number of nearest neighbors, i.e. $n_p / n_a = \varepsilon / \mu$

As described in the question, for fcc structure, $n_p / n_a = 4/8 = 1/2 = \varepsilon / \mu$

$$\therefore \quad \frac{\theta}{T_N} = \frac{\mu + \varepsilon}{\mu - \varepsilon} = \frac{1 + \varepsilon/\mu}{1 - \varepsilon/\mu} = \frac{1 + 1/2}{1 - 1/2} = \frac{3/2}{1/2} = 3 \Rightarrow \underline{\underline{\theta = 3T_N}}$$

4. (25 points)

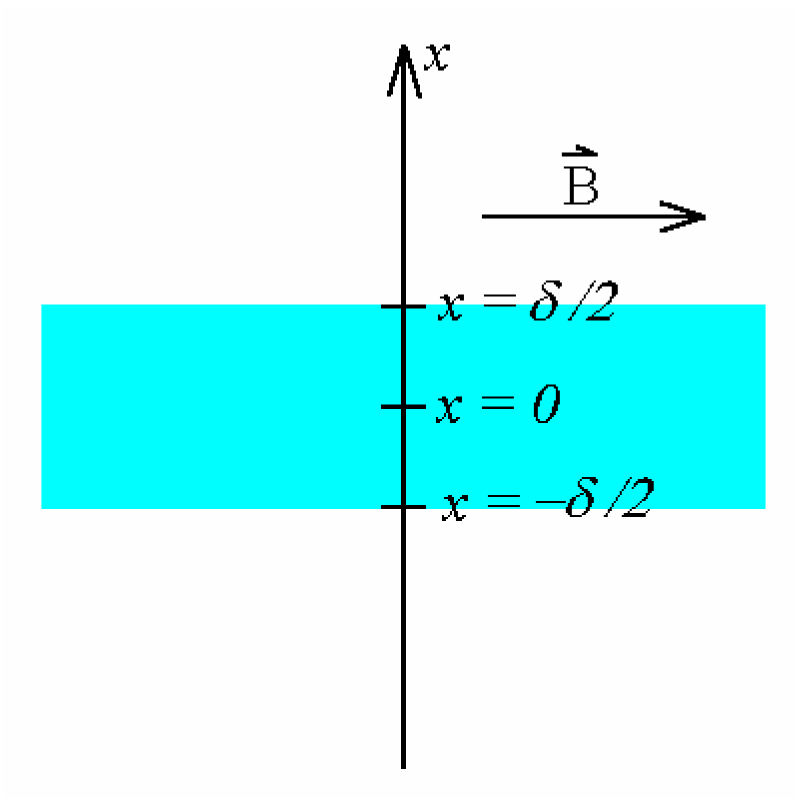
The penetration equation of a superconductivity may be written as $\lambda^2\nabla^2 B = B$, where λ is the penetration depth. (a) Show that B(x) inside a superconducting plate perpendicular to the x axis and of thickness δ is given by

$$B(x) = B_a \frac{\cosh(x/\lambda)}{\cosh(\delta/2\lambda)} \quad ,$$

Where B_a is the field outside the plate and parallel to it; here x=0 is at the center of the plate. (b) The effective magnetization M(x) in the plate is defined by $B(x) - B_a = 4\pi M(x)$. Show that, in CGS, $4\pi M(x) = -B_a(1/8\lambda^2)(\delta^2 - 4x^2)$, for $\delta \ll \lambda$. In SI we replace the 4π by μ_0.

Solutions

(a)



$$\lambda^2\nabla^2 B = B \Rightarrow \frac{\partial^2 B}{\partial x^2} - \frac{1}{\lambda^2}B = 0$$

$$\Rightarrow B = Ae^{x/\lambda} + Ce^{-x/\lambda}$$

At $x = \delta/2$ and $x = -\delta/2$, $B = B_a$

$$\therefore\ Ae^{\delta/2\lambda} + Ce^{-\delta/2\lambda} = B_a \qquad ---(1)$$
$$Ae^{-\delta/2\lambda} + Ce^{\delta/2\lambda} = B_a \qquad ---(2)$$
$$(1) \Rightarrow A = B_a e^{-\delta/2\lambda} - Ce^{-\delta/\lambda}$$

Substitute this into (2),

$$(B_a e^{-\delta/2\lambda} - Ce^{-\delta/\lambda})e^{-\delta/2\lambda} + Ce^{\delta/2\lambda} = B_a$$
$$\Rightarrow C(e^{\delta/2\lambda} - e^{3\delta/2\lambda}) = B_a(1 - e^{-\delta/\lambda})$$
$$\Rightarrow C(1 - e^{-\delta/\lambda})(e^{\delta/2\lambda} + e^{-\delta/2\lambda}) = B_a(1 - e^{-\delta/\lambda})$$
$$\Rightarrow C = \frac{B_a}{e^{\delta/2\lambda} + e^{-\delta/2\lambda}} = \frac{2B_a}{\cosh\frac{\delta}{2\lambda}}$$

$$\therefore\ A = B_a e^{-\delta/2\lambda} - Ce^{-\delta/\lambda} = B_a e^{-\delta/2\lambda} - \frac{e^{-\delta/\lambda}B_a}{e^{\delta/2\lambda} + e^{-\delta/2\lambda}}$$
$$= B_a \frac{1 + e^{-\delta/\lambda} - e^{-\delta/\lambda}}{e^{\delta/2\lambda} + e^{-\delta/2\lambda}}$$
$$= \frac{B_a}{e^{\delta/2\lambda} + e^{-\delta/2\lambda}}$$
$$= \frac{B_a}{2\cosh\frac{\delta}{2\lambda}}$$

$$\therefore\ B(x) = Ae^{x/\lambda} + Ce^{-x/\lambda} = \frac{B_a}{2\cosh\frac{\delta}{2\lambda}}e^{x/\lambda} + \frac{B_a}{2\cosh\frac{\delta}{2\lambda}}e^{-x/\lambda}$$
$$= \frac{B_a}{2\cosh\frac{\delta}{2\lambda}}(e^{x/\lambda} + e^{-x/\lambda})$$
$$= B_a\frac{\cosh\frac{x}{\lambda}}{\cosh\frac{\delta}{2\lambda}}$$

(b)

$$
\begin{aligned}
4\pi M(x) \;=\; B(x) \;-\; B_a \;&=\; B_a \frac{\cosh\frac{x}{\lambda}}{\cosh\frac{\delta}{2\lambda}} - B_a \\
&=\; B_a\left(\frac{\cosh\frac{x}{\lambda}}{\cosh\frac{\delta}{2\lambda}} - 1\right) \\
&\approx\; B_a\left(\frac{1+\frac{1}{2}\left(\frac{x}{\lambda}\right)^2}{1+\frac{1}{2}\left(\frac{\delta}{2\lambda}\right)^2} - 1\right) \qquad\qquad (\delta << \lambda) \\
&=\; B_a\left(\frac{1+\frac{1}{2}\left(\frac{x}{\lambda}\right)^2 - \left[1+\frac{1}{2}\left(\frac{\delta}{2\lambda}\right)^2\right]}{1+\left(\frac{\delta}{2\lambda}\right)^2}\right) \\
&\approx\; B_a\left[\frac{1}{2}\left(\frac{x}{\lambda}\right)^2 - \frac{1}{2}\left(\frac{\delta}{2\lambda}\right)^2\right] \\
&=\; \underline{\underline{-\,\frac{B_a}{8\lambda^2}\left(\delta^2 - 4x^2\right)}}
\end{aligned}
$$