

Level 3 Condensed Matter Physics- Part I

Weekly problem 1 solutions

(1) Given a system of free electrons with chemical potential μ the probability of an eigenstate of energy E being occupied is given by the Fermi-Dirac distribution

$$f(E) = \frac{1}{e^{(E-\mu/k_B T)} + 1} \quad (1.1)$$

At low temperature the Fermi function becomes a step function (electron energy states below the chemical potential are filled, those above are empty), whereas at finite temperatures, the step function becomes progressively more smeared out. **[2 marks]**

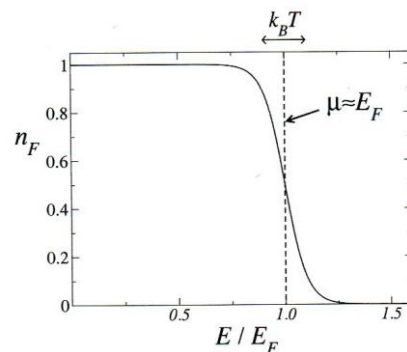
(2) We will consider electron waves in a box of size $V = L^3$ with the box having periodic boundary conditions. The plane wavefunctions of the electron waves are of the form $e^{i\mathbf{k}\cdot\mathbf{r}}$ with the wavevectors of the electrons taking the values $(2\pi/L)(n_1, n_2, n_3)$. These plane waves have corresponding energies

$$E(k) = \frac{\hbar^2 |k|^2}{2m}$$

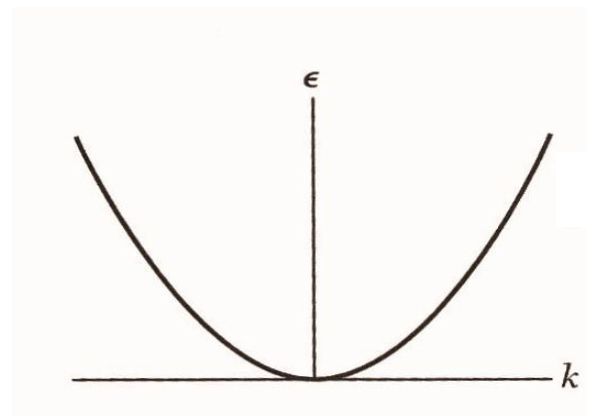
where m is the electron mass. We can define the Fermi energy, E_F as equal to the chemical potential at $T = 0$ and related to the Fermi wavevector k_F via

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

A graph of energy against wavevector gives a parabola centred at the origin. **[3 marks]**



The Fermi-Dirac distribution for $k_B T \ll E_F$. The dashed line marks the chemical potential μ , which is approximately E_F . At $T = 0$ the distribution is a step function but at finite temperature it gets smeared out over a range of energies of width a few $k_B T$.



(3) There are 4 monovalent copper atoms in a cubic unit cell of volume a^3 giving a free electron density of $n = 8.50 \times 10^{28}$ and a corresponding Fermi wavevector of $k_F = 1.35 \times 10^{10} \text{ m}^{-1}$, a Fermi energy E_F of 7.00 eV and a corresponding Fermi temperature ($T_F = E_F/k_B$) of 81,200 K. This shows that at any temperature below T_F copper will behave as a quantum degenerate system i.e. a quantum system even at room temperature and up to its melting point. **[3 marks]**

(4) The energy eigenvalues are

$$E = \frac{\hbar^2 k^2}{2m}$$

The mean value over the volume of the Fermi sphere in k space is

$$\langle E \rangle = \frac{\int_0^{k_F} \frac{\hbar^2 k^2}{2m} (4\pi k^2) dk}{\left(\frac{4\pi}{3} k_F^3\right)} = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 = \frac{3}{5} E_F.$$

Level 3 Condensed Matter Physics- Part I

Weekly problem 2 solutions

(1) The group velocity is the velocity of electrons in Bloch states in energy bands. For ordinary traveling waves we have $v_g = \frac{\partial \omega}{\partial k}$ and in Bloch states where $E = \hbar\omega$ we have $v_g = \frac{1}{\hbar} \frac{dE}{dk}$

[1 mark].

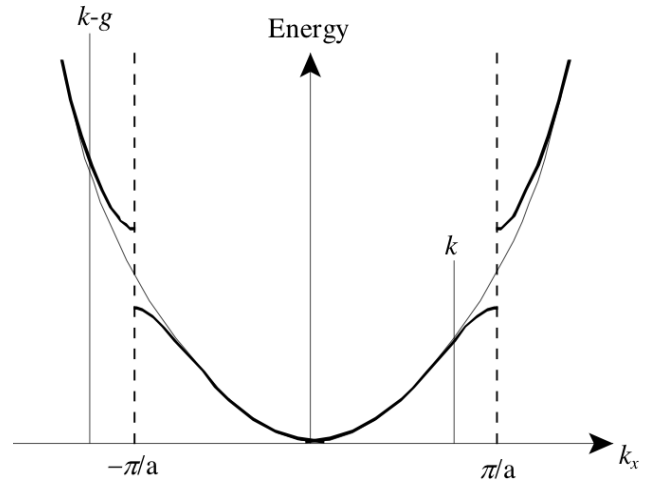
Thus, the velocity depends on the gradient of the $E(k)$ relationship and this in the nearly-free electron approximation is not constant across the Brillouin zone.

[1 mark]

The diagram, right, shows the typical $E(k)$ behaviour for nearly free electrons in a metal across the first Brillouin zone from $-\frac{\pi}{a}$ to $+\frac{\pi}{a}$.

[1 marks]

Unlike the free electron parabola, the electron group velocity can vary, from zero at the zone centre and zone boundaries up to a maximum close to the middle of the zone at $\pm \frac{\pi}{2a}$. [1 mark]



(2) We know that

$$v_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} \frac{d}{dk} (Ck^2 - Dk^4) = \frac{1}{\hbar} (2Ck - 4Dk^3) = \frac{1}{\hbar} 2Ck(1 - 2Dk^2).$$

[1 mark]

The group velocity is zero at $k = 0$ and at $k = \pm \pi/a$. [1 mark]

Setting $k = \pi/a$ and equating v_g to zero implies that $D = \frac{1}{2} \frac{a^2}{\pi^2}$. [1 mark]

The group velocity starts off as zero at the start of the Brillouin zone centre and increases to a maximum value close to the middle of the zone before decreasing again to zero at the Brillouin zone boundary.

(3) Evaluating and substituting for D gives $\frac{d^2E}{dk^2} = 2C - 6C \frac{a^2 k^2}{\pi^2}$. Since the system is isotropic (i.e. the energy E depends only on the magnitude of k) this gives an effective mass of $\hbar^2 / \left[2C - 6C \frac{a^2 k^2}{\pi^2} \right]$. Evaluating at $k = 0$ gives $m_{eff} = \frac{\hbar^2}{2C}$ and at $k = \pm \frac{\pi}{a}$ gives $m_{eff} = -\frac{\hbar^2}{4C}$.

[3 marks]

Level 3 Condensed Matter Physics- Part I
Weekly problem 3 solutions

(1) Assume that the uniform \mathbf{B} -field is along the z -axis. Then:

$$\mathbf{A}(\mathbf{r}) = \frac{\mathbf{B} \times \mathbf{r}}{2} = \frac{1}{2} \begin{vmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} & \hat{\mathbf{k}} \\ 0 & 0 & B \\ x & y & z \end{vmatrix} = \frac{1}{2} [-(By)\hat{\mathbf{i}} + (Bx)\hat{\mathbf{j}}]$$

[1 mark]

From the definition of the magnetic vector potential, the magnetic field \mathbf{B} is:

$$\mathbf{B} = \vec{\nabla} \times \mathbf{A} = \frac{1}{2} \begin{vmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} & \hat{\mathbf{k}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ -By & Bx & 0 \end{vmatrix} = B\hat{\mathbf{k}}$$

The correct form of the magnetic field is obtained, which validates the choice of magnetic vector potential \mathbf{A} .

[1 mark]

(2) From the previous question $\mathbf{A}(\mathbf{r})$ has components only in the xy -plane. We can express these in component form using polar coordinates:

$$\mathbf{A}(\mathbf{r}) = A_R \hat{\mathbf{R}} + A_\theta \hat{\boldsymbol{\theta}}$$

Making use of the relationship between Cartesian and polar coordinates we can write:

$$\begin{aligned} -\frac{By}{2} &= -\frac{BR\sin\theta}{2} = A_R \cos\theta - A_\theta \sin\theta \\ \frac{Bx}{2} &= \frac{BR\cos\theta}{2} = A_R \sin\theta + A_\theta \cos\theta \end{aligned}$$

Solving these simultaneous equations we obtain $A_R = 0$ and $A_\theta = BR/2$, i.e. $\mathbf{A}(\mathbf{r})$ points in the $\hat{\boldsymbol{\theta}}$ direction and has magnitude that depends on R only. This shows that $\mathbf{A}(\mathbf{r})$ is rotationally invariant.

Note that it is possible to select other gauges as well, e.g. $\mathbf{A}(\mathbf{r}) = (0, Bx, 0)$. However, the symmetric gauge is used since its rotational symmetry is well-suited for studying the magnetic properties of an electron in a spherically symmetric atom.

[2 marks]

(3) Let ψ denote a wavefunction. Then using the result for $\mathbf{A}(\mathbf{r})$ from question (1):

$$\mathbf{p} \cdot \mathbf{A}\psi = \frac{-i\hbar}{2} B \left[-\frac{\partial(y\psi)}{\partial x} + \frac{\partial(x\psi)}{\partial y} \right] = \frac{i\hbar}{2} B \left[y \frac{\partial\psi}{\partial x} - x \frac{\partial\psi}{\partial y} \right]$$

[1 mark]

$$\mathbf{A} \cdot \mathbf{p}\psi = \frac{-i\hbar}{2} \left[-(By) \frac{\partial \psi}{\partial x} + (Bx) \frac{\partial \psi}{\partial y} \right] = \frac{i\hbar}{2} B \left[y \frac{\partial \psi}{\partial x} - x \frac{\partial \psi}{\partial y} \right]$$

[1 mark]

It is therefore clear that \mathbf{p} and \mathbf{A} commute.

(4) The current density is given by:

$$\mathbf{J}(\mathbf{r}) = -e\rho(\mathbf{r})\mathbf{v}$$

where \mathbf{v} is the velocity of the electrons. This follows from the fact that $\rho(\mathbf{r})|\mathbf{v}|$ number of electrons with charge $-e$ will flow out of unit cross-sectional area within unit period of time. The change in velocity due to the magnetic field is $e\mathbf{A}(\mathbf{r})/m$, so that the induced current density is:

$$\mathbf{J}(\mathbf{r}) = \frac{e^2}{m} \rho(\mathbf{r})[\mathbf{r} \times \mathbf{B}]$$

[2 marks]

Note that the $[\mathbf{r} \times \mathbf{B}]$ term implies that there is a connection between $\mathbf{J}(\mathbf{r})$ and diamagnetism, which has energy proportional to $(\mathbf{B} \times \mathbf{r})^2$. In fact, $\mathbf{J}(\mathbf{r})$ is called the diamagnetic current density- it can be interpreted as the induced current density within the atom that opposes the applied magnetic field. Note also that for the symmetric gauge $\vec{\nabla} \cdot \mathbf{A} = 0$, and therefore $\vec{\nabla} \cdot \mathbf{J} = 0$ as well. This implies that the atom is in steady state, and there is no net flow of electrons out of the atom due to the magnetic field.

[2 marks]

Level 3 Condensed Matter Physics- Part I

Weekly problem 4 solutions

(1) How much work has been done?

A magnetic field acting upon a magnetic dipole will produce a torque, $\tau = \mu \times \mathbf{B}$. When the magnetic dipole rotates through an angle $d\theta$ the torque does work,

$$dW = \tau d\theta = \mu B \sin\theta d\theta. \quad [1 \text{ mark}]$$

Setting this work equal to the change in potential energy we obtain,

$$dE = dW = \mu B \sin\theta d\theta, \text{ and by integrating we obtain,}$$

$$E = -\mu B [\cos\theta]_{\theta_0}^{\theta} + E_0 \quad [1 \text{ mark}]$$

Choosing the potential energy to be zero when the magnetic dipole is perpendicular to the field, i.e. $E = 0$ when $\theta_0 = 90^\circ$, we obtain the potential energy of the magnetic dipole as required,

$$E = -\mu B \cos\theta = -\boldsymbol{\mu} \cdot \mathbf{B} \quad [1 \text{ mark}]$$

(2) Energy differences due to magnetism

The potential energy is at its minimum when $\theta = 0^\circ$ and at its maximum when $\theta = 180^\circ$.

$$E_{\max} = -\mu B \cos\theta = -2 \times \mu_B \times 1 \times \cos(180^\circ) = -2 \times 9.27 \times 10^{-24} \times 1 \times -1 = 18.5 \times 10^{-24} \text{ J}$$

Similarly, the minimum potential energy when $\theta = 0^\circ$ yields $E_{\min} = -18.5 \times 10^{-24} \text{ J}$. [2 marks]

The potential energy difference between these two states of the atom is therefore

$\Delta E = 37.1 \times 10^{-24} \text{ J}$, which at a room temperature of 300 K compares to a thermal energy of $k_B T \approx 4.14 \times 10^{-21} \text{ J}$. Thus, the potential energy difference is only approx. 1% of the thermal energy available at room temperature. This means both states will exist with almost equal populations at room temperature. [1 mark]

(3) Diamagnetism in Bismuth

(a) We use the Langevin's expression for diamagnetic susceptibility $\chi_d = -\frac{\mu_0 N Z e^2 \langle r^2 \rangle}{6m_e}$

We determine N from the equation where m is the molar mass of bismuth.

$$N = \frac{N_A \rho}{m} = \frac{6.023 \times 10^{23} \times 9.78 \times 10^3}{208.98 \times 10^{-3}} = 2.82 \times 10^{28} \text{ m}^{-3} \quad [1 \text{ mark}]$$

Therefore

$$\chi_d = -\frac{\mu_0 N Z e^2 \langle r^2 \rangle}{6m_e} = -\frac{4\pi \times 10^{-7} \times 2.82 \times 10^{28} \times 83 \times (1.6 \times 10^{-19})^2 \times (0.16 \times 10^{-9})^2}{6 \times 9.11 \times 10^{-31}} = -3.5 \times 10^{-4}$$

[1 mark]

(b) The magnetic moment (m) of the sample can be calculated from the magnetisation (total magnetic moment per unit volume), M , but we need to convert from sample mass (m_s) to sample volume using the density ρ involving an equation which contains too many m's

$m = \frac{Mm_s}{\rho}$ and using the definition for susceptibility

$$m = \frac{\chi_d H m_s}{\rho} = \frac{-3.5 \times 10^{-4} \times 3 \times 10^3 \times 1 \times 10^{-3}}{9.78 \times 10^3} = -1.07 \times 10^{-7} \text{ A m}^2$$

[2 marks]

Level 3 Condensed Matter Physics- Part I

Weekly problem 5 solutions

(1) **L-S coupling**; here the coupling of the **L** vectors of the individual electrons combine to form a total angular momentum **L**, while the spin momentum vectors combine independently to form a total spin momentum vector **S**. This means that the calculated **S** is not affected by the value of **L** i.e. the spin-spin and orbit-orbit couplings are much stronger than the spin-orbit coupling for each electron. This leads to a total angular momentum **J** of an atom is the vector sum of the two non-interacting momenta **L** and **S**, $\mathbf{J} = \mathbf{L} + \mathbf{S}$. [1 mark]

(2) We are given that,

$$M = M_S \left[\frac{(2J+1)}{2J} \coth \left(\frac{(2J+1)}{2J} y \right) - \frac{1}{2J} \coth \left(\frac{y}{2J} \right) \right]$$

where $y = \frac{g_J \mu_B J B}{(k_B T)}$ and $M_S = n g_J \mu_B J$. At small magnetic fields and/or high temperatures y is very small. This means we can use the result,

$$\coth x \approx \frac{1}{x} + \frac{x}{3} \text{ for } x \rightarrow 0$$

To obtain,

$$\begin{aligned} M &\approx n g_J \mu_B J \left[\frac{2J+1}{2J} \left(\frac{2J}{(2J+1)y} + \frac{(2J+1)}{2J} \times \frac{y}{3} \right) - \frac{1}{2J} \left(\frac{2J}{y} + \frac{1}{2J} \times \frac{y}{3} \right) \right] \\ &= n g_J \mu_B J \left(\frac{(J+1)}{J} \times \frac{y}{3} \right). \end{aligned}$$

Substituting in for y gives,

$$M \approx \frac{n g_J^2 \mu_B^2 J(J+1) B}{3 k_B T}.$$

[1 mark]

Substituting $B = \mu_0 H$ into this expression and re-arranging gives the paramagnetic susceptibility,

$$\chi_P = \frac{M}{H} = \frac{n g_J^2 \mu_0 \mu_B^2 J(J+1)}{3 k_B T},$$

Which has the form of Curie's law, $\chi = C/T$

[1 mark]

(3) $\text{Ti}^{2+} 3d^2$ (note that the azimuthal quantum number $l = 2$ for the d -shell):

m_l	-2	-1	0	1	2
s				+1/2	+1/2

Ground state:

$$S = \sum s = 2 \times \frac{1}{2} = 1, \quad L = \sum m_l = 2 + 1 = 3, \\ J = |L - S| = |3 - 1| = 2.$$

Excited states: $J = |L - S| + 1 = 3, J = L + S = 4$ [2 marks]

Total magnetic moment of an atom, $|m_J| = g_J \mu_B \sqrt{J(J+1)}$ and

$$g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}.$$

$$J = 2, g_J = 1 + \frac{2(2+1) - 3(3+1) + 1(1+1)}{4(2+1)} = 0.67, |m_2| = 0.67 \times \sqrt{2(2+1)} \mu_B \\ = 1.64 \mu_B.$$

$$J = 3, g_J = 1 + \frac{3(3+1) - 3(3+1) + 1(1+1)}{6(3+1)} = 1.08, |m_2| = 1.08 \times \sqrt{3(3+1)} \mu_B \\ = 3.74 \mu_B.$$

$$J = 4, g_J = 1 + \frac{4(4+1) - 3(3+1) + 1(1+1)}{8(4+1)} = 1.25, |m_2| = 1.25 \times \sqrt{4(4+1)} \mu_B \\ = 5.59 \mu_B.$$

[1 mark]

(4) Energy states: $E_{SO}(J) = \frac{\lambda}{2} [J(J+1) - L(L+1) - S(S+1)]$

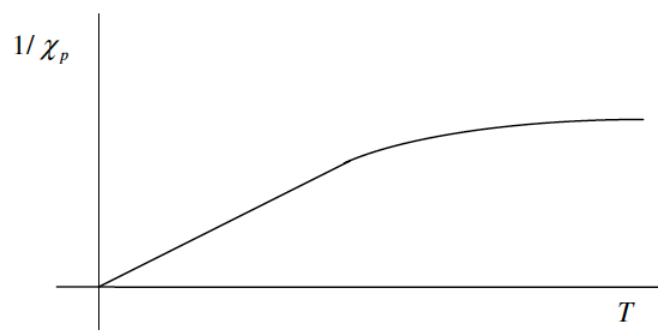
$$J = 2, E_{SO}(2) = \frac{4.5}{2} [2(2+1) - 3(3+1) - 1(1+1)] = -18 \text{ meV}$$

$$J = 3, E_{SO}(3) = \frac{4.5}{2} [3(3+1) - 3(3+1) - 1(1+1)] = -4.5 \text{ meV}$$

$$J = 4, E_{SO}(4) = \frac{4.5}{2} [4(4+1) - 3(3+1) - 1(1+1)] = 13.5 \text{ meV}$$

[2 marks]

(5) Given the form of the probability, $P(J) \propto (2J+1) \exp(-E_{SO}(J)/k_B T)$, it would be expected that, at very low temperatures, only the ground $J = 2$ state, would be substantially populated and the ground state magnetic moment would dominate the paramagnetic susceptibility with $\frac{1}{\chi_P} = \frac{3k_B T}{\mu_0 N m_2^2}$. At higher temperatures we would expect the contribution from the $J = 3$ state, and given the greater atomic moment, this would cause the measured paramagnetic susceptibility to be larger than that expected for the $J = 2$ state. Hence the inverse susceptibility would have the form:



[2 marks]