

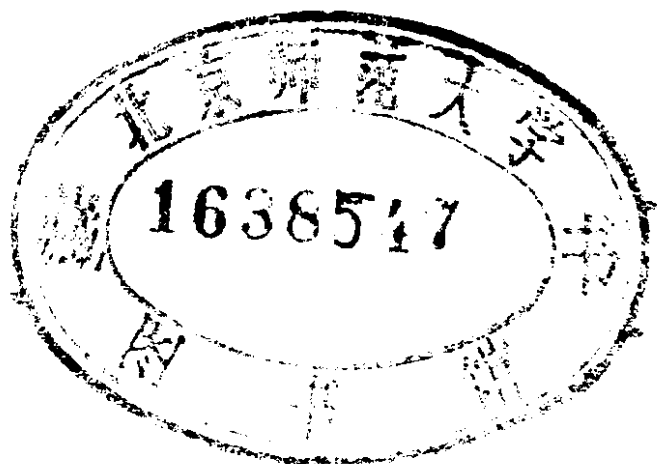
固態物理學問題詳解

C. 基特尔 原著

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问 题

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内 容

本书系 C. 基特尔著《固态物理学导论》一书的习题详解。

固态物理学问题详解

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Chapter 1 (1) Crystal Structure

1. **Tetrahedral angles.** The angles between the tetrahedral bonds of diamond are the same as the angles between the body diagonals of a cube, as in Fig. 12. Use elementary vector analysis to find the value of the angle.
2. **Indices of planes.** Consider the planes with indices (100) and (001); the lattice is fcc, and the indices refer to the conventional cubic cell. What are the indices of these planes when referred to the primitive axes of Fig. 13?
3. **Hcp structure.** Show that the c/a ratio for an ideal hexagonal close-packed structure is $(\frac{8}{3})^{1/2} = 1.633$. If c/a is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.

Chapter 2 (2) Reciprocal Lattice and (Crystal Diffraction)

1. **Interplanar separation.** Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$ is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$. (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.
2. **Hexagonal space lattice.** The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{x} + (a/2)\hat{y} ; \quad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{x} + (a/2)\hat{y} ; \quad \mathbf{a}_3 = c\hat{z} .$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.

(b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y} ; \quad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y} ; \quad \mathbf{b}_3 = (2\pi/c)\hat{z} ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.

(c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

3. **Volume of Brillouin zone.** Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b})\mathbf{a}$.

4. **Width of diffraction maximum.** We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\rho_m = m\mathbf{a}$, where m is an integer. By analogy with (20) the total scattered radiation amplitude will be proportional to $F = \sum \exp[-ima \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k})]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]}$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x}$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 = F^*F = \frac{\sin^2 \frac{1}{2}M(\mathbf{a} \cdot \Delta\mathbf{k})}{\sin^2 \frac{1}{2}(\mathbf{a} \cdot \Delta\mathbf{k})}$$

(b) We know that a diffraction maximum appears when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin \frac{1}{2}M(\mathbf{a} \cdot \Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M . The same result holds true for a three-dimensional crystal.

5. **Structure factor of diamond.** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the

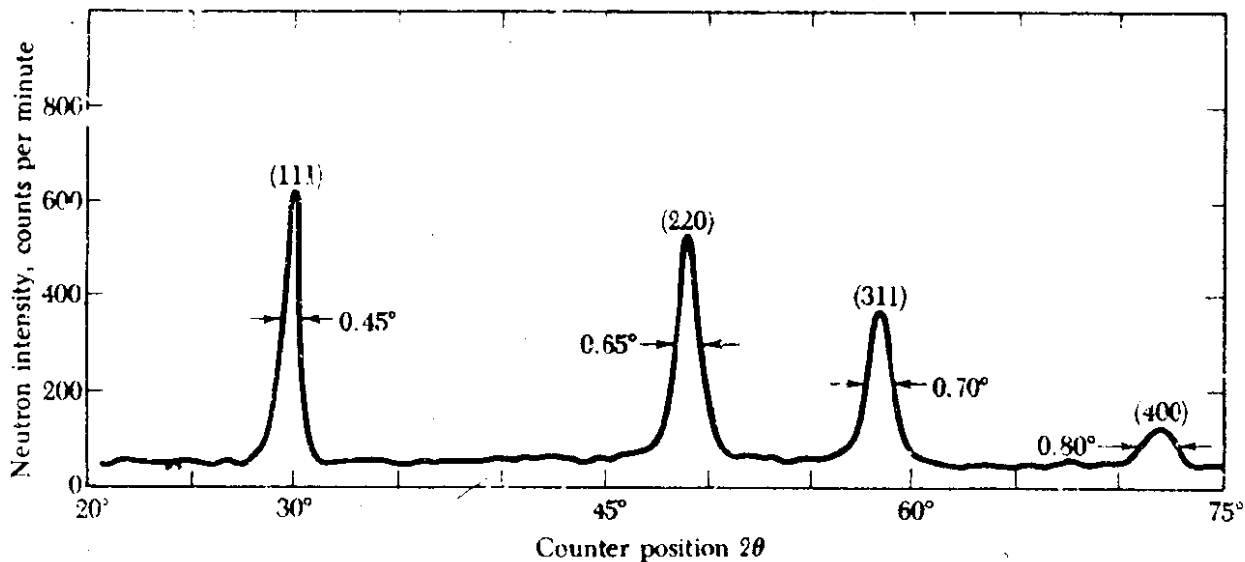


Figure 19 Neutron diffraction pattern for powdered diamond. (After C. Bacon.)

allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (Fig. 19). (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

6. **Form factor of atomic hydrogen.** For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_0^3)^{-1} \exp(-2r/a_0)$, where a_0 is the Bohr radius. Show that the form factor is $f_G = 16/(4 + G^2 a_0^2)^2$.

7. **Diatomc line.** Consider a line of atoms $ABAB \dots AB$, with an $A-B$ bond length of $\frac{1}{2}a$. The form factors are f_A, f_B for atoms A, B , respectively. The incident beam of x-rays is perpendicular to the line of atoms. (a) Show that the interference condition is $n\lambda = a \cos \theta$, where θ is the angle between the diffracted beam and the line of atoms. (b) Show that the intensity of the diffracted beam is proportional to $|f_A - f_B|^2$ for n odd, and to $|f_A + f_B|^2$ for n even. (c) Explain what happens if $f_A = f_B$.

Chapter 3 (3) Crystal Binding

1. **Quantum solid.** In a quantum solid the dominant repulsive energy is the zero-point energy of the atoms. Consider a crude one-dimensional model of crystalline He⁴ with each He atom confined to a line segment of length L . In the ground state the wave function within each segment is taken as a half wavelength of a free particle. Find the zero-point kinetic energy per particle.
2. **Cohesive energy of bcc and fcc neon.** Using the Lennard-Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures. The lattice sums for the bcc structures are:

$$\sum_j' p_j^{-12} = 9.11418 ; \quad \sum_j' p_j^{-6} = 12.2533 .$$

3. **Solid molecular hydrogen.** For H₂ one finds from measurements on the gas that the Lennard-Jones parameters are $\epsilon = 50 \times 10^{-16}$ erg and $\sigma = 2.96$ Å. Find the cohesive energy in kJ per mole of H₂; do the calculation for an fcc structure. Treat each H₂

molecule as a sphere. The observed value of the cohesive energy is 0.751 kJ/mol, much less than we calculated, so that quantum corrections must be very important.

4. **Possibility of ionic crystals R^+R^- .** Imagine a crystal that exploits for binding the coulomb attraction of the positive and negative ions of the same atom or molecule R . This is believed to occur with certain organic molecules, but it is not found when R is a single atom. Use the data in Tables 5 and 6 to evaluate the stability of such a form of Na in the NaCl structure relative to normal metallic sodium. Evaluate the energy at the observed interatomic distance in metallic sodium, and use 0.78 eV as the electron affinity of Na.
5. **Linear ionic crystal.** Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbors. (a) Show that at the equilibrium separation

$$(CGS) \quad U(R_0) = -\frac{2Nq^2 \ln 2}{R_0} \left(1 - \frac{1}{n}\right) .$$

(b) Let the crystal be compressed so that $R_0 \rightarrow R_0(1 - \delta)$. Show that the work done in compressing a unit length of the crystal has the leading term $\frac{1}{2}C\delta^2$, where

$$(CGS) \quad C = \frac{(n-1)q^2 \ln 2}{R_0}$$

To obtain the results in SI, replace q^2 by $q^2/4\pi\epsilon_0$. Note: We should not expect to obtain this result from the expression for $U(R_0)$, but we must use the complete expression for $U(R)$.

6. **Cubic ZnS structure.** Using λ and ρ from Table 7 and the Madelung constants given in the text, calculate the cohesive energy of KCl in the cubic ZnS structure described in Chapter 1. Compare with the value calculated for KCl in the NaCl structure.
7. **Divalent ionic crystals.** Barium oxide has the NaCl structure. Estimate the cohesive energies per molecule of the hypothetical crystals Ba^+O^- and $Ba^{++}O^{--}$ referred to separated neutral atoms. The observed nearest-neighbor internuclear distance is $R_0 = 2.76 \text{ \AA}$; the first and second ionization potentials of Ba are 5.19 and 9.96 eV; and the electron affinities of the first and second electrons added to the neutral oxygen atom are 1.5 and -9.0 eV. The first electron affinity of the neutral oxygen atom is the energy released in the reaction $O + e \rightarrow O^-$. The second electron affinity is the energy released in the reaction $O^- + e \rightarrow O^{--}$. Which valence state do you predict will occur? Assume R_0 is the same for both forms, and neglect the repulsive energy.

Chapter 4 (4) Phonons I. Crystal Vibrations

1. **Vibrations of square lattice.** We consider transverse vibrations of a planar square lattice of rows and columns of identical atoms, and let $u_{l,m}$ denote the displacement normal to the plane of the lattice of the atom in the l th column and m th row (Fig. 13). The mass of each atom is M , and C is the force constant for nearest neighbor atoms.
 - (a) Show that the equation of motion is

$$M(d^2u_{lm}/dt^2) = C[(u_{l+1,m} + u_{l-1,m} - 2u_{lm}) + (u_{l,m+1} + u_{l,m-1} - 2u_{lm})] .$$



Figure 13 Square array of lattice constant a . The displacements considered are normal to the plane of the lattice.

(b) Assume solutions of the form

$$u_{lm} = u(0) \exp[i(lK_x a + mK_y a - \omega t)] ,$$

where a is the spacing between nearest-neighbor atoms. Show that the equation of

motion is satisfied if

$$\omega^2 M = 2C(2 - \cos K_x a - \cos K_y a) .$$

This is the dispersion relation for the problem. (c) Show that the region of \mathbf{K} space for which independent solutions exist may be taken as a square of side $2\pi/a$. This is the first Brillouin zone of the square lattice. Sketch ω versus K for $K = K_x$ with $K_y = 0$, and for $K_x = K_y$. (d) For $Ka \ll 1$, show that

$$\omega = (Ca^2/M)^{1/2}(K_x^2 + K_y^2)^{1/2} = (Ca^2/M)^{1/2}K$$

so that in this limit the velocity is constant.

2. *Monatomic linear lattice.* Consider a longitudinal wave

$$u_s = u \cos(\omega t - sKa)$$

which propagates in a monatomic linear lattice of atoms of mass M spacing a , and nearest-neighbor interaction C .

(a) Show that the total energy of the wave is

$$E = \frac{1}{2}M \sum_s (du_s/dt)^2 + \frac{1}{2}C \sum_s (u_s - u_{s+1})^2 ,$$

where s runs over all atoms.

(b) By substitution of u_s in this expression, show that the time-average total energy per atom is

$$\frac{1}{2}M\omega^2 u^2 + \frac{1}{2}C(1 - \cos Ka)u^2 = \frac{1}{2}M\omega^2 u^2 ,$$

where in the last step we have used the dispersion relation (9) for this problem.

3. *Continuum wave equation.* Show that for long wavelengths the equation of motion (2) reduces to the continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} ,$$

where v is the velocity of sound.

4. *Basis of two unlike atoms.* For the problem treated by (18) to (26), find the amplitude ratios u/v for the two branches at $K_{\max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

5. *Kohn anomaly.* We suppose that the interplanar force constant C_p between planes s and $s + p$ is of the form

$$C_p = A \frac{\sin pk_0 a}{pa} ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0 : there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

6. *Diatomic chain.* Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2 .

7. **Atomic vibrations in a metal.** Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $\mathfrak{N}/4\pi R^3$, which defines R . (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$. (b) Estimate the value of this frequency for sodium, roughly. (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.

*8. **Soft phonon modes.** Consider a line of ions of equal mass but alternating in charge, with $e_p = e(-1)^p$ as the charge on the p th ion. The interatomic potential is the sum of two contributions: (1) a short-range interaction of force constant $C_{1R} = \gamma$ that acts between nearest neighbors only, and (2) a coulomb interaction between all ions. (a) Show that the contribution of the coulomb interaction to the atomic force constants is $C_{pC} = 2(-1)^p e^2/p^3 a^3$, where a is the equilibrium nearest-neighbor distance. (b) From (16a) show that the dispersion relation may be written as

$$\omega^2/\omega_0^2 = \sin^2 \frac{1}{2}Ka + \sigma \sum_{p=1}^{\infty} (-1)^p (1 - \cos pKa)p^{-3},$$

where $\omega_0^2 \equiv 4\gamma/M$ and $\sigma = e^2/\gamma a^3$. (c) Show that ω^2 is negative (unstable mode) at the zone boundary $Ka = \pi$ if $\sigma > 0.475$ or $4/7\zeta(3)$, where ζ is a Riemann zeta function. Show further that the speed of sound at small Ka is imaginary if $\sigma > (2 \ln 2)^{-1} = 0.721$. Thus ω^2 goes to zero and the lattice is unstable for some value of Ka in the interval $(0, \pi)$ if $0.475 < \sigma < 0.721$. Notice that the phonon spectrum is not that of a diatomic lattice because the interaction of any ion with its neighbors is the same as that of any other ion.

Chapter 5 (5) Phonons II. Thermal Properties

1. **Singularity in density of states.** (a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of N atoms with nearest neighbor interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{(\omega_m^2 - \omega^2)^{1/2}},$$

where ω_m is the maximum frequency. (b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = (L/2\pi)^3 (2\pi/A)^{3/2} (\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

2. *Runs thermal dilation of crystal cell.* (a) Estimate for 300 K the root mean square thermal dilation $\Delta V/V$ for a primitive cell of sodium. Take the bulk modulus as 7×10^{10} erg cm⁻³. Note that the Debye temperature 158 K is less than 300 K, so that the thermal energy is of the order of $k_B T$. (b) Use this result to estimate the root mean square thermal fluctuation $\Delta a/a$ of the lattice parameter.
3. *Zero point lattice displacement and strain.* (a) In the Debye approximation, show that the mean square displacement of an atom at absolute zero is $\langle R^2 \rangle = 3\hbar\omega_D^2/8\pi^2\rho v^3$, where v is the velocity of sound. Start from the result (4.29) summed over the independent lattice modes: $\langle R^2 \rangle = (\hbar/2\rho V)\Sigma\omega^{-1}$. We have included a factor of $\frac{1}{2}$ to go from square amplitude to square displacement. (b) Show that $\Sigma\omega^{-1}$ and $\langle R^2 \rangle$ diverge for a one-dimensional lattice, but that the mean square strain is finite. Consider $\langle (\partial R/\partial x)^2 \rangle = \frac{1}{2}\Sigma K^2 u_0^2$ as the mean square strain, and show that it is equal to $\hbar\omega_D^2 L/4\pi M N v^3$ for a line of N atoms each of mass M , counting longitudinal modes only. The divergence of R^2 is not significant for any physical measurement.
4. *Heat capacity of layer lattice.* (a) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2 . (b) Suppose instead, as in many layer structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?
- *5. *Grüneisen constant.* (a) Show that the free energy of a phonon mode of frequency ω is $k_B T \ln [2 \sinh (\hbar\omega/2k_B T)]$. It is necessary to retain the zero-point energy $\frac{1}{2}\hbar\omega$ to obtain this result. (b) If Δ is the fractional volume change, then the free energy of the crystal may be written as

$$F(\Delta, T) = \frac{1}{2}B\Delta^2 + k_B T \sum \ln [2 \sinh (\hbar\omega_K/2k_B T)] ,$$

where B is the bulk modulus. Assume that the volume dependence of ω_K is $\delta\omega/\omega = -\gamma\Delta$, where γ is known as the Grüneisen constant. If γ is taken as independent of the

*This problem is somewhat difficult.

mode K , show that F is a minimum with respect to Δ when $B\Delta = \gamma \sum_j \hbar \omega_j \coth(\hbar \omega_j / 2k_B T)$, and show that this may be written in terms of the thermal energy density as $\Delta = \gamma U(T)/B$. (c) Show that on the Debye model $\gamma = -\partial \ln \theta / \partial \ln V$. Note: Many approximations are involved in this theory: the result (a) is valid only if ω is independent of temperature; γ may be quite different for different modes.

- *6. *Density of modes of square lattice.* The dispersion relation of a square lattice with nearest-neighbor interactions was found in Problem 4.1 to be $\omega^2 M = 2C(2 - \cos K_x a - \cos K_y a)$. Note that the Brillouin zone can be divided into eight equivalent sectors. If you have access to a microcomputer, divide a sector into around 100 squares, evaluate ω at the center of each square (or at common corners), and plot a histogram of the number of squares per unit frequency range. Sketch $D(\omega)$ as a function of ω . In the calculation take $2C = 1$ and $M = 1$.

Chapter 6 (6) Free Electron Fermi Gas

1. *Kinetic energy of electron gas.* Show that the kinetic energy of a three-dimensional gas of N free electrons at 0 K is

$$U_0 = \frac{3}{5} N \epsilon_F \quad (60)$$

2. *Pressure and bulk modulus of an electron gas.* (a) Derive a relation connecting the pressure and volume of an electron gas at 0 K. Hint: Use the result of Problem 1 and the relation between ϵ_F and electron concentration. The result may be written as $p = \frac{2}{3}(U_0/V)$. (b) Show that the bulk modulus $B = -V(\partial p/\partial V)$ of an electron gas at 0 K is $B = 5p/3 = 10U_0/9V$. (c) Estimate for potassium, using Table 1, the value of the electron gas contribution to B .

3. *Chemical potential in two dimensions.* Show that the chemical potential of a Fermi gas in two dimensions is given by:

$$\mu(T) = k_B T \ln [\exp(\pi n \hbar^2 / m k_B T) - 1] \quad (61)$$

for n electrons per unit area. Note: The density of orbitals of a free electron gas in two dimensions is independent of energy: $D(\epsilon) = m/\pi \hbar^2$, per unit area of specimen.

4. **Fermi gases in astrophysics.** (a) Given $M_{\odot} = 2 \times 10^{33}$ g for the mass of the Sun, estimate the number of electrons in the Sun. In a white dwarf star this number of electrons may be ionized and contained in a sphere of radius 2×10^9 cm; find the Fermi energy of the electrons in electron volts. (b) The energy of an electron in the relativistic limit $\epsilon \gg mc^2$ is related to the wavevector as $\epsilon \cong pc = \hbar kc$. Show that the Fermi energy in this limit is $\epsilon_F \approx \hbar c(N/V)^{1/3}$, roughly. (c) If the above number of electrons were contained within a pulsar of radius 10 km, show that the Fermi energy would be $\approx 10^6$ eV. This value explains why pulsars are believed to be composed largely of neutrons rather than of protons and electrons, for the energy release in the reaction $n \rightarrow p + e^-$ is only 0.8×10^6 eV, which is not large enough to enable many electrons to form a Fermi sea. The neutron decay proceeds only until the electron concentration builds up enough to create a Fermi level of 0.8×10^6 eV, at which point the neutron, proton, and electron concentrations are in equilibrium.
5. **Liquid He³.** The atom He³ has spin $\frac{1}{2}$ and is a fermion. The density of liquid He³ is 0.081 g cm^{-3} near absolute zero. Calculate the Fermi energy ϵ_F and the Fermi temperature T_F .
6. **Frequency dependence of the electrical conductivity.** Use the equation $m(dv/dt + v/\tau) = -eE$ for the electron drift velocity v to show that the conductivity at frequency ω is

$$\sigma(\omega) = \sigma(0) \left(\frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \right), \quad (62)$$

where $\sigma(0) = ne^2\tau/m$.

- *7. **Dynamic magnetoconductivity tensor for free electrons.** A metal with a concentration n of free electrons of charge $-e$ is in a static magnetic field $B\hat{z}$. The electric current density in the xy plane is related to the electric field by

$$j_x = \sigma_{xx}E_x + \sigma_{xy}E_y; \quad j_y = \sigma_{yx}E_x + \sigma_{yy}E_y.$$

Assume that the frequency $\omega \gg \omega_c$ and $\omega \gg 1/\tau$, where $\omega_c = eB/mc$ and τ is the collision time. (a) Solve the drift velocity equation (46) to find the components of the magnetoconductivity tensor:

$$\sigma_{xx} = \sigma_{yy} = i\omega_p^2/4\pi\omega; \quad \sigma_{xy} = -\sigma_{yx} = \omega_c\omega_p^2/4\pi\omega^2,$$

where $\omega_p^2 = 4\pi ne^2/m$. (b) Note from a Maxwell equation that the dielectric function tensor of the medium is related to the conductivity tensor as $\epsilon = 1 + i(4\pi/\omega)\sigma$. Consider an electromagnetic wave with wavevector $\mathbf{k} = k\hat{z}$. Show that the dispersion relation for this wave in the medium is

$$c^2k^2 = \omega^2 - \omega_p^2 \pm \omega_c\omega_p^2/\omega . \quad (63)$$

At a given frequency there are two modes of propagation with different wavevectors and different velocities. The two modes correspond to circularly polarized waves. Because a linearly polarized wave can be decomposed into two circularly polarized waves, it follows that the plane of polarization of a linearly polarized wave will be rotated by the magnetic field.

- *8. **Cohesive energy of free electron Fermi gas.** We define the dimensionless length r , as r_0/a_H , where r_0 is the radius of a sphere that contains one electron, and a_H is the Bohr radius \hbar^2/e^2m . (a) Show that the average kinetic energy per electron in a free electron Fermi gas at 0 K is $2.21/r_s^2$, where the energy is expressed in rydbergs,

*This problem is somewhat difficult.

with $1 \text{ Ry} = me^4/2\hbar^2$. (b) Show that the coulomb energy of a point positive charge e interacting with the uniform electron distribution of one electron in the volume of radius r_0 is $-3e^2/2r_0$, or $-3/r_s$ in rydbergs. (c) Show that the coulomb self-energy of the electron distribution in the sphere is $3e^2/5r_0$, or $6/5r_s$ in rydbergs. (d) The sum of (b) and (c) gives $-1.80/r_s$ for the total coulomb energy per electron. Show that the equilibrium value of r_s is 2.45. Will such a metal be stable with respect to separated H atoms?

9. **Static magnetoconductivity tensor.** For the drift velocity theory of (51), show that the static current density can be written in matrix form as

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \frac{\sigma_0}{1 + (\omega_c\tau)^2} \begin{pmatrix} 1 & -\omega_c\tau & 0 \\ \omega_c\tau & 1 & 0 \\ 0 & 0 & 1 + (\omega_c\tau)^2 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} . \quad (64)$$

In the high magnetic field limit of $\omega_c\tau \gg 1$, show that

$$\sigma_{yx} = nec/B = -\sigma_{xy} . \quad (65)$$

In this limit $\sigma_{xx} = 0$, to order $1/\omega_c\tau$. The quantity σ_{yx} is called the Hall conductivity.

10. **Maximum surface resistance.** Consider a square sheet of side L , thickness d , and electrical resistivity ρ . The resistance measured between opposite edges of the sheet is called the surface resistance: $R_{sq} = \rho L/Ld = \rho/d$, which is independent of the area L^2 of the sheet. (R_{sq} is called the resistance per square and is expressed in ohms per square, because ρ/d has the dimensions of ohms.) If we express ρ by (44), then $R_{sq} = m/nde^2\tau$. Suppose now that the minimum value of the collision time is determined by scattering from the surfaces of the sheet, so that $\tau \approx d/v_F$, where v_F is the Fermi velocity. Thus the maximum surface resistivity is $R_{sq} \approx mv_F/nd^2e^2$. Show for a monatomic metal sheet one atom in thickness that $R_{sq} \approx \hbar/e^2 = 4.1 \text{ k}\Omega$, where $1 \text{ k}\Omega$ is 10^3 ohms.

*11. **Small metal spheres.** Consider free electrons in a spherical square well potential of radius a , with an infinitely high boundary. (a) Show that the wave function of an orbital of angular momentum ℓ and projection m has the form

$$\psi = R_{k\ell}(r)Y_{\ell m}(\theta, \varphi) , \quad (66)$$

where the radial wave function has the form

$$R_{k\ell}(r) = (k/r)^{1/2}J_{\ell+1/2}(kr) ,$$

and Y is a spherical harmonic. Here J is a Bessel function of half-integral order and satisfies the boundary condition $J_{\ell+1/2}(ka) = 0$. The roots give the energy eigenvalues ϵ of the levels above the bottom of the well, where $\epsilon = \hbar^2k^2/2m$. (b) Show that the order of the levels above the ground orbital is

$$1s, 1p, 1d, 2s, 1f, 2p, 1g, 2d, 1h, 3s, 2f, \dots ,$$

where s, p, d, f, g, h denote $\ell = 0, 1, 2, 3, 4, 5$.

Chapter 7 (7) Energy Bands

Square lattice, free electron energies. (a) Show for a simple square lattice (two dimensions) that the kinetic energy of a free electron at a corner of the first zone is higher than that of an electron at midpoint of a side face of the zone by a factor of 2. (b) What is the corresponding factor for a simple cubic lattice (three dimensions)? (c) What bearing might the result of (b) have on the conductivity of divalent metals?

2. **Free electron energies in reduced zone.** Consider the free electron energy bands of an fcc crystal lattice in the approximation of an empty lattice, but in the reduced zone scheme in which all k 's are transformed to lie in the first Brillouin zone. Plot roughly in the [111] direction the energies of all bands up to six times the lowest band energy at the zone boundary at $k = (2\pi/a)(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Let this be the unit of energy. This problem shows why band edges need not necessarily be at the zone center. Several of the degeneracies (band crossings) will be removed when account is taken of the crystal potential.
3. **Kronig-Penney model.** (a) For the delta-function potential and with $P \ll 1$, find at $k = 0$ the energy of the lowest energy band. (b) For the same problem find the band gap at $k = \pi/a$.
4. **Potential energy in the diamond structure.** (a) Show that for the diamond structure the Fourier component U_G of the crystal potential seen by an electron is equal to zero for $G = 2A$, where A is a basis vector in the reciprocal lattice referred to the conventional cubic cell. (b) Show that in the usual first-order approximation to the solutions of the wave equation in a periodic lattice the energy gap vanishes at the zone boundary plane normal to the end of the vector A .

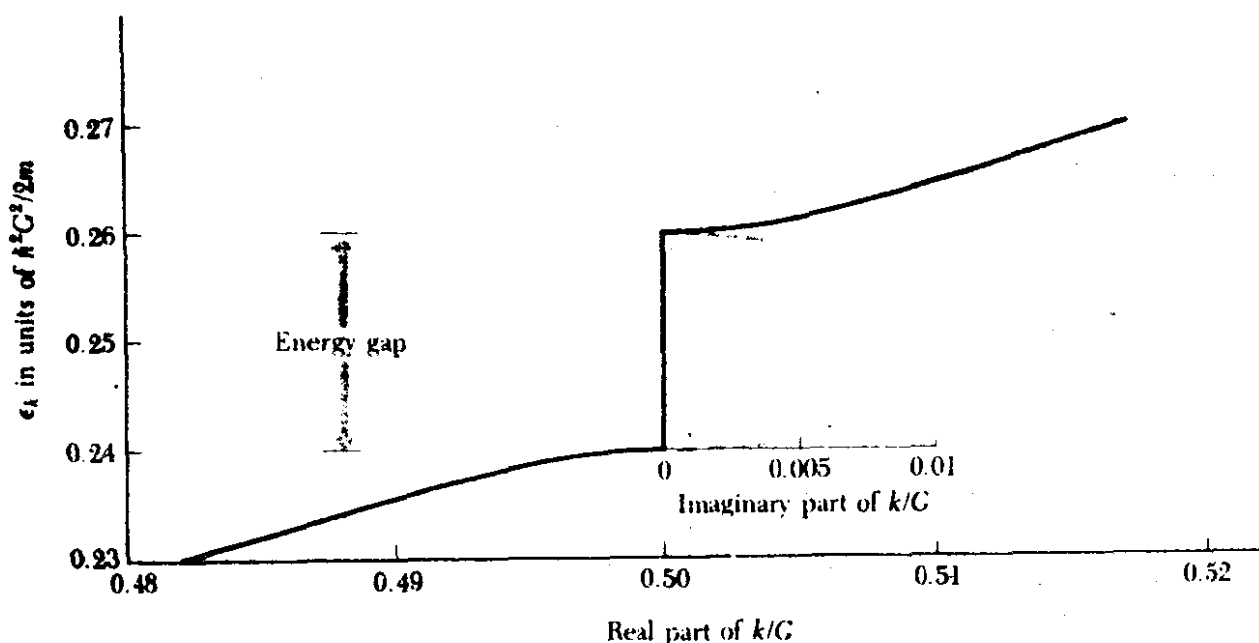


Figure 12 In the energy gap there exist solutions of the wave equation for complex values of the wavevector. At the boundary of the first zone the real part of the wavevector is $\frac{1}{2}G$. The imaginary part of k in the gap is plotted in the approximation of two plane waves, for $U = 0.01 \hbar^2 G^2 / 2m$. In an infinite unbounded crystal the wavevector must be real, or else the amplitude will increase without limit. But on a surface or at a junction there can exist solutions with complex wavevector.