Problems and exams of the Course

Electrons in Crystals

Università di Trieste

The problems here belong to three distinct classes

(i) problems given to the students for the final exam or for an intermediate exam are denoted with a * in the list;

(ii) Problem solved during tutorials;

(iii) Longer problems for homework.

A typical exam requires solving two problems in three hours
The student should give all the details of calculation, as well as motivating the route chosen to solve the problem.
Problems (questions in a problem) for which only the final results is given are normally not counted in establishing the score.
Numerical evaluations should be given with 3 significant figures if not otherwise indicated.
Other exercises may be found on the N. Ashcroft e N. D. Mermin, Solid State Physics, Saunders-College (1976) [AM] and on the C. Kittel, Introduction to Solid State Physics, Wiley (1996).
Here we give a list of problems from AM: : Chap. **1**, n. 5; **2**, 1; **4**, 6; **8**, 1 and 2; **10**, 1, 2 and 3; **12**, 1, 2, 6 and 7; **13**, 1; **16**, 2 and 3.
Another book with problems is L. Mihály e M. C. Martin, Solid State Physics: Problems and Solutions (Wiley, 1996).

Contents

1 * Crystalline organic conductor

A crystalline organic conductor has a plasma frequency $\omega_p = 2.50 \times 10^{15} s^{-1}$ and a relaxation time $\tau = 5.03 \times 10^{-15}$, at room temperature.

1. Calculate the static electric conductivity σ of this conductor using the data given above. Use c.g.s. units.
2. Express σ in MKSA, that is in (ohm cm)$^{-1}$.
Note that : One may use: 1 Volt = 1/300 statvolt (cgs potential unit) and 1 Ampere = $3{\times}10^9$ statampere (cgs current unit).
3. Assuming that transport is due to one kind of carrier (electrons),with density $n = 7.5 \times 10^{20} cm^{-3}$, obtain the effective mass m^* of the carriers (i) in grams and (ii) in units of the electron mass.
4. Calculate the r_s parameter for the carriers, using the definition $1/n = 4\pi r_s^3 a_0^3/3$.
5. Calculate the Fermi energy of the carriers in eV.
6. Calculate the Fermi temperature.
7. Calculate the specific heat of these carriers treated as free electrons with mass m^*, assuming that $T \ll T_F$). Give C_v in $calorie/(mole\ ^oK)$. Is the assumption $T \ll T_F$ corrects?

2 * Surface plasmon

Consider an homogeneous metal occupying the region $z > 0$, with the remaining half space $z < 0$ being vacuum. Use Drude formula for the dielectric function of the metal $\varepsilon(\omega)$, any spacial dependence being neglected.
Consider density waves in the metal with no volume charge density, $\rho(z) = 0$, $z > 0$. They will satisfy Poisson equation

$$\nabla^2 V(\mathbf{r}) = 0 \tag{1}$$

both for $z > 0$ and for $z < 0$. Use the notation $\mathbf{s} \equiv (x, y)$, so that $\mathbf{r} = (\mathbf{s}, z)$.

1. Consider, for $z > 0$, $V(\mathbf{r}) = V_0 e^{-\kappa z} cos(\mathbf{Q} \cdot \mathbf{s})$. Find which is the relation that there must be between $\mathbf{Q}$ and κ in order to satisfy Eq. 1.
2. Calculate the electric field for the potential above.
3. Consider, for $z < 0$, $V'(\mathbf{r}) = V_0' e^{\kappa' z} cos(\mathbf{Q}' \cdot \mathbf{s})$. Again, what is t he relation between $\mathbf{Q}$ and κ in order to satisfy Eq. 1.
4. Calculate the electric field for the potential above.
5. Using the continuity of the parallel electric field $\mathbf{E}_p \equiv (E_x, E_y, 0)$ at $z = 0$, obtain the relation between V_0 and V_0' and between κ e κ'.
6. Using the continuity of the transverse displacement $\mathbf{D}_t \equiv (0, 0, D_z)$ a $z = 0$, obtain a condition on the frequency ω of the waves.
7. For rare collisions, that is $\omega\tau \gg 1$, obtain an explicit expression of the propagation frequency of the waves in terms of the electron average density n, their mass m and charge e.
8. Compute the frequency for aluminum at room conditions.

3 * Plasmon in a *jellium* sphere at the density of Sr

Let us consider a *jellium* sphere, that is (i) a sphere of radius R centered at the origin with a uniform positive charge density [the *background*] and (ii) N electrons moving in the electric potential of the background. The system is globally uncharged (electrically neutral) and the electrons are distributed with a uniform density on a sphere of radius R which at rest is also centered at the origin.
Describe the oscillatory motion [*plasmon*] corresponding to small rigid displacements of the electronic sphere with respect to the background sphere, that is of its center with respect to the origin.

1. Give the charge density of the background, using the parameters and informations given above, and denoting the absolute value of the electron charge with e.

2. Using Gauss theorem, calculate the electric field due to the background both inside and outside the background sphere.

3. Using the result of the previous point give the electric field due to the electronic sphere inside it, when centered in $\mathbf{d}$.

4. Calculate the force on a test charge internal to both spheres, when the electronic sphere is centered in $\mathbf{d}$ and $d < 2R$.

5. Consider now $d \ll R$ and neglect the role of the electrons which fall outside of the background sphere. Using the answer to the previous point give the force on an electron internal to both sphere when the displacement of the electronic sphere is $\mathbf{d}$ e write down its equation of motion.

6. Solve the equation above and evaluate (numerically) the frequency of oscillation (plasmon frequency) for $R = 5$ Å and $N = 125$.

7. Can the above mode be excited by light any of the following ranges: infrared, visible, ultraviolet.[Optional question].

4 One-dimensional electron gas

Consider a system of N noninteracting point fermions moving in 1D in [0,L]. Let's study the problem with each of the following boundary conditions:

(a) Born — von Karman (also know as PBC): $\psi(x+L) = \psi(x)$

(b) Hard wall $\psi(L) = \psi(0) = 0$.

In each of cases (a) and (b):

1. Give eigenfunctions and eigenvalues.
2. Calculate the one body density $n(x)$ giving also a qualitative plot and discussing what happens in the thermodynamic limit ($N,\ L \longrightarrow \infty$; $N/L = n$).
3. Calculate the Fermi energy $E_F(N, L)$ and its behavior in the thermodynamic limit.
4. Calculate the total energy $E_{tot}(N, L)$. Discuss whether it is possible to break it in a *volume* term
$$E_V(N, L) = N\mathcal{E}_V\left(\frac{N}{L}\right)$$
and a *surface* term
$$E_S(N, L) = \mathcal{E}_S\left(\frac{N}{L}\right),$$
plus terms that vanish in the thermodynamic limit. Check if there is a relation between the total energy and the Fermi energy.

Suggestion

1. It might be useful to remember:
$$\sum_{n=1}^{m} n^2 = \frac{1}{6}m(m+1)(2m+1)$$
$$\sum_{n=1}^{m} a^n = \frac{a - a^{m+1}}{1-a}$$
2. and the definition of the Bessel function:
$$j_0(x) = \frac{\sin x}{x}.$$

5 Boundary conditions and thermodynamic limit

Let's consider N free noninteracting electrons in one dimension and moving on $0 \leq x \leq L$. The average particle density is $n = N/L$. In the following for simplicity we assume $N = 4M + 2$, with M a positive integer.

1. First, obtain the one particle orbitals $\phi_k(x)$ with periodic boundary conditions $\phi_k(x + L) = \phi_k(x)$. Calculate the allowed k's, then considering that for each k there are two possible spin projections calculate:

   - the occupied k's;
   - the energy per particle [use the identities below].
   - Discuss what is the relation between the result of the previous point [for N electrons on the segment L] and that for a system in the thermodynamic limit [i.e., $N \to \infty$ ed $L \to \infty$ with $N/L = n$=constant].

2. Solve now the problem at (1) with the boundary conditions $\phi_k(x+L) = e^{i2\pi\alpha}\phi_k(x)$, just for the allowed k's and the occupied k's.

   - Consider [without attempting a direct calculation – f is generic] the average value of $f(k)$ over the occupied k's,

     $$\langle f \rangle = \frac{1}{N} \sum_{k,occup.} f(k).$$

     This quantity depends on α since the allowed k 's do. Thus, $\langle f \rangle = g(\alpha)$.
   - Show that $\overline{g}$, the average of $g(\alpha)$ over α,

     $$\overline{g} = \int_{-1/2}^{1/2} d\alpha \; g(\alpha),$$

     with N finite, coincides with $\langle f \rangle$ in the thermodynamic limit and $n = N/L$. This is true for any f, not only for the energy. [It is suggested to exploit the fact that the the integral over α of the k-sum is a sum of integrals that covers the interval .....]
   - To be able to obtain the result above it is necessary to be able to write $\langle f \rangle$ in the thermodynamic limit as an integral.

In this simple case, the average on the boundary conditions for N and L finite provides a result equivalent to the one for a system in the thermodynamic limit and at density $n = N/L$!

6 He^3 film.

An He^3 film is a system in which helium atoms (1/2 spin Fermions) move in a two dimensional word (on a plane). Assume to be close to zero temperature. The areal density is $\rho = 2.24 \times 10^{-9} g/cm^2$ and set the atomic mass of helium to 3.

1. Evaluate the areal density n in $atoms/cm^2$ for the above film.
2. Calculate r_s, the radius (in units of Bohr radii) of the disk that contains one atom in average, as function of n. Estimate r_s.
3. Calculate the radius k_F of Fermi disk, in terms of n and then express it as function of r_s.
4. Calculate the Fermi energy ϵ_F in terms of r_s, in Ry.
5. Evaluate Fermi energy for the present film in eV.
6. Evaluate Fermi temperature in ^{o}K.

7 * Simple Metal

A metal has a specific heat of 1879 erg $\text{cm}^{-3}\text{K}^{-1}$ at T=3 K. Describe the metal as an electron gas.

1. Calculate the electronic density n in cm^{-3}.
2. Calculate the Fermi energy in eV.
3. Calculate ω_P in s^{-1}.
4. Is it larger the Fermi energy or the plasmon energy $\hbar\omega_p$?
5. A T=77 K, $\omega_p\tau = 1644$. What is the value of the real part of the dielectric function (order of magnitude).
6. At the same temperature, what is the order of magnitude of the imaginary part of the dielectric function.

8 * Hexagonal lattice

Consider the honeycomb lattice (a collection of hexagonal tiles) with the lattice points at the vertexes of the hexagons. One of the hexagon sides is parallel to the y axis. The lower and upper vertexes of such a side are occupied respectively by atoms of type A and B.

1. The lattice is a Bravais with a basis: what is the Bravais? Give a pair of primitive vectors Bravais ($\mathbf{a}_1$ ed $\mathbf{a}_2$) for such a Bravais.

2. Give the basis vectors ($\mathbf{b}_1$ ed $\mathbf{b}_2$).

3. Say what is the reciprocal lattice of this Bravais and its primitive vectors ($\mathbf{g}_1$ ed $\mathbf{g}_2$).

4. Calculate the geometrical form factor at the generic vector of the reciprocal lattice $\mathbf{G} = n_1\mathbf{g}_1 + n_2\mathbf{g}_2$, when f_A and f_B (real numbers) are the atomic form factors, which here are independent from the wave vector [we are thinking of neutron diffraction].

5. For which $\mathbf{G}$ the geometrical form factor $F(\mathbf{G})$ is real, regardless of the value of the ratio $\alpha = f_A/f_B$?

6. If $f_B = -f_A$, are there $\mathbf{G}$'s for which $F(\mathbf{G}) = 0$? If so say which ones and show them in a sketch if the reciprocal lattice.

9 * Square lattice with a basis

Consider a square lattice with side (of the square) a, and basis $\vec{0}$, $\vec{d} = a(1/2, 1/2)$. The basis locations are occupied by atoms with potential $\phi_1(r)$ and $\phi_2(r)$.

1. Write the crystalline potential $U(\mathbf{r})$ as a lattice sum.
2. Write $U(\mathbf{r})$ in terms of its Fourier components.
3. Set $\phi_1(q) = [\alpha(q) + \beta(q)]/2$ and $\phi_2(q) = [\alpha(q) - \beta(q)]/2$ and express the Fourier components of $U(\mathbf{r})$ in terms of α and β.
4. What are the simplifications that arise from the assumption above for the Fourier components $U_{\mathbf{G}}$ of the potential. How many subsets of $\{\mathbf{G}\}$ is possible to distinguish?
5. If $\alpha = 0$, in reciprocal space the potential has the symmetry of which lattice? With which lattice parameter and which axes.
6. As above but for $\beta = 0$.
7. Write the scattering amplitude of such a lattice setting for the atomic form factors of the two kinds of atom $f_1(q) = [\gamma(q) + \delta(q)]/2$ and $f_2(q) = [\gamma(q) - \delta(q)]/2$. If $\gamma = 0$, which operations (rotations and translations and in which order) bring the reciprocal lattice to a known Bravais?

10 * Electrons in 2 dimensions

Consider electrons in 2D in a potential

$$U(\mathbf{r}) = -2U\left\{\cos[gx] + 2\cos\left[\frac{gx}{2}\right]\cos\left[\frac{\sqrt{3}}{2}gy\right]\right\},$$

con $U > 0$.

1. Write $U(\mathbf{r})$ in terms of its Fourier components. How many are the non vanishing components and at which wavevectors $\mathbf{G}$? Give the value of such $U_{\mathbf{G}}$?
2. Give a basis for this Bravais. Sketch both the Bravais and its reciprocal lattice.
3. What's the value of the potential at (i) the origin, (ii) midway between the origin and a first neighbor, (iii) at any of the farthest points from the origin within the Wigner-Seitz cell.
4. Assume that there are two electrons in the primitive cell and that the electrons are independent. For $U = 0$ (free electrons) express k_F and the energy per electron ϵ_{el} in terms of g.
5. Again for $U = 0$, build up the ground sate *occupying* the wavevectors in the first Brillouin zone, rather than inside the Fermi disk. Express the energy per electrons ϵ_{rv} in terms of g.
[Use symmetry to express the energy as a sum over 1/12 of the FBZ (for instance in the irreducible corner $0 < \phi < \pi/6$).]
6. What are the ratios (i) $k_F/(g/2)$ e (ii) $\epsilon_{el}/\epsilon_{rv}$?
7. If $g = 7.25\text{Å}^{-1}$, what is (in Å) the lattice parameter of the Bravais?
8. And the value of ϵ_{el} in Ry?

11 * Band filling in a 2D square lattice.

Consider Schrödinger's single particle equation for an electron moving on a plane under in a potential

$$U(x,y) = -2U\left[cos\left(\frac{2\pi}{a}x\right) + cos\left(\frac{2\pi}{a}y\right)\right].$$

1. First say where are minima and maxima of $U(x,y)$. Give a sketch of Bravais formed by all the minima (maxima).
2. Which are the non vanishing $U_{\mathbf{G}}$ and their value? (*Hint:*: write trigonometric functions in terms of exponentials).
3. Sketch the First Brillouin Zone(FBZ).
4. Assume U "small" and calculate with first order perturbation theory the change in the plane waves (energies) at the corners of the FBZ, $k = (\pi/a)(\pm 1, \pm 1)$. Define as belonging to first band the solution with the lowest energy.
5. Repeat the calculation for the points at the center of the sides of the FBZ. The two solution found for the energy give give the first two bands at these points.
6. What is the condition under which the second band at the side center becomes lower in energy than the first band at the corner of the FBZ?
7. In a system with 2 electrons in the primitive cell and when the condition found immediately above is fulfilled, how many bands are occupied? Would you be able to sketch the Fermi surface in the FBZ when $U \to 0$?

Equivalent exercise: change the potential into

$$U(x,y) = -2U\left[cos\left(\frac{2\pi}{a}x\right) cos\left(\frac{2\pi}{a}y\right)\right].$$

N.B. For the alternative choice of the potential the coordinates of the corners will need to be changed from those of the first choice.

12 * 1D Tight binding

Consider electrons moving in 1D. First tackle the problem of an electron in the potential $V(x) = -e^2 U\delta(x/a_B)$, $(U > 0)$, with e e a_B the electron charge and the Bohr radius.

1. What are the units of U?
2. Write Schrödinger's equation for the electron in the potential above in atomic unit ($e = \hbar = m = 1$), which you will use throughout the exercise.
3. Find the normalized wavefunction of the bound state exploiting (i) the continuity of the wavefunction and (ii) the know discontinuity of its first derivative at $x = 0$. Are there any other bound states, in addition to the one that you found?
4. Consider now a 1D Bravais with a periodic potential $v(x) = -U \sum_n \delta(x - n)$ and treat it by tight binding. Using the textbook definitions for a system with a 1S orbital calculate the shift β as functions of U.
5. calculate the $\alpha(n)$ as function of U.
6. Calculate the so-called transfer integral $\gamma(n)$, as function of U.
7. Calculate the effective mass at the band minimum.

13 * Tight binding in a triangular lattice

Consider a triangular lattice with an atom per site with only an s orbital and treat the problem within the *tight binding* approximation. Neglect overlap and assume that only first neighbors are important so that only β e the first transfer γ need be considered, $\beta, \gamma > 0$ following the convention in AM. The orbital unperturbed energy is $-\epsilon_0$, with $\epsilon_0 > 0$.
Use as real space basis $\mathbf{a}_1 = a(1,0)$, $\mathbf{a}_2 = a(1/2, \sqrt{3}/2)$ and as reciprocal lattice basis $\mathbf{g}_1 = (4\pi/\sqrt{3}a)(\sqrt{3}/2, -1/2)$ and $\mathbf{g}_2 = (4\pi/\sqrt{3}a)(0,1)$

1. Sketch the First Brillouin Zone (FBZ). Use the notation $\Gamma = (0,0)$, $A = (4\pi/3a, 0)$, $B = (0, 2\pi/\sqrt{3}a)$
2. Calculate the energy dispersion $\epsilon(\mathbf{k})$ of the tight binding energy band and express functions in such a way that only real functions appear.
3. Sketch the band energy along the segment in k-space $\overline{\Gamma A}$, specifying the value of the energy at Γ and at A and respecting the qualitative features of the dispersion at these points.
4. As above but along $\overline{\Gamma B}$.
5. Calculate the elements of the inverse mass tensor at any of the points above where it makes sense.
6. What are the values of the off-diagonal elements of the mass tensor at the points found in 5)?
7. Say at which of the points found at 5) is found the heaviest effective mass.

14 * Orbits of Bloch electrons in a magnetic field

Consider a solid in the simple cubic structure, with a single 1s orbital per site, that has a tight binding band $\epsilon(\mathbf{q}) = -2\gamma[cos(q_x a)+cos(q_y a)+cos(q_z a)]$, with a the lattice parameter and suitably chosen zero of energy. A uniform static magnetic filed $\mathbf{H} = H\hat{z}$ is present.

1. Write the Bloch electron velocity in the plane (x,y).
2. Write the condition satisfied by an orbit (in $\mathbf{q}$ space) for $q_z = 0$ and energy E, $\epsilon(\mathbf{q}) = E$.
3. What's the orbit when $E = -2\gamma[3 - \delta^2/2]$ and $\delta \ll 1$?
4. Give an expression for the period of the orbit when $\gamma a^2 = \hbar^2/2m^*$?
5. Consider now the case $E = -2\gamma$ and due to the symmetry of the problem restrict your attention to the region satisfying ($q_x \geq 0$, $q_y \geq 0$). Obtain in this region the relation between q_x and q_y on the orbit and sketch it in the First Brillouin Zone (FBZ).
6. Indicate the direction of motion along the orbit.
7. Rewrite the velocity in the (x,y) plane calculated at 1) in terms of q_x, only exploiting the previous results.
8. Use the previous answer to integrate $q_x(t)$ on one quarter of the orbit to get $T/4$, with T the period of the orbit. [*Note:* $\int dx/sin(x) = ln(tan(x/2))$]. Whats the value of T?

Alternative choice : Choose the zero of energy in such a way that the minimum of the band is -12γ.

1. Write the Bloch electron velocity in the plane (y,z).
2. Write the condition satisfied by an orbit (in $\mathbf{q}$ space) for $q_z = 0$ and energy E, $\epsilon(\mathbf{q}) = E$.
3. What's the orbit when $E = -4\gamma[3 - \delta^2/4]$ and $\delta \ll 1$?
4. What's the orbit period in terms of the quantities given so far?
5. What should be γ, in eV, in order to have the same period as for a free electron?
6. What the equation of the orbit when $q_z = 2\pi/a$ and $E = -4\gamma[-1 + \delta^2]$, with $\delta \ll 1$.
7. What's the point of the orbit closest to the origin of the last orbit considered?
8. Are you able to sketch qualitatively the orbit on the face of the FBZ containing the orbit?

15 * Properties of an anisotropic metal.

Consider a metal, with one valence electron per primitive cell, with a band:

$$\varepsilon(\mathbf{k}) = \varepsilon_0 + \frac{\hbar^2}{2}\left(\frac{k_x^2 + k_y^2}{m_t} + \frac{k_z^2}{m_l}\right).$$

1. Calculate the effective mass tensor $\mathbf{M}$.
2. Calculate the energy density of states $g(\varepsilon)$.
3. Denoting the electronic number density, in cm^{-3}, with n, calculate the Fermi energy density of states.
4. If $n = 10^{22} cm^{-3}$ and $m_l = 2m_e = 4m_t$, evaluate (i) the Fermi energy in ^{o}K and (ii) the density of states at the Fermi energy in $cm^{-3}eV^{-1}$.

Apply a magnetic field $\mathbf{H} = H(\sin\theta, 0, \cos\theta)$ to such a solid.

5. Write and solve the semi classical equation s of motion for Bloch electrons.
6. Give the expression of the cyclotron effective mass m_c^* that one can obtain from **5)** above, imposing that the period has the same form as for free electrons with m_c^* replacing m_e.

Consider now $\theta = 0$.

7. For such choice of θ give the $\mathbf{k}$-space orbits,exploiting the energy conservation and verifying that the results that you obtain is equivalent to the one at **5**.
8. Verify that the value of m_c^* found at **6** equals $\frac{\hbar^2}{2\pi}\frac{\partial A}{\partial \varepsilon}$, where A is the area enclosed in the orbit.

16 * Hall effect for an e-h system

Consider a conductor with electron density n and home density p in an electric field $\mathbf{E} = (E_x, 0, 0)$ and a magnetic filed $\mathbf{H} = (0, 0, H)$, in a Hall geometry. Holes and electrons have masses m_e e m_b and collision times τ_e e τ_b. Let us set $b = (\tau_e/m_e)/(\tau_b/m_b)$.

1. Write the evolution equation of the average electron and hole momenta at stationarity, for each Cartesian component.
2. As we have an open circuit along y, $j_y = j_y^{(e)} + j_y^{(b)} = 0$. Use this condition to obtain two equations that contain only $j_x^{(e)}$ and $j_x^{(b)}$.
3. Derive a relation between $j_x^{(e)}$ and $j_x^{(b)}$ when $n = p$.
4. Calculate the Hall coefficient $E_y/(j_x H)$ when $n = p$.
5. What's the value of E_y when the mobilities of electrons and hole are equal, ($\mu = e\tau/m$), and e $n = p$?

17 * Conductivity tensor in a metal

Consider the expression for the conductivity tensor in the relaxation time approximation

$$\sigma_{ij} = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \tau(\epsilon(\mathbf{k})) \left[\frac{-\partial g^o}{\partial \epsilon(\mathbf{k})}\right] v_i(\mathbf{k}) v_j(\mathbf{k})$$

for a metal. Assume that there is only one band crossed by the Fermi surface.

1. Assume $T_F \gg T$ (and that the Fermi energy is far from the band extrema). Take the τ out of the integration on the basis that it is dependent on the energy. Say why you can do it.
2. Exploiting the fact that the velocity is the gradient of the energy rewrite 'Eq. 1 so as to display the $\mathbf{k}$ gradient of $g^o(\epsilon(\mathbf{k}))$.
3. Integrate by part the previous expression, taking into account the fact that all the function appearing in the integral are periodic and that the integral is over the whole Brillouin zone.
4. Rearrange the previous expression in such a way that the inverse mass tensor $\left[\frac{1}{m(\mathbf{k})}\right]_{ij}$ appears.
5. Assuming that you are close to an extremum and that $m_{ij}(\mathbf{k}) = m_{ij}$ is independent from $\mathbf{k}$ over the integration region, calculate the integral to obtain σ_{ij} in terms of n (the carrier density in the band), τ, and the mass tensor.
6. If the mass tensor is diagonal, $m_{ij} = \delta_{ij} m^*$, what is the form of the conductivity tensor?
7. Utilizing the expression obtained in 4) and the fact that the mass tensor is the gradient of a function periodic in $\mathbf{k}$ rewrite the conductivity in terms of the holes rather that electrons.