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 = 3×10^9 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 $R = 5\mathring{A}$ 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

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

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 * Proprieties 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.

18 * Linear chain of H atoms: s and p bands within the "tight-binding" approximation

Consider a linear chain of equispaced H atoms along the z axis: $\mathbf{R}_n = (0,0,z_n) = (0,0,na)$, n=0, ±1, ±2, ... Our aim is to study the bands deriving from the first degenerate excited states, that is $2s$ and $2p$. It is convenient to consider p_x, p_y, and p_z (rather than $p_{0,\pm1}$), so that they can be written as $\psi_{2p_x} = x\phi_p(r)$, $\psi_{2p_y} = y\phi_p(r)$, and $\psi_{2p_z} = z\phi_p(r)$ respectively. In the "tight-binding" method the energies of the 4 bands coming from these states are given by (neglecting all overlap integrals):

$$|(\mathcal{E}(k) - E_0)\delta_{ij} + \beta_{ij} + \widetilde{\gamma}_{ij}(k)| = 0$$

where E_0 is the energy of the atomic $2s$ and $2p$ levels, and:

$$\begin{aligned}
\widetilde{\gamma}_{ij}(k) &= \sum_n e^{\imath k z_n}\gamma_{ij}(z_n) \approx \gamma_{ij}(a)e^{\imath ka} + \gamma_{ij}(-a)e^{-\imath ka} \qquad (first-neighbourapprox.)\\
\gamma_{ij}(z_n) &= -\int d\mathbf{r}\ \psi_i(\mathbf{r})\psi_j(\mathbf{r}-\mathbf{R}_n)\Delta U(\mathbf{r}) \qquad (``hopping''integral)\\
\beta_{ij} &= \gamma_{ij}(0)
\end{aligned}$$

and the indexes i, j run over the 4 atomic basis orbitals.

1. Write the expression of the function $\Delta U(\mathbf{r})$ (apply the independent electron approximation, and consider the crystal potential as due only to the pointlike nuclei). Discuss the symmetry of $\Delta U(\mathbf{r})$, and show that the expansion of $\Delta U(\mathbf{r})$ around the origin and up to third-order terms included is given by

$$\Delta U(\mathbf{r}) \approx c_0 + c_1(x^2+y^2) + c_2 z^2.$$

2. Show that the matrix β_{ij} is diagonal, determine how many and which are its independent entries. (*N.B.: the explicit calculation of the integral is not required).*
3. Show that also the hopping integrals $\gamma_{ij}(\mathbf{R})$ and $\gamma_{ij}(-\mathbf{R})$ can be expressed in terms of a few independent entries, that in the tight-binding jargon are called: $\langle ss\sigma\rangle = \gamma_{ss}(a)$, $\langle sp\sigma\rangle = \gamma_{sp_z}(a)$, $\langle pp\sigma\rangle = \gamma_{p_zp_z}(a)$, $\langle pp\pi\rangle = \gamma_{p_xp_x}(a)$. (*N.B.: again, explicit calculation of integrals is not required*)
4. Show that the matrix $\widetilde{\gamma}_{ij}$ is block-diagonal, write how many and which are the independent entries, and write them down explicitly as a function of the above mentioned $\langle ss\sigma\rangle$, $\langle sp\sigma\rangle$, $\langle pp\sigma\rangle$, and $\langle pp\pi\rangle$.
5. Write down explicitly the equation that determines the band dispersion, and discuss its solutions, pointing out their degeneration, provided there is. Draw a qualitative plot in the first Brillouin zone. Which parameters determine the band *amplitude?*
6. What would change, within the same approximations, if we had helium atoms instead of hydrogen?

19 Density-density response function for a gas of non-interacting electrons

Consider a set of N non-interacting electrons in a volume $V = L^d$ in d-dimensions, with periodic boundary conditions (PBC). Applying an external potential $U(\mathbf{r}) = \int \frac{d\mathbf{q}}{(2\pi)^d} U(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}$ the electron density changes from $n(\mathbf{r}) = n_0 \equiv \frac{N}{V}$ to $n(\mathbf{r}) = n_0 + n_1(\mathbf{r}) + \cdots$, n_1 being linear in U.

1. Compute the density-density linear response function $\chi(q)$, which links the Fourier transform of the first-order density change $n_1(\mathbf{r})$ to the Fourier components of U,

$$n_1(\mathbf{q}) = \chi(q) U(\mathbf{q}).$$

   To this end, proceed as suggested below:

   (a) Use (static) perturbation theory to compute the first-order change $\psi^1_{\mathbf{k}}(\mathbf{r})$ of the non-interacting electrons

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi^0_{\mathbf{k}}(\mathbf{r}) + \psi^1_{\mathbf{k}}(\mathbf{r}) + \cdots.$$

   By definition $\psi^1_{\mathbf{k}}(\mathbf{r})$ is linear in U.

   (b) Compute the density change $n_1(\mathbf{r})$ induced by the potential U using

$$n(\mathbf{r}) = \sum_{\mathbf{k}} f_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})^2 = n_0 + n_1(\mathbf{r}) + \cdots,$$

   $f_{\mathbf{k}}$ being the occupation number of the orbital $\mathbf{k}$.

   (c) Compute the Fourier transform of $n_1(\mathbf{r})$, obtained at the previous point and obtain from it

$$\begin{aligned} \chi(q) &= V^{-1} \sum_{\mathbf{k}} f_{\mathbf{k}} \left(\frac{1}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}} + \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}}\right) \\ &= V^{-1} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}/2} - f_{\mathbf{k}+\mathbf{q}/2}}{\epsilon_{\mathbf{k}-\mathbf{q}/2} - \epsilon_{\mathbf{k}+\mathbf{q}/2}}. \end{aligned} \tag{2}$$

   (d) In doing all the algebraic manipulations in the previous points do bear in mind that $\psi^0_{\mathbf{k}} = \frac{1}{\sqrt{V}} e^{i\mathbf{q}\cdot\mathbf{r}}$. $\epsilon_{\mathbf{k}}$ is the energy of the orbital $\psi^0_{\mathbf{k}}$.

2. Specialize the treatment at the case $d = 2$ and compute explicitly $\chi(q)$ for unpolarized electrons ($f_{\mathbf{k}} = 2$ for $k \leq k_F$) [Stern function] proceeding as follows:

   (a) Use the relation 2 and rewrite the sum over the discrete $\mathbf{k}$ compatible with the PBC as an integral in polar coordinates.

   (b) First compute the angular integral.

   (c) Then compute the radial integral [i.e., the integral in k].

   (d) You should obtain:

$$\begin{aligned} \chi(q) &= -\frac{m}{\pi\hbar^2}, \qquad q < 2q_F \\ \chi(q) &= -\frac{m}{\pi\hbar^2}[1 - \sqrt{1 - 4q_F^2/q^2}], \quad q > 2q_F \end{aligned}$$

Note: you need to be able to integrate the functions $\int dt/(1+t^2)$ and $\int dt/(1-t^2)$.

20 * Peierls instability.

Consider a 1D non-interacting electron gas. The definition of the (density-density) static response function in Fourier transform space is

$$\chi_0(q) = \frac{2}{L}\sum_k \left[\frac{f(k-q/2)-f(k+q/2)}{\varepsilon(k-q/2)-\varepsilon(k+q/2)}\right],$$

$\varepsilon(k)$ being the energy level of the non-interacting electrons, and $f(k) = \theta(k_F - |k|)$ the Fermi functions at $T = 0$.

1. Compute $\chi_0(q)$ starting from the above formula, writing down all relevant passages.
2. Draw a semi-quantitative plot of $\chi_0(q)$ as a function of $Q = q/k_F$, $Q \geq 0$. Comment on the shape of the plot for $Q \leq 0$, without drawing it.
3. The density response to an external energy field V is given by $\rho(q) = \chi_0(q)V(q)$. What do you expect it happens if one applies an arbitrarily small field with $V(2k_F) \neq 0$? What will be the periodicity of the perturbed system? (Remember that in 1D $k_F = \pi n_0/2$, $n_0 = N/L$.)
4. The kinetic energy per electron of an homogeneous electron gas in 1D is $t(n_0) = Cn_0^2$, $C = (\hbar^2\pi^2)/(24m)$. Write down $E^{LDA}[n]$, the total energy functional in the Local Density Approximation (LDA) for an inhomogeneous system.
5. Using the following alternative definition for the response function of a homogeneous 1D fluid:
$$\chi_0^{-1}(x,y) = -\left[\frac{\delta^2 E[n]}{\delta n(x)\delta n(y)}\right]_{n(x)=n_0},$$
where χ_0^{-1} is such that
$$\int dz\ \chi_0(x,z)\chi_0^{-1}(z,y) = \delta(x,y),$$
compute the LDA response function in k-space.
6. Compare the result of the previous point with that of the first, on the plot done at point 2, and identify in which limit the two results coincide and why.

Note: Remember that in a translationally invariant system $\chi_0(x,y) = \chi_0(x-y)$.

21 1D chain of rare-gas atoms

Consider a linear chain of Krypton atoms and assume that they interact with a pair force of the Lennard-Jones form $\phi(|x|) = 4\epsilon[(\sigma/x)^{12} - (\sigma/x)^6]$.

1. Write the potential energy per particle $u(a)$ when the particles lie regularly at a spacing of a, i.e. when $x_n = na$. Compute: (i) the equilibrium distance a_0 as a function of σ and (ii) the cohesive energy as a function of ϵ.

2. Compute the phonon dispersion relation [i.e. $\omega(q)$ as a function of q], under the hypothesis that interactions beyond first-neighbours can be neglected. Express explicitly the dispersion law as a function of ϵ, σ, M, where M is the mas of the rare gas atom.

   All the atoms have zero speed at $t = 0$. In symbols, if $u(n,t)$ is the displacement at time t of the n-th atom from the equilibrium position na_0, we are using the initial conditions

$$u(n,0) = l\delta_{n,0},$$
$$\dot{u}(n,0) = 0, \forall n.$$

   A. Compute the time evolution of the chain at $t > 0$.
   B. Compute at which time $t_1 > 0$ [in seconds] the 0-th atoms is to be found again in its equilibrium position [$u(0,t_1) = 0$].
   C. Compute the speed [in cm/s] which the 0-th atom has when it goes through the equilibrium position at $t = t_1$.

Hints:

- The parameters for the Lennard-Jones potential for the rare gases can be found on Ashcroft-Mermin [AS].

- Numerical values of the Riemann zeta functions [$\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$] can be found, for instance, in the book [HMF]:*Handbook of Mathematical Functions*, Edited by M. Abramowitz and I. A. Stegun (Dover, New York).

- Remember that the phonons are the normal modes of oscillation of the chain, in the harmonic approximation. Hence any displacement of the atoms from the equilibrium position [provided it is sufficiently small that the harmonic approximation still holds] can be analyzed in terms of phonons. One has then to find the linear combination of normal oscillations that satisfies the conditions listed in (1).

- Remember the identity $\sum_q exp(iqna_0) = N\delta_{n,0}$ where the sum over q is on the 1st BZ and one considers a chain of N atoms with periodic boundary conditions.

- Remember the definition of Bessel Function

$$J_n(z) = \frac{1}{\pi}\int_0^{\pi} dx\ cos(nx - zsinx).$$

  Zeros and other properties of the Bessel Functions can be found in the HMF book above mentioned, or in other specific books.

22 * Stability of monatomic crystals at $T > 0$

Consider a harmonic crystal with one atom per cell, in D dimensions (we are clearly interested especially in $D = 1, 2, 3$.)

1. Show that the phonon density of states at low frequencies ($\omega_s(\mathbf{k}) = c_s(\hat{\mathbf{k}})k$ per $\omega < \omega_c$) has an $g(\omega) = A\omega^{D-1}$ behaviour.
[To be more precise one should find $A = [D\Omega_D]/[(2\pi)^D c^D]$, with Ω_D the *solid angle* in D dimensions and c a suitable average over angles and polarizations of a function of $c_s(\hat{\mathbf{k}})$: which one?]
2. Consider now the square mean displacement of the atoms from the equilibrium position, defined as

$$\overline{\mathbf{u}^2} = \frac{1}{N}\sum_{\mathbf{R}}\langle \mathbf{u}^2(\mathbf{R})\rangle,$$

with $\langle \ldots \rangle$ the average at a given temperature. Express $\overline{\mathbf{u}^2}$ as a sum over the normal-modes frequencies.
[We suggest to use the following:
(i) $\mathbf{u}(\mathbf{R}) = (1/\sqrt{N})\sum_{\mathbf{k},s}\mathbf{u}_s(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}}$, with $\mathbf{u}_s(\mathbf{k})$ *normal* coordinates and $\mathbf{k} \in$ FBZ; (ii) $\mathbf{u}_s(\mathbf{k}) \propto \boldsymbol{\epsilon}_s(\mathbf{k})$, and $\boldsymbol{\epsilon}_s(\mathbf{k}) = \boldsymbol{\epsilon}_s(-\mathbf{k})$; (iii) the mean value at a given temperature of the potential energy of a normal oscillator is clearly equal to half of the average value of the total energy $\hbar\omega_s(\mathbf{k})(n_s(\mathbf{k}) + 1/2)$.]
3. Rewrite $\overline{\mathbf{u}^2}$ as an integral over the frequencies, introducing the density of states.
4. Specialize the previous formula to a finite system, simply by limiting the integral over the frequencies to $\omega > \omega_t = 2\pi c/L$, where the cutoff frequency ω_t is $L = N^{1/D}/\rho^{1/D}$, with ρ the atomic density and within adimensional constants of order 1.
5. Estimate, for $T > 0$, the dominating contribution to $\overline{\mathbf{u}^2}$ due to the low-frequency modes ($\omega_t < \omega < \omega_c$), in the regime $\beta\hbar\omega \ll 1$.
6. What happens to $\overline{\mathbf{u}^2}$ for $D = 2$ when $N \to \infty$?
7. As above but for $D = 1$.

23 1D chains with long-range interactions: vibration modes and stability

Consider a system of particles forced to move in 1D [for instance the x axis] interacting via a pair potential $\phi(|x_n - x_m|; |n-m|)$.

1. Write the potential energy per particle $u(a)$ when the particles are arranged in a regular fashion spaced by a, that in when $x_n = na$.

2. Consider small oscillations of the particles around the regular arrangement described at point 1, that is $x_n = na + \delta_n$ with $|\delta_n| \ll a$. Write then the total potential energy in powers of the δ_n, up to the second order included. The zero-order term of course coincides with $Nu(a)$, if you consider a piece of the chain with N particles [and Born - von Karman boundary conditions].

   2.a) Show that the first-order term is always missing, so that the configuration $x_n = na$ is always an extreme of the energy for each a.

   2.b) Writhe the dynamical matrix $D(|n-m|)$, determining the second order term, as a function of the $\phi''(|n|a; |n|)$, where the double prime denotes the second derivative of ϕ with respect to its first argument.

   2.c) Using the result of point 2.b) write the dispersion relation for the small oscillations [harmonic vibrations] as a function of the $\phi''(|n|a; |n|)$, assuming that the particles mass is M; that is, write explicitly $\omega^2(k)$.

3. Consider a pair potential of the type

$$\phi(|x|; |n|) = \frac{C}{|x|^\alpha} + \frac{e^2}{|x|}(-1)^n,$$

   which includes both repulsive [$C > 0$ and let us consider for the time being $\alpha > 0$ so that we have a repulsion that declines with distance] and Coulombic interactions.

   3.a) Write the dispersion relation in this specific case, using the notation: $G = \alpha(\alpha+1)C/a^{\alpha+2}$, with G being a force constant, $\sigma = e^2/(Ga^3)$ an adimensional parameter measuring the relative importance of the Coulombic interaction with the repulsive interaction, and $\omega_0^2 = 4G/M$. One should obtain

$$\frac{\omega^2(k)}{\omega_0^2} = \sum_{n=1}^{\infty} \frac{1}{n^{\alpha+2}} sin^2(\frac{kna}{2}) + \sigma \sum_{n=1}^{\infty} \frac{(-1)^n}{n^3}[1 - cos(kna)]$$

   .

   3.b) Consider the relation obtained in 3.a) at the zone boundary, i.e. for $k = \pi/a$. To this end introduce the Riemann Zeta function $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$. Bear also in mind the identity $\sum_{n=1}^{\infty}(-1)^n n^{-s} = -\zeta(s)(1-2^{1-s})$, easily provable separating the sum in even and odd terms and by summing and subtracting once the even terms.

3.c) Using the result of 3.b) show that the square of the frequency becomes negative for $\sigma \geq \sigma_c^\pi = 4\zeta(\alpha+2)/(7\zeta(3))$. This indicates an instability of the 1D crystal. That is, the configuration assumed as the equilibrium one is just an extremum and is not a minimum.

3.d) Consider the dispersion for small k, i.e. for $k \to 0$. Assuming that $\alpha > 1$, compute explicitly the speed of sound. Show that it becomes imaginary for $\sigma \geq \sigma_c^0 = \zeta(\alpha)/(2ln2)$, drawing conclusions similar to the previous point.

4. Clearly for $\sigma \geq \sigma_c^\pi$ one finds imaginary frequencies close to the zone boundary and for $\sigma \geq \sigma_c^0$ also at the zone center. This type of instability, anyway, concerns crystal deformations at fixed *density*, that is at fixed a.

4.a) Try to study the stability with respect to the changes in a, considering the equilibrium energy $u(a)$ of point 1. Show that the requirement that $u(a)$ is a minumum yields an equilibrium parameter $a_0 = [\alpha C\zeta(\alpha)/(e^2 ln2)]^{1/(\alpha-1)}$, with the additional condition $\alpha > 1$. [Compare with the assumption at 3.d)].

4.b) Consider small oscillations around the equilibrium points obtained at (4.a). Then, at a_0 there will be one G_0 and thus $\sigma_0 = \zeta(\alpha)/((\alpha+1)\ln 2)$. Show that in this case the speed of sound is always a real quantity. With reference to point 3.c, try to discuss what happens at the zone boundary for integer values of α, with $\alpha > 1$. [If one wishes to attack this last point it will be necessary to compute numerically $\zeta(n)$, which can be found tabulated in the book *Handbook of Mathematical Functions*, edit. M. Abramowitz and I. Stegun, (Dover, NY, 1972).]

24 * Kohn anomaly

Consider a linear chain of identical atoms with a equilibrium spacing a. Let $u(n)$ be the displacement from the equilibrium position (na) of the n–th atom. There are springs acting over all atoms, so that the force on the n–th atom is given by $F(n) = \sum_m C_m[u(n+m) - u(na)]$.

1. Write th equation of motion of a generic atom.
2. Show that solutions of the form $e^{i(qna-\omega_q t)}$ satisfy the equations of motion, obtaining an expression for ω_q^2.
3. Assume that

$$C_m = C\frac{sin(mk_0a)}{ma}$$

and compute $d\omega_q^2/dq$.
4. How much is $d\omega_q^2/dq$ at $q = k_0$?
5. Draw a qualitative plot of ω_q as a function of q around $q = k_0$.

25 * 1D chain with further-neighbours interactions

Consider the oscillation modes of a linear atomic chain having mass M, in the case in which there exist interactions beyond first neighbours.

1. Write the energy of the chain denoting with $u(na)$ the displacement from the equilibrium position na of the $n-$th atom and with C_m the force constant of order m, $m \geq 1$.
Remember that the interaction energy between the $n-$th atom and its $m-$th neighbour is $(1/2)C_m\,[u(na) - u[(n+m)a]]^2$.
2. Write the dispersion relation $\omega(k)$.
3. Consider $C_1 = C$, with $C_m = 0$ for $m > 1$, and plot $\tilde{\omega}(q) \equiv \omega\sqrt{M/C}/2$, where $q \equiv ka/2$, for $0 \leq q \leq \pi/2$.
4. Consider now $C_1 = C$, $C_2 = C/4$ with $C_m = 0$ for $m > 2$ and plot again $\tilde{\omega}(q)$. [It is enough to concentrate on the differences from the case at the point 3 for small q and for $q = \pi/2$.]
5. Consider now $C_1 = C$, $C_2 = C/4$, $C_3 = -C/5$ with $C_m = 0$ for $m > 3$, and plot again $\tilde{\omega}(q)$. [It is suggested to consider explicitly the behaviour at small q and the points $q = \pi/6, \pi/3, \pi/2$.]

26 * Square harmonic crystal

Consider a square crystal wit lattice parameter a. Each atom has mass M and is connected to its first neighbors via springs having elastic constant G_x in the x direction and G_y in the y direction.

1. Write the potential energy U of the crystal when the atoms perform small oscillations around the lattice sites. [The springs have rest length a and the motion is strictly 2D.]
2. Write the equation of motion for a generic atom.
3. Solve the equation obtained in (2) using a plane wave ansatz and characterize the two modes so obtained.
4. Here and in what follows take $G_y = 4G_x$. Plot the two modes: (i) along the path (in units of π/a) (0,0) $\rightarrow$ (1,0) $\rightarrow$ (1,1) $\rightarrow$ (0,1) $\rightarrow$ (0,0) and (ii) along the path (again in units of π/a) (0,0) $\rightarrow$ (1,1). [The paths are meant to be straight lines connecting the given points.]
5. Write the dispersion relations for the two modes when $\sqrt{q_x^2 + q_y^2}\, a \ll 1$.
6. Compute the phonon specific heat at low T, in a similar way to the way used in 3D and considering that $\int_0^\infty dx\, x/(e^x - 1) = \pi^2/6$.
7. Write the dynamical matrix as a matrix respect to the Cartesian indexes (x,y) and lattice indexes (m,n). [*Note:* the Bravais translations are $\mathbf{R} = (m, n)a$].

27 * Effective masses in a semiconductor

The experimental analysis of a certain semiconductor shows that the density of states in energy of a specific band has, close to the band edge $\mathbf{k}^*$ of that band, the expected square root behaviour $g(\epsilon) = C\sqrt{\epsilon}$, where $\epsilon = |E - E^*|$ and $C = 6.97 \times 10^{20}\, cm^{-3}/eV^{3/2}$. In what follows we shall assume that the laboratory coordinate system coincides with the principal axes system $(\hat{x}_1,\, \hat{x}_2,\, \hat{x}_3)$ of the mass tensor at $\mathbf{k}^*$.

1. How much is the determinant of the mass tensor in units of m_e^3?
2. Performing experiments in a magnetic field one finds that rotating $\mathbf{H}$ around the $\hat{x}_3$ axis the cyclotron effective mass does not change. How many different eigenvalues has, at most, the mass tensor? Argue your answer in full details.
3. Knowing that for a magnetic field orthogonal to the $\hat{x}_3$ axis the cyclotron mass is $m^*(\mathbf{H}) = 0.253 m_e$ compute the eigenvalues of the mass tensor (in units of m_e).
4. Do you have an idea on which semiconductor could it be?
5. What is the shape of the orbits for a magnetic field lying along the $\hat{x}_3$ axis?
6. And for a magnetic field lying along the $\hat{x}_1$ axis?
7. What will be the measured cyclotron frequency (in cm^{-1}) for a magnetic field with $\hat{H} = (1/\sqrt{2}, 0, 1/\sqrt{2})$?

28 * Divalent impurities

Consider a semiconductor with a dielectric constant $\epsilon = 12.5$ and conduction effective mass $m = 0.067 m_e$, doped with few divalent donors, that can thus be regarded as independent. Remember that the total binding energy of the He atom is $E = 5.81 Ry$.

1. Write the expression and the numerical value (in eV) of the binding energy ε_1, respect to the conduction band for a single electron on the donor.
2. Write the expression and the numerical value (in eV) of the binding energy ε_2, after the addition of a second electron to the donor.
3. Estimate the effective Bohr radius (in $\AA$) of the impurity with one electron and judge if the "hydrogenic" approximation is reasonable. Do you expect that with two electrons the approximation gets better or worse?
4. Compute the average occupation of these (independent) donor centers computing a suitable average. How much is it at $T = 0$?
5. Determine the position of the chemical potential at $T \to 0$, in the hypothesis that only the mentioned donors are there.
6. If N_d is the density of the donor dopants and one adds (monovalent) acceptor dopants as well with density $N_a = N_d$, where will the chemical potential will go as $T \to 0$?

29 * Impurity-induced conductivity

Consider the crystalline semiconductor GaAs (gallium arsenide). This is a direct-gap semiconductor ($E_g \simeq 1.52\ eV$ at room T: neglect the dependence of E_g on T). The conduction band has a measured effective mass of $m_c = 0.068 m_e$ and the valence band of $m_v = 0.41 m_e$. The measured dielectric constant is $\epsilon = 14.6$.
Assume that the semiconductor is doped with donor and assume that one can describe the state of the excess electrons thus introduced using the *hydrogenic* model.

1. Compute the binding energy E_d (in eV) of the excess electrons with respect to the conduction band.
2. Compute the effective Bohr radius a_B^* (in $\mathring{A}$) of such electrons, assuming that each one is in the *hydrogenic* ground state centered on a donor.
3. Is the value computed for a_B^* compatible with the hydrogenic model used?
4. Assume that when the average distance between the donor centres becomes comparable with a_B^* the electrons *screen* each other, ceasing to be bound and ending up in the conduction band. For which critical value n_{cr} of the donor (electron) density will this happen? Compute n_{cr} in cm^{-3}.
[Hint: write the average donor/electron density as $n_d = [(4\pi/3)a^3]^{-1}$ and take a as a measure of the average distance between donors. Other possible methods to estimate n_{cr} are not, however, discouraged.]
5. Estimate the carrier density ($n_c + p_v$, in cm^{-3}) at $T = 10K^o$ in the intrinsic (undoped) semiconductor using the data provided in the introduction.
6. Compare the carrier densities obtained at point 4 and 5 and write whether at $T = 100K^o$ and for $n_d > n_{cr}$ the doped semiconductor is in the extrinsic (dopant-dominated) or intrinsic regime.
7. At $T = 0$ and for a donor density $n_d > n_{cr}$, is doped $GaAs$ an insulator, a semiconductor or a metal? Why?

30 * Electrons in GaAs/AlGaAs-based quantum wells

It is possible to make in the laboratory GaAs/AlGaAs-based heterostructures in which an (almost) 2D electron gas can be created.
It is known that the dielectric constant of these systems is $\epsilon = 12.5$. Moreover, cyclotron resonance experiments using a field $B = 10^4 gauss$ reveal a cyclotron frequency $\omega_c = 1.76 \times 10^{11} s^{-1}$ for the electrons.
One can assume that the said electrons move in a dielectric *continuum*.

1. Compute the electron effective mass m^* in units of the electron mass m_e.
2. How much is the energy per electron ε and the Fermi energy E_F (in eV) for such a 2D electron gas if the density is $n = 3.18 \times 10^9 cm^{-2}$?
3. How much is T_F in K?
4. Draw a qualitative plot of the Fermi function as a function of the energy for $0 \leq E \leq 0.1eV$, plotting $f(E)$ as a function of E/E_F.
5. The importance of electron interaction can be measured via the ratio γ between (i) the potential energy of two electrons at the typical average distance $a = \sqrt{1/(\pi n)}$ and (ii) the Fermi energy E_F. How much is γ in this electron gas?

31 * Charge transfer in coupled quantum wells

Consider two strictly 2D symmetrical quantum wells at a distance d.
[Each quantum well traps electrons forcing them to move exclusively on a plane. The first well (A) can be modeled as the plane perpendicular to the z-axis an passing through $z = 0$, the second (B) is parallel to the first and passes through $z = d$. Initially each plane is electrically neutral with an electron (number) areal density $N/A = \rho$ neutralized by a uniform positive background with charge areal density $e\rho$. Note that the substrates are fixed, while the electrons are free to transfer from a plane to the other.]
Without any loss of generality we shall consider the possibility that electron transfer from B to A. The electron charge distributions remain always uniform in each plane.

1. Write the variation of the electrostatic energy per unit area $E_H(n, d)$ caused by the transfer of $n \leq \rho$ electron (per unit area) from B to A. [Hint: the charge transfer leads to a net charge density $-en$ on plane A and $+en$ on plane B. Consider the energy per unit area accumulated in the electric field, or equivalently the work per unit area needed to separate the two charged planes from distance 0 to a distance d.]
2. In the Hartree-Fock scheme the electrons in each plane interact with each other with an energy per unit area of the form $E_I(\rho_I) = C\rho_I^2 - D\rho_I^{3/2}$, I=A, B, with $C = e^2\pi a_B/2$ and $D = e^2(4/3)\sqrt{2/\pi}$; evidently $\rho_B = \rho - n$ and $\rho_A = \rho + n$. Write the energies per unit area due to the interactions in the two planes $E_A(\rho + n)$ and $E_B(\rho - n)$.
3. Write the total energy per unit area $E_T(\rho, n, d) = E_A + E_B + E_H$
4. Write (i) the change in total energy corresponding to a charge transfer from B to A $\Delta(\rho, n, d) = E_T(\rho, n, d) - E_T(\rho, 0, d)$ and (ii) consider specifically the case of total transfer $n = \rho$, namely compute $\Delta_t = \Delta(\rho, \rho, d)$.
5. Are there, at a fixed distance d, situations where the total transfer is energetically favourable (i.e., $\Delta_t < 0$)? If so, write the condition that must be satisfied by the density ρ.
6. In case of an affirmative answer at the previous point, consider the special case in which $d = 200\mathring{A}$ and the effective Bohr radius $a_B = 100\mathring{A}$, and estimate the maximum density ρ^* (in cm^{-2}) at which the transfer can be observed.
7. How much is the radius r_s^* of the Wigner disk corresponding to the density of the previous point? $[\pi(r_s^* a_B)^2 = \rho^{*-1}]$

32 * Properties of molecules with a triplet excited state.

Consider molecules with a triplet excited state at an energy superior of Δ with respect to the singlet ground state. Both states have zero orbital angular momentum. All other excited states can be neglected at the temperatures of interest. Imagine a non-interacting gas of such molecules at temperature T.

1. Write the Helmholtz free energy per molecule of such a gas in the presence of a magnetic field $\mathbf{B} = B\hat{z}$.
2. Compute the average magnetization per molecule.
3. Calculate the molecular magnetic susceptibility.
4. Write the limiting expression for the magnetic susceptibility when (i) $\beta\Delta \ll 1$ and (ii) $\beta\Delta \gg 1$.
5. Compute the entropy per molecule at $B = 0$ and try to draw a qualitative plot of it as a function of $K_B T/\Delta$.
6. Compute the molecular specific heat and draw a qualitative plot of it as a function of $K_B T/\Delta$.

33 * Magnetism of the electron gas and Stoner condition.

A 3D homogeneous electron gas is subject to a magnetic field B pointing in the z direction. Consider a stat in which N_+ electrons have positive spin component (along z) and N_- negative and define the spin polarization $\zeta = (N_+ - N_-)/N$ with $N = N_+ + N_-$. The energy of each spin component ($\sigma = \pm$) is made up by three contributions: (i) kinetic energy $N_\sigma(3/5)(\hbar^2 K_{F,\sigma}^2)/(2m)$, (ii) exchange energy $N_\sigma(3e^2 K_{F,\sigma})/(4\pi)$, and the coupling energy between the spin magnetic moments and B; clearly $K_{F,\sigma}$ is the Fermi wavevector of the spin component with projection σ.

1. Write the energy of the spin-up electrons.
2. Write the energy of the spin-down electrons.
3. Write the total energy and write down the condition that determines the equilibrium polarization at constant N and V.
4. Specialize the condition found at the previous point to the case $\zeta \ll 1$ and give an explicit formula the equilibrium ζ.
5. Find for which values of r_s, considering B of about 10^4 gauss, the value of ζ found at the previous point is indeed small.
6. What is the condition for which the state with $\zeta = 0$ becomes unstable (a maximum for the energy!).

34 Specific heat in a Heisenberg ferromagnet.

Consider a 3D Heisenberg ferromagnet, in the absence of external magnetic fields. Assume that the spins have *magnitude* S and lie on a BCC lattice with lattice parameter a_L. Also assume *only nearest-neighbours* exchange interactions, with exchange coupling constant J.

1. Consider excitations from the ground state in the form of spin waves. Find the dispersion relations of the excitation energies for small values of the wave vector $\mathbf{k}$, writing explicitly the excitation energy $\epsilon(\mathbf{k})$ of the spin wave as a function of S, a_L, J, k.

2. Consider the specific heat per unit volume, at constant volume, c_v^M, due to the magnetic excitations, *in the limit of low temperatures*, assuming that the low-energy excitations are due to spin waves and have the form found in the previous point.
   Express c_v^M in terms of S, a_L, J, K_B, T. [*Note: the problem is very similar to that of the low-temperature specific heat due to lattice vibrations, where one considers spin waves (or magnons) in place of phonons.*]

3. Taken as known the lattice specific heat c_v^L at low T [in terms of $K_B, T, \hbar, c$, with c a suitable average of the speed of sound].
   Assuming that the crystal considered here is an insulator and thus that the total specific heat $c_v = c_v^M + c_v^L$ comes only from the lattice and magnetic contributions, estimate at which temperature T^* [written in terms of $K_B, \hbar, c, S, a_L, J$] one has $c_v^M = c_v^L$.

4. With reference to point 3, write down the condition that must be obeyed by the temperature so that the magnetic specific heat dominates on the lattice specific heat and thus is easily observable.

Note: The Riemann zeta function, $\zeta(s) = \sum_{1,\infty} n^{-s}$, n an integer, can be found tabulated in the book: Jahnke-Emde-Lösche, *Tables of higher functions*, McGraw-Hill, NY 1960.

35 * Peierls instability in a 1D conductor.

Consider a system of ions and electrons forced to move along a line. The ions have unit charge and there is one electron per ion, so that the system is globally neutral. Assume that the ions lie in the positions $X_n^0 = na$ ant that the electron energy levels$\epsilon^0(q)$ are known. As a simplification we shall assume $\epsilon^0(q) = \hbar^2 q^2/2m$. In the ground state all and only the levels with $|q| \leq q_F$ are occupied, with $q_F = \pi/2a$ and the energy per electron turns out to be $E_e^0 = \epsilon_F/3$.
Consider a lattice deformation

$$\begin{aligned} X_n &= X_n^0 + u(n), \\ u(n) &= \Delta\, cos(2q_F na) = \Delta\, cos(\pi n) \end{aligned}$$

where Δ is a parameter.

1. What is the periodicity of the deformed lattice?
2. Compute the variation of the ion-ion energy (per ion) E_a, describing the interionic interaction as due to springs having an elastic constant C (and rest length a), connecting each ion to its first neighbors.
3. The lattice deformation induces an additional electron-ion potential of the form

$$U_{ei} = 2A\Delta cos(2q_F x) = A\Delta(e^{i2q_F x} + e^{-i2q_F x}).$$

U_{ei} couples states with wavevectors differing by $2q_F \equiv G_1$, with an amplitude $U_{G_1} = A\Delta$. In the two-level scheme, each eigenvalue $\epsilon^0(q)$ originates two perturbed levels. Clearly at each q the electrons occupy the lowest level $\epsilon(q) \equiv \epsilon_-(q)$. Compute the energy per electron in the deformed lattice

$$E_e = \frac{1}{q_F}\int_0^{q_F} dq\ \epsilon(q).$$

(In order to compute the integral easily it is suggested to change the integration variable to $y = q_F - q$).
4. Compute the equilibrium Δ^* by minimizing the total energy $E(\Delta) = E_a + E_e$ with respect to Δ, namely by imposing that

$$\frac{dE(\Delta)}{d\Delta} = 0.$$

5. Exploit the expression for Δ^* to show that $E(\Delta^*) - E(0) < 0$. This shows that the deformed system has lower energy and hence is the equilibrium state. Is this deformed system a metal or an insulator?
6. Simplify the expression of Δ^* assuming that $C\epsilon_F/A^2$ is much greater than one, so that $\sinh(x) \approx e^x/2$. Then rewrite $C\epsilon_F/A^2$ as a function of the density of states in q at the Fermi level, $N_0 = g(\epsilon_F)/2$, and of the effective electron-electron potential $V_0 = A^2 a/2C$. Does the expression found remind you of something?
Notes:
1. Remember that: $\int dt\ \sqrt{1+t^2} = (1/2)[t\sqrt{1+t^2} + \text{arcsinh}(t)]$, and $(d/dx)\text{arcsinh}(x) = 1/\sqrt{1+x^2}$.

2. Remember that in D dimensions the free-electron density of states is

$$g(\epsilon) = \frac{Dn}{2\epsilon_F} \left[\frac{\epsilon}{\epsilon_F}\right]^{D/2-1},$$

n being the density.