

$$\hbar = 1.054 \times 10^{-34} \text{ Js} \quad m_e = 9.11 \times 10^{-31} \text{ kg} \quad |e| = 1.602 \times 10^{-19} \text{ C}$$

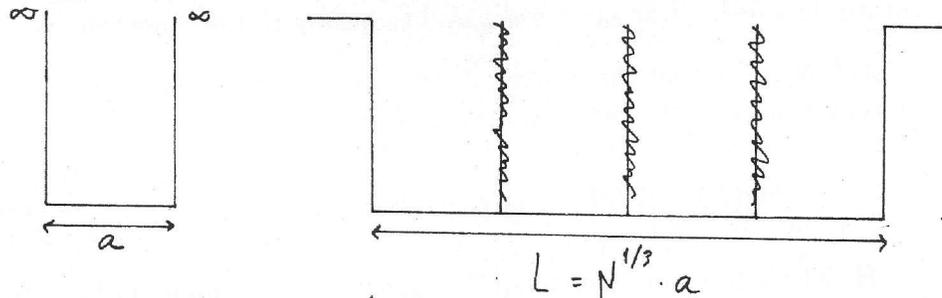
1. (20 points) Consider the free electron gas model for metals. For a system of N free electrons in a volume V at 0 K,
- a) Show that the kinetic energy of the electrons is (E_F is the Fermi energy)

$$U_0 = \frac{3}{5} N E_F.$$

- b) Derive an expression connecting the pressure P and the volume V of the system.
- c) Show that the bulk modulus, defined as $B = -V(\partial P/\partial V)$, is given by

$$B = \frac{5}{3} P.$$

2. (20 points) Binding in simple metals such as Na arises from the lowering of kinetic energy of valence electrons when the atoms are brought together. Estimate the cohesive energy per atom as a function of the lattice constant a using the following simplified model, depicted in the figure: (i) Treat the valence electrons in the isolated atoms as being in infinite potential wells of width a (left panel); (ii) assume that when a large number N of atoms are brought together to form the solid, the walls of the wells disappear, so that the valence electrons are free to roam through the entire sample of macroscopic volume $V = L^3$ (right panel).



- a) Assuming one valence electron per atom, show that the cohesive energy per atom is approximately given by

$$E_{\text{cohesive}} \simeq \frac{4}{5} (3\pi^2)^{2/3} \frac{\hbar^2}{2m_e a^2}.$$

[Hint: Make the approximation $\frac{3}{5 \times (3\pi^2)^{1/3}} = 0.1939 \dots \simeq 0.2$.]

- b) On the basis of this model, estimate the cohesive energy of simple metals. How does it compare with the cohesive energy in van der Waals solids?

3. (20 points) Consider the first Brillouin zone of a crystal with a simple hexagonal lattice in three dimensions with lattice constants a and c . Let \mathbf{G}_c denote the shortest reciprocal lattice vector parallel to the c axis of the crystal lattice.

a) Show that for a hexagonal close-packed crystal structure the Fourier component $U(\mathbf{G}_c)$ of the crystal potential $U(\mathbf{r})$ is zero.

b) Is $U(2\mathbf{G}_c)$ also zero?

c) Why is it possible in principle to obtain an insulator made up of *divalent* atoms at the lattice points of a simple hexagonal lattice?

d) Why is it not possible to obtain an insulator made up of *monovalent* atoms in a hexagonal-close-packed structure?

4. (20 points) Consider a nanometric wire in the form of a rectangular parallelepiped, with two sides $L_x \simeq L_y \simeq 1$ nm and the long axis $L_z = 1$ cm. The single-particle eigenstates of the system may be written as

$$\psi = \sin(n_x \pi x / L_x) \sin(n_y \pi y / L_y) \exp(i2\pi N z).$$

The energy $E_{\mathbf{n}}(N)$ of the eigenstate is, with $\mathbf{n} = (n_x, n_y)$ and $\epsilon_{\mathbf{n}}$ the energy level of a particle in an infinite 2D well of dimensions $L_x \times L_y$,

$$E_{\mathbf{n}}(N) - \epsilon_{\mathbf{n}} = (2\pi\hbar N)^2 / 2m = AN^2 = \frac{1}{2}mv^2,$$

where v is the electron velocity along the z -axis. Here $A = (2\pi\hbar)^2 / 2m$ and $N = \sqrt{[(E - \epsilon) / A]}$. States labelled by the same \mathbf{n} are said to belong to the same "subband."

a) Using $\delta E_{\mathbf{n}} = 2AN\delta N$, show that the density of states in each subband, with account of the two spin orientations and the two \pm values of N , is

$$D_{\mathbf{n}}(E) = (2/\pi\hbar)[1/v_{\mathbf{n}}(E)]\Theta(E - \epsilon_{\mathbf{n}}),$$

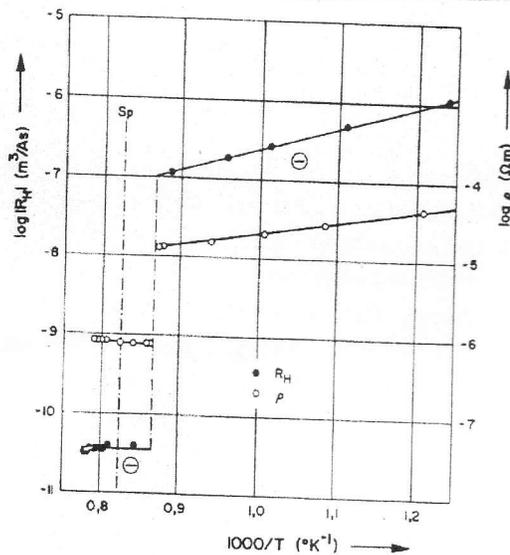
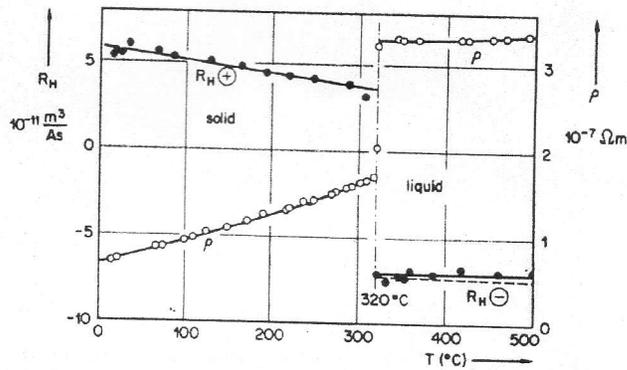
where $\Theta(x)$ is the Heaviside function (step function), zero for $x < 0$ and unity for $x > 0$.

b) The contribution from subband \mathbf{n} to the current in the nanometric wire is $I_{\mathbf{n}} = (N_+ - N_-)ev_F(\mathbf{n})$, where $v_F(\mathbf{n})$ is the Fermi velocity, $N_+ - N_- = D_{\mathbf{n}}(E_F)eV$, and V is the bias voltage. Show that the *total* current may be written as

$$I = (2e^2/\pi\hbar)n_{\text{occ}}V,$$

where n_{occ} is the number of subbands which carry electrons. Hence the conductance (defined as $G = I/V$, the current divided by the voltage drop) is $(4e^2/h)n_{\text{occ}}$. Note that it is quantized.

5. (20 points)



The figure shows experimental data for the resistivity $\rho(T)$ and the Hall coefficient $R_H(T)$ of two materials around their melting points T_m (at T_m both ρ and R_H vary discontinuously). One of the materials is Cd, a metal, while the other is Ge, which in the crystalline phase is a semiconductor while in the liquid phase it becomes a metal.

- By carefully discussing the T -dependence of the measured quantities, indicate which of the two graphs pertains to Cd, and which to Ge. Note that in one of the graphs the vertical scales are linear while in the other they are logarithmic, and that in one graph the horizontal axis is T , while in the other it is $\propto 1/T$.
- Why is it that for both materials the temperature dependence of ρ is much weaker above T_m than below?
- What is the sign of R_H according to the free-electron theory? Since in the upper panel R_H changes sign upon melting, either below or above T_m (which one?) the sign is different from the simple theoretical prediction. Can you speculate (in very general and qualitative terms) as to the origin of this failure of the free-electron theory?