Statistical Physics & Condensed Matter Theory I: Exercise

The Bohm-Staver formula

In class, we have discussed the harmonic chain, without discussing the true origin of the restoring force in realistic situations. In this problem, we look into phonons in more detail.

Consider thus a three-dimensional crystal. The atoms consist of large ions surrounded by light electrons. The dynamics of the ions, which have a mass M much greater (order 10^5) than the electron mass, is thus much slower. As an approximation, we can say that the fast-moving (and fast equilibrating) electrons are always 'pinned' to the ions in order to maintain charge neutrality. What then provides the restoring force is the electron gas itself, whose energy depends on its density.

a)

Let us start by establishing the properties of the free electron gas. Consider the free three-dimensional case, with single-particle energy $\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$. For a given Fermi momentum k_F (and thus Fermi energy $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$ and Fermi velocity $v_F = \hbar k_F/m$), show that the number of electrons per unit volume (spin-1/2) is $\frac{N_e}{V} = \frac{1}{3\pi^2} k_F^3 \equiv \rho_e$. Show that the energy per unit volume is $\frac{E_e^0}{V} = \frac{\hbar^2}{10\pi^2 m} k_F^5 = \frac{\hbar^2}{10\pi^2 m} (3\pi^2)^{5/3} \rho_e^{5/3}$ and that the energy per particle is $\frac{E_e^0}{N} = \frac{3\hbar^2}{10m} k_F^2 = \frac{3}{5}\varepsilon_F$.

b)

Let us now adopt a continuum description with $\rho_{ion}(\mathbf{r}, t)$ being the density of atoms per unit volume. In each volume element, we assume that the atoms move with a uniform velocity $\mathbf{v}(\mathbf{r}, t)$. Their density must obey the continuity equation $\partial_t \rho_{ion}(\mathbf{r}, t) + \nabla \cdot (\rho_{ion}(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)) = 0$. We can interpret $M\rho_{ion}(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)$ as the total momentum per unit volume of the ions, which we write $\boldsymbol{\pi}(\mathbf{r}, t)$, so

$$M\partial_t \rho_{ion}(\mathbf{r}, t) + \nabla \cdot \boldsymbol{\pi}(\mathbf{r}, t) = 0 \quad \rightarrow \quad M\partial_t^2 \rho_{ion}(\mathbf{r}, t) + \nabla \cdot \dot{\boldsymbol{\pi}}(\mathbf{r}, t) = 0$$

On the other hand $\boldsymbol{\pi}$ must obey Newton's law, with the force originating from the pressure of the electrons; the total force is in fact the pressure gradient, so (using the definition of pressure)

$$\dot{\boldsymbol{\pi}} = -\nabla P = \nabla \left(\frac{\partial E_e^0}{\partial V}|_{N_e} \right).$$

Calculate $P = -\frac{\partial E_e^0}{\partial V}|_{N_e}$ using your results above, and show that it equals $\frac{2}{3}\frac{E_e^0}{V} = \frac{2}{5}\varepsilon_F \rho_e$.

Taking $\rho_e(\mathbf{r}, t) = Z\rho_{ion}(\mathbf{r}, t)$ to be the density of electrons (Z being the atomic number of the ions), and making the approximation of small density fluctuations $\rho_{ion}(\mathbf{r}, t) = \rho_{ion}^0 + \delta\rho_{ion}(\mathbf{r}, t)$ (with ρ_{ion}^0 constant), show that $\dot{\boldsymbol{\pi}} = -\frac{2}{3}\varepsilon_f \nabla \rho_e = -\frac{2}{3} Z \varepsilon_F \nabla \delta\rho_{ion}$. Finally, show (dropping terms of order $(\delta\rho_{ion})^2$) that the density fluctuations obey the harmonic equation

$$M\partial_t^2 \delta\rho_{ion} - \frac{2}{3} Z \varepsilon_F \nabla^2 \delta\rho_{ion} = 0.$$

c)

Show that this entails the existence of density fluctuations propagating with velocity

$$v_s = \left(\frac{Zm}{3M}\right)^{1/2} v_F,$$

which is known as the **Bohm-Staver formula** for the velocity of acoustic phonons in solids. Give an order of magnitude estimate for v_s for a realistic solid, using the fact that in typical metals $v_F \sim 1 - 2 \times 10^6 m/s$.

You now know that classical acoustic (sound) wave propagation in solids is thus really driven by quantum-mechanical effects on the electrons.