Lecture 19: Phonons

We discuss the longitudinal sound wave of jellium. We view it as a charged plasma where the oscillation of the positively charged jellium is screened by the electrons. The plasma frequency $\omega_{\text{pl}}^2 = 4\pi n_0 e^2/M$ where M, which is the nuclear mass, is screened by replacing e^2 by $e^2/\varepsilon(q, \omega = 0)$ and we use the Thomas Fermi screening

$$\frac{1}{\varepsilon(q)} = \frac{q^2}{q^2 + \kappa^2}, \tag{1}$$

where $\kappa^2 = 4\pi e^2(2N(0))$, and $N(0)$ is the single spin electronic density of states at the Fermi level. This gives

$$\begin{aligned} \omega^2(q) &= \omega_{\text{pl}}^2/\varepsilon(q) \\ &= c^2 q^2 \end{aligned} \tag{2}$$

where

$$\begin{aligned} c^2 &= \frac{4\pi n_o e^2}{M\kappa^2} \\ &= \frac{1}{3}\frac{m}{M} v_F^2 \ . \end{aligned} \tag{3}$$

Then the sound velocity is reduced from the Fermi velocity by a factor $\sqrt{\frac{m}{3M}}$. This is a useful small parameter when discussing phonons and electrons.

Next we introduce a local displacement vector $\mathbf{d}(\mathbf{r}, t)$ for the jellium. A modulation of $\mathbf{d}(\mathbf{r}, t)$ causes density modulation given by

$$\delta n(\mathbf{r}, t) = -n_0 \boldsymbol{\nabla} \cdot \mathbf{d}(\mathbf{r}, t) \ . \tag{4}$$

Then we can write the Lagrangian as

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}\int d^3\mathbf{r}\left[Mn\left(\frac{d}{dt}\mathbf{d}\right)^2 - \frac{B}{n_0^2}(\delta n)^2\right] \\ &= \frac{1}{2}\int d^3\mathbf{r}\left[Mn\left(\frac{d}{dt}\mathbf{d}\right)^2 - B\left(\boldsymbol{\nabla}\cdot\mathbf{d}\right)^2\right] \qquad (5)\end{aligned}$$

where B is the bulk modulus. This gives the usual classical wave equation with sound velocity $c^2 = B/Mn_0$.

We introduce the canonical momentum density

$$\boldsymbol{\pi}(\mathbf{r},t) = Mn_0\frac{\partial\mathbf{d}(\mathbf{r},t)}{\partial t} \qquad (6)$$

and the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\int d^3\mathbf{r}\frac{1}{Mn_0}\left(\boldsymbol{\pi}\cdot\boldsymbol{\pi} + B(\boldsymbol{\nabla}\cdot\mathbf{d})^2\right) \quad . \qquad (7)$$

The problem is quantized by demanding the canonical commutation relation between $\mathbf{d}$ and $\boldsymbol{\pi}$. This is satisfied by the Fourier expansion

$$\mathbf{d}(\mathbf{r},t) = -\frac{i}{\sqrt{Mn_0}}\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}\hat{k}\sqrt{\frac{\hbar}{2\omega_k}}\left(b_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_k t} - b_k^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega_k t}\right) \quad . \qquad (8)$$

Then

$$\mathcal{H} = \frac{1}{2}\sum_{\mathbf{k}}\hbar\omega_k\left(b_k^\dagger b_k + \frac{1}{2}\right) \qquad (9)$$

and

$$\left[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger\right] = \delta_{\mathbf{k},\mathbf{k}'} \quad . \qquad (10)$$

In real solids there are transverse acoustic modes in addition to the longitudinal mode discussed above. If there are two or more atoms per unit cell, there are optical modes as well. All these can be quantized by extending the above procedure.

Reading: Marder 13.2, 13.3