Ph135 - Problem Set 4

November 12, 2019

Problem 1

In the dilute gas limit, $n\lambda_T^3 \ll 1$, so $\mu = T\ln(n\lambda_T^3) \ll 0$, which means

$$f_0 = \frac{1}{e^{(\epsilon-\mu)/T}+1} \approx \frac{1}{e^{(\epsilon-\mu)/T}}. \tag{1}$$

By the relaxation time approximation of the Boltzmann equation,

$$f = f_0 - \tau\frac{\partial\vec{r}}{\partial t}\cdot\nabla_{\vec{r}}T\frac{\partial f_0}{\partial T}, \tag{2}$$

where

$$\frac{\partial f_0}{\partial T} = -\frac{\partial f_0}{\partial\epsilon}\frac{\epsilon-\mu}{T}, \tag{3}$$

and so

$$\lambda = -2e\tau\int d\epsilon\rho(\epsilon)\langle(\hat{x}\cdot\nabla_{\vec{p}}\epsilon_{\vec{p}})^2\rangle_{\text{direction}}\frac{\partial f_0}{\partial\epsilon}\frac{\epsilon-\mu}{T}. \tag{4}$$

Now

$$\rho(\epsilon) = 2\cdot 4\pi(\frac{\sqrt{2m}}{2\pi\hbar})^3\sqrt{\epsilon}, \tag{5}$$

and

$$\frac{\partial\epsilon}{\partial k} = \frac{\hbar^2 k}{m} = \sqrt{\frac{2\epsilon}{m}}, \tag{6}$$

we therefore have

$$\lambda = -2e\tau\int d\epsilon\frac{2^{3/2}}{3\sqrt{m}\pi^2\hbar^3}\epsilon^{3/2}\frac{\partial f_0(\epsilon)}{\partial\epsilon}\frac{\epsilon-\mu}{T}, \tag{7}$$

and

$$\lambda = \frac{2^{5/2}e\tau}{3\sqrt{m}\pi^2\hbar^3}\int\epsilon^{3/2}\frac{1}{T}\frac{1}{e^{(\epsilon-\mu)/T}}\frac{\epsilon-\mu}{T}d\epsilon = \frac{e\tau}{\sqrt{2m}\pi^{3/2}\hbar^3}e^{\mu/T}(5T^{3/2}-2\mu T^{1/2}). \tag{8}$$

We substitute $\mu = T\ln(n\lambda_T^3)$ into the above equation, we get that

$$\lambda = \frac{10ne\tau}{m} - \frac{4ne\tau}{m}\ln(n\lambda_T^3), \tag{9}$$

where

$$\lambda_T = \left(\frac{2\pi\hbar^2}{mT}\right)^{1/2}. \tag{10}$$

Now we estimate the numerical value of the thermoelectric coefficient for a reasonably doped semiconductor, e.g., Silicon. First, let's do a dimensional analysis for λ, since λ relates current density with temperature gradient $\vec{j} = -\lambda\nabla T$, we have that $[\lambda] = (C\cdot s^{-1}\cdot m^{-2})/(K\cdot m^{-1}) = C\cdot m^{-1}\cdot s^{-1}\cdot K^{-1}$. Next, we plug in the numerical values for Silicon, $n \approx 1.08\times 10^{18}m^{-3}$ at 300K. To estimate the scattering time τ, we use the Drude formula eq.(2), for the mass m, we need to use the effective mass of the electron in Silicon, which is $m_e^* \approx 0.2 m_e$, which is the mass that the electrons seem to have when responding to forces in the Silicon band structure. Then

$$\tau = \frac{m_e^*}{ne^2\rho} \approx \frac{2.0 \times 10^{-31}\mathrm{kg}}{1.08 \times 10^{18}\mathrm{m}^{-3} \times (1.6 \times 10^{-19}\mathrm{C})^2 \times 0.1\Omega \cdot \mathrm{m}} \approx 7.2 \times 10^{-11} s. \tag{11}$$

Hence

$$\lambda \approx \frac{10 k_B n e \tau}{m} \approx \frac{10 \times 1.38 \times 10^{-23}\mathrm{m}^2 \cdot \mathrm{kg} \cdot \mathrm{s}^{-2} \cdot \mathrm{K}^{-1} \times 1.08 \times 10^{18}\mathrm{m}^{-3} \times 1.6 \times 10^{-19}\mathrm{C} \times 7.2 \times 10^{-11}\mathrm{s}}{2.0 \times 10^{-31}\mathrm{kg}}, \tag{12}$$

and $\lambda \approx 8.6 \times 10^{-3}\mathrm{C} \cdot \mathrm{m}^{-1} \cdot \mathrm{s}^{-1} \cdot \mathrm{K}^{-1}$.

Problem 2

(a) Denote by $x_{A,n}$ ($x_{B,n}$) the displacement of the n-th atom A (B) from the equilibrium. The potential energy takes the form

$$V = \frac{k}{2} \sum_n \left[(x_{B,n} - x_{A,n})^2 + (x_{A,n+1} - x_{B,n})^2 \right]. \tag{13}$$

After a Fourier transformation

$$\begin{aligned} x_{A,n} &= \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dq e^{iqna} x_{A,q}, \\ x_{B,n} &= \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dq e^{iqna} x_{B,q}, \end{aligned} \tag{14}$$

the potential energy takes the form

$$V = \frac{k}{2} \sum_n \left| \frac{a}{2\pi} \int dq e^{iqna} (x_{B,q} - x_{A,q}) \right|^2 + \sum_n \left| \frac{a}{2\pi} \int dq e^{iqna} (x_{A,q} e^{iqa} - x_{B,q}) \right|^2 \tag{15}$$

Since

$$\begin{aligned} \left| \frac{a}{2\pi} \int dq e^{iqna} (x_{B,q} - x_{A,q}) \right|^2 &= \left(\frac{a}{2\pi} \right)^2 \int dq \int dq' \sum_n e^{i(q-q')na} (x_{A,q} - x_{B,q})(x_{A,q'} - x_{B,q'})^* \\ &= \left(\frac{a}{2\pi} \right)^2 \int dq \int dq' \frac{2\pi}{a} \delta(q-q') (x_{A,q} - x_{B,q})(x_{A,q'} - x_{B,q'})^* \\ &= \frac{a}{2\pi} \int dq |x_{A,q} - x_{B,q}|^2, \end{aligned} \tag{16}$$

and

$$\begin{aligned} \left| \frac{a}{2\pi} \int dq e^{iqna} (x_{A,q} e^{iqa} - x_{B,q}) \right|^2 &= \left(\frac{a}{2\pi} \right)^2 \int dq \int dq' \sum_n e^{i(q-q')na} (x_{A,q} e^{iqa} - x_{B,q})(x_{A,q'} e^{iq'a} - x_{B,q'})^* \\ &= \left(\frac{a}{2\pi} \right)^2 \int dq \int dq' \frac{2\pi}{a} \delta(q-q') (x_{A,q} e^{iqa} - x_{B,q})(x_{A,q'} e^{iq'a} - x_{B,q'})^* \\ &= \frac{a}{2\pi} \int dq |x_{A,q} e^{iqa} - x_{B,q}|^2. \end{aligned} \tag{17}$$

We thus have

$$\begin{aligned} V &= \frac{k}{2} \frac{a}{2\pi} \int dq |x_{A,q} - x_{B,q}|^2 + \frac{k}{2} \frac{a}{2\pi} \int dq |x_{A,q} e^{iqa} - x_{B,q}|^2 \\ &= \frac{k}{2} \frac{a}{2\pi} \int dq (2|x_{A,q}|^2 + 2|x_{B,q}|^2 - (1 + e^{iqa}) x_{A,q} x_{B,q}^* - (1 + e^{-iqa}) x_{B,q} x_{A,q}^*), \end{aligned} \tag{18}$$

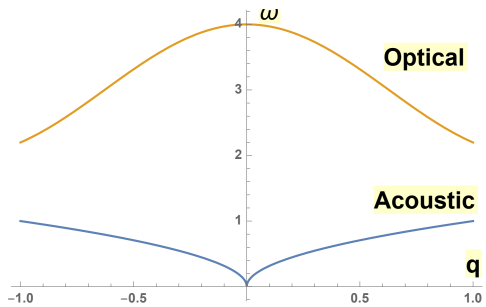

Figure 1: Dispersion relation of phonons in the chain

and the Hamiltonian is given by

$$H = \frac{a}{2\pi}\int dq\left(\frac{|p_{A,k}|^2}{2m_A} + \frac{|p_{B,k}|^2}{2m_B} + 2|x_{A,q}|^2 + 2|x_{B,q}|^2 - (1+e^{iqa})x_{A,q}x^*_{B,q} - (1+e^{-iqa})x_{B,q}x^*_{A,q}\right). \tag{19}$$

The equations of motion are given by

$$\begin{aligned}
\frac{dp_{A,q}}{dt} &= -\frac{i}{\hbar}[p_{A,q}, H] \\
&= -\frac{i}{\hbar}\frac{a}{2\pi}\int dq\left(2[p_{A,q}, x_{A,q}x^*_{A,q}] - (1+e^{iqa})[p_{A,q}, x_{A,q}x^*_{B,q}] - (1+e^{-iqa})[p_{A,q}, x_{B,q}x^*_{A,q}]\right) \\
&= -\frac{k}{2}\left(4x_{A,q} - 2(1+e^{-iqa})x_{B,q}\right) \\
&= -k\left(2x_{A,q} - (1+e^{-iqa})x_{B,q}\right), && (20) \\
\frac{dx_{A,q}}{dt} &= -\frac{i}{\hbar}[x_{A,q}, H] = \frac{p_{A,q}}{m_A}, && (21)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{dp_{B,q}}{dt} &= -\frac{k}{2}\left(4x_{B,q} - 2(1+e^{iqa})x_{A,q}\right), && (22) \\
\frac{dx_{B,q}}{dt} &= \frac{p_{B,q}}{m_B}. && (23)
\end{aligned}$$

In matrix form,

$$\begin{aligned}
\frac{d}{dt}\begin{pmatrix} x_{A,q} \\ x_{B,q} \end{pmatrix} &= -\begin{pmatrix} 2k/m_A & -k(1+e^{-iqa})/m_A \\ -k(1+e^{iqa})/m_B & 2k/m_B \end{pmatrix}\begin{pmatrix} x_{A,q} \\ x_{B,q} \end{pmatrix} \\
&\equiv -\Omega\begin{pmatrix} x_{A,q} \\ x_{B,q} \end{pmatrix} && (24)
\end{aligned}$$

The normal mode frequencies are given by the eigenvalues of the matrix Ω, which are

$$\omega^2_{\pm} = k\left(\frac{m_A+m_B}{m_Am_B} \pm \sqrt{\left(\frac{m_A+m_B}{m_Am_B}\right)^2 - \frac{4}{m_Am_B}\sin^2(\frac{qa}{2})}\right). \tag{25}$$

Since $\omega_-(q=0) = 0$, it corresponds to the acoustic branch, and ω_+ corresponds to the optical branch.

(b) As $q \to 0$,

$$\omega_-(q) = aq\sqrt{\frac{k}{2(m_A+m_B)}} + O(q^2). \tag{26}$$

Thus the speed of sound is given by

$$\begin{aligned} c &= \frac{\partial \omega_-}{\partial q}\Big|_{q\to 0} \\ &= a\sqrt{\frac{k}{2(m_A+m_B)}}. \end{aligned} \tag{27}$$

(c) At low temperature, the optical branch isn't excited, so we only need to consider the contribution of the acoustic branch to the total energy, which is given by

$$\begin{aligned} U &= 2L\int_0^{\pi/a}\frac{dq}{2\pi}\hbar\omega_-(q)\frac{1}{e^{\beta\hbar\omega_-(q)}-1} \\ &\approx 2L\int_0^{\pi/a}\frac{dq}{2\pi}\hbar c q\frac{1}{e^{\beta\hbar c q}-1} \\ &= \frac{k_B^2T^2L}{\pi\hbar c}\int_0^{\frac{\pi\hbar c\beta}{a}} dx\frac{x}{e^x-1} \\ &= \frac{k_B^2T^2L}{\pi\hbar c}\frac{\pi^2}{6} = \frac{k_B^2T^2\pi L}{6\hbar c}. \end{aligned} \tag{28}$$

The heat capacity is then given by

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{k_B^2T\pi L}{3\hbar c}. \tag{29}$$

Problem 3

Let $|\psi\rangle$ be a trial wave function of the form

$$|\psi\rangle = \sum_{i=1}^N \alpha_i|i\rangle \tag{30}$$

We try to minimize

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{i,j}\alpha_i\alpha_j^* h_{ji}}{\sum_{i,j}\alpha_i\alpha_j^* M_{ji}}. \tag{31}$$

Therefore,

$$\begin{aligned} &\frac{\partial}{\partial\alpha_k^*}\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \\ =&\frac{\partial}{\partial\alpha_k^*}\frac{\sum_{i,j}\alpha_i\alpha_j^* h_{ji}}{\sum_{i,j}\alpha_i\alpha_j^* M_{ji}} \\ =&\frac{(\sum_i\alpha_i h_{ki})(\sum_{i,j}\alpha_i\alpha_j^*M_{ji}) - (\sum_{i,j}\alpha_i\alpha_j^*h_{ji})(\sum_i\alpha_i M_{ki})}{(\sum_{i,j}\alpha_i\alpha_j^*M_{ji})^2} = 0, \end{aligned} \tag{32}$$

which implies that

$$(h\alpha)(\alpha^\dagger M\alpha) = (\alpha^\dagger h\alpha)(M\alpha). \tag{33}$$

Since $\alpha^\dagger M\alpha$ and $\alpha^\dagger h\alpha$ are just numbers,

$$h\alpha = EM\alpha, \tag{34}$$

and

$$M^{-1/2}hM^{-1/2}(M^{1/2}\alpha) = E(M^{1/2}\alpha). \tag{35}$$

Hence the best lowest-energy N solutions that are superpositions of the form $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |i\rangle$ have energies that given by the eigenvalues of the matrix:

$$H_{\text{eff}} = M^{-1/2}hM^{1/2}. \tag{36}$$

Denote by $\alpha' = M^{1/2}\alpha$ the corresponding eigenstate of H_{eff},

$$M^{-1/2}hM^{-1/2}\alpha' = E\alpha', \tag{37}$$

then

$$|\psi\rangle = \sum_{i=1}^{N}(M^{-1/2}\alpha')|i\rangle. \tag{38}$$