

Problem 1. Momentum operator Show that the state $\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$ is an eigenstate of the momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla$ and find the eigenvalue.

Solution. A state $|a\rangle$ is an eigenstate of an operator A if $A|a\rangle = a|a\rangle$, where a is a number and eigenvalue of $|a\rangle$ [1, p. 12]. Note that

$$\hat{\mathbf{p}}\psi_k(\mathbf{r}) = -i\hbar\nabla e^{i\mathbf{k}\cdot\mathbf{r}} = -i\hbar(i\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} = \hbar\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}} = \hbar\mathbf{k}\psi_k(\mathbf{r}),$$

so we have shown that $\psi_k(\mathbf{r})$ is an eigenvector of $\hat{\mathbf{p}}$ with eigenvalue $\hbar\mathbf{k}$. □

Problem 2. Density of states for free electrons

2(a) What is the fermi wavevector and fermi energy as a function of particle density for a free electron gas in one and two dimensions (define density appropriately)?

Solution. In three dimensions, the total number of occupied states inside the fermi sphere is given by Eq. (2.8) of the lecture notes,

$$N = 2 \frac{4\pi k_F^3/3}{(2\pi/L)^3}, \quad (1)$$

where k_F is the fermi wavevector, $L^3 = V$ is the volume, and 2 is the number of electron spin states. By inspection, then, the one- and two-dimensional equivalents to this equation are

$$N = 2 \frac{k_F}{2\pi/L} \quad (d=1), \quad N = 2 \frac{\pi k_F^2}{(2\pi/L)^2} \quad (d=2),$$

where k_F is the length of a one-dimensional fermi line and πk_F^2 is the area of a fermi circle of radius k_F . The one-dimensional volume is L , and the two-dimensional volume is L^2 . Solving for the wavevectors and writing them in terms of particle density $n = N/V$, we obtain

$$k_F = \pi n \quad (d=1), \quad k_F = \sqrt{2\pi n} \quad (d=2).$$

The fermi momentum is $p_F = \hbar k_F$ and the fermi energy is $E_F = p_F^2/2m$ [2, p. 36]. Both definitions hold regardless of dimension. So the fermi energy in one and two dimensions is

$$E_F = \frac{\pi^2 \hbar^2 n^2}{2m} \quad (d=1), \quad E_F = \frac{\pi \hbar^2 n}{m} \quad (d=2).$$

2(b) Calculate the density of states in energy for free electrons in one and two dimensions.

Solution. According to Eq. (2.10) of the lecture notes, the density of states $g(E)$ can be found by

$$g(E) dE = 2 \cdot \frac{\text{Volume of shell in } k \text{ space}}{\text{Volume of } k \text{ space per state}} = 2 \frac{4\pi k^2 dk}{(2\pi)^3/V},$$

where the final equality is for the three-dimensional case. For one and two dimensions, the equivalent expressions are

$$g(E) dE = 2 \frac{dk}{2\pi/L} \quad (d=1), \quad g(E) dE = 2 \frac{2\pi k dk}{(2\pi)^2/L^2} \quad (d=2).$$

Noting that

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \Rightarrow \quad \frac{dk}{dE} = \sqrt{\frac{m}{2\hbar^2 E}},$$

which again is true regardless of dimension. So we find

$$\begin{aligned} (d=1) \quad g(E) &= \frac{L}{\pi} \frac{dk}{dE} = \frac{L}{\pi} \sqrt{\frac{m}{2\hbar^2 E}}, \\ (d=2) \quad g(E) &= \frac{L^2 k}{\pi} \frac{dk}{dE} = \frac{L^2}{\pi} \sqrt{\frac{2mE}{\hbar^2}} \sqrt{\frac{m}{2\hbar^2 E}} = \frac{L^2 m}{\pi \hbar^2}. \end{aligned}$$

Per unit volume, we have

$$g(E) = \frac{1}{\pi} \sqrt{\frac{m}{2\hbar^2 E}} \quad (d=1), \quad g(E) = \frac{L^2 m}{\pi \hbar^2} \quad (d=2).$$

2(c) Show how the 3D density of states can be rewritten as

$$\frac{3}{2} \frac{n}{E_F} \sqrt{\frac{E}{E_F}} \quad (2)$$

with $n = N/V$.

Solution. The 3D density of states per unit volume is given by Eq. (2.11) in the lecture notes,

$$g(E) = \frac{V}{\pi^2} \frac{m}{\hbar^2} \sqrt{\frac{2mE}{\hbar^2}}.$$

We will work backward to reach this form from Eq. (2).

Equation (1) can be written as follows:

$$N = 2 \frac{4\pi/3}{(2\pi)^3/V} \left(\frac{2mE_F}{\hbar^2} \right)^{3/2} \quad \Rightarrow \quad n = \frac{(2mE_F)^{3/2}}{3\pi^2 \hbar^3} \quad \Rightarrow \quad E_F^3 = \frac{(3\pi^2 \hbar^3 n)^2}{(2m)^3},$$

where we have used $k = \sqrt{2mE/\hbar^2}$. Feeding the last expression into Eq. (2), we obtain

$$g(E) = \frac{3}{2} n \sqrt{\frac{E}{E_F^3}} = \frac{3}{2} n \sqrt{E \frac{(2m)^3}{(3\pi^2 \hbar^3 n)^2}} = \frac{1}{\pi^2} \frac{m}{\hbar} \sqrt{\frac{2mE}{\hbar^2}}$$

as desired. □

Problem 3. Thermodynamic properties of a free electron metal

Problem 4. Acoustic phonon dispersion in the monatomic chain By substituting Eq. (2.24) in Eq. (2.23) derive the dispersion relation Eq. (2.25) for the one-dimensional monatomic chain.

Solution. Equation (2.23) is

$$m \frac{\partial^2 u_n}{\partial t^2} = K(u_{n+1} - u_n) + K(u_{n-1} - u_n), \quad (3)$$

and Eq. (2.24) is

$$u_n(t) = u_0 \cos[qr_n - \omega(q)t]. \quad (4)$$

Using $r_n = na$ from p. 17 of the lecture notes, note that

$$\begin{aligned} \frac{2}{u_0}(u_{n+1} - u_n) &= 2 \{ \cos[q(n+1)a - \omega(q)t] - \cos[qna - \omega(q)t] \} \\ &= e^{iqna} e^{iqa} e^{-i\omega(q)t} + e^{-iqna} e^{-iqa} e^{i\omega(q)t} - e^{iqna} e^{-i\omega(q)t} - e^{-iqna} e^{i\omega(q)t} \\ &= e^{iqna} e^{-i\omega(q)t} (e^{iqa} - 1) + e^{-iqna} e^{i\omega(q)t} (e^{-iqa} - 1), \end{aligned}$$

and likewise

$$\frac{2}{u_0}(u_{n-1} - u_n) = \frac{e^{iqna} e^{-i\omega(q)t} (e^{-iqa} - 1) + e^{-iqna} e^{i\omega(q)t} (e^{iqa} - 1)}{2}.$$

Feeding these results into Eq. (3) yields

$$\begin{aligned} \frac{2m}{Ku_0} \frac{\partial^2 u_n}{\partial t^2} &= e^{iqna} e^{-i\omega(q)t} (e^{iqa} - 1) + e^{-iqna} e^{i\omega(q)t} (e^{-iqa} - 1) + e^{iqna} e^{-i\omega(q)t} (e^{-iqa} - 1) + e^{-iqna} e^{i\omega(q)t} (e^{iqa} - 1) \\ &= e^{iqna} e^{-i\omega(q)t} (e^{iqa} + e^{-iqa} - 2) + e^{-iqna} e^{i\omega(q)t} (e^{-iqa} + e^{iqa} - 2) \\ &= (e^{iqna} e^{-i\omega(q)t} + e^{-iqna} e^{i\omega(q)t}) (e^{iqa} + e^{-iqa} - 2) \\ &= 2 \cos[qna - \omega(q)t] [2 \cos(qa) - 2]. \end{aligned} \quad (5)$$

Differentiating Eq. (4), we find

$$\frac{\partial^2 u_n}{\partial t^2} = \frac{\partial}{\partial t} \left(\frac{\partial u_n}{\partial t} \right) = \frac{\partial}{\partial t} \{ u_0 \omega(q) \sin[qr_n - \omega(q)t] \} = -u_0 \omega^2(q) \cos[qr_n - \omega(q)t].$$

Making this substitution in Eq. (5) gives us

$$-\frac{m\omega^2(q)}{K} = 2[\cos(qa) - 1],$$

implying

$$m\omega^2(q) = 2K[1 - \cos(qa)] = 4K \sin^2\left(\frac{qa}{2}\right),$$

which is Eq. (2.25). □

Problem 5. Acoustic and optic phonons in the diatomic chain In the diatomic chain, we take the unit cell to be of length a , and take x_A and x_B to be the coordinates of the A and B atoms within the unit cell. Hence, in the n th cell,

$$r_{n,A} = na + x_A;$$

$$r_{n,B} = na + x_B$$

Problem 6. Lattice specific heat

6(a) From Eq. (2.44) derive the formula for the Debye specific heat Eq. (2.45).

Solution. Equation (2.44) is

$$U_D = \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2 v^3} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

From Eq. (2.43), $C_V = (\partial U / \partial T)_V$. As on p. 23 of the lecture notes, we multiply the right side by three since there are three acoustic branches. So

$$C_V = 3 \left(\frac{\partial U_D}{\partial T} \right)_V = 3 \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2 v^3} \hbar\omega \frac{\partial}{\partial T} \left(\frac{1}{e^{\hbar\omega/k_B T} - 1} \right). \quad (6)$$

Let $x = \hbar\omega/k_B T$. Then

$$\frac{\partial}{\partial T} \left(\frac{1}{e^{\hbar\omega/k_B T} - 1} \right) = \frac{\partial x}{\partial T} \frac{\partial}{\partial x} \left(\frac{1}{e^x - 1} \right) = \left(-\frac{\hbar\omega}{k_B T^2} \right) \left(-\frac{e^x}{(e^x - 1)^2} \right) = \frac{\hbar\omega}{k_B T^2} \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2}.$$

So Eq. (6) becomes

$$C_V = 3 \int_0^{\omega_D} d\omega \frac{V\hbar^2\omega^4}{2\pi^2 v^3 k_B T^2} \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2} = 3 \int_0^{\omega_D} d\omega \frac{V k_B^3 T^2}{2\pi^2 \hbar^2 v^3} \frac{x^4 e^x}{(e^x - 1)^2}.$$

We can write $x = \Theta_D/T$, where $\Theta_D = \hbar\omega_D/k_B$ as on p. 23 of the lecture notes. Then, changing our variable of integration,

$$\begin{aligned} C_V &= 3 \int_0^{\Theta_D/T} \frac{k_B T dx}{\hbar} \frac{V k_B^3 T^2}{2\pi^2 \hbar^2 v^3} \frac{x^4 e^x}{(e^x - 1)^2} = 3 \int_0^{\Theta_D/T} \frac{k_B T dx}{\hbar} \frac{V k_B^3 T^2}{2\pi^2 \hbar^2 v^3} \frac{x^4 e^x}{(e^x - 1)^2} = 3 \frac{V k_B^4 T^3}{2\pi^2 \hbar^3 v^3} \int_0^{\Theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2} \\ &= 3 \frac{V \omega_D^3}{2\pi^2 v^3} k_B \frac{T^3}{\Theta_D^3} \int_0^{\Theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2}. \end{aligned} \quad (7)$$

From Eq. (2.38),

$$\omega_D^3 = \frac{6\pi^2 v^3 N}{V} \implies 3N = \frac{V \omega_D^3}{2\pi^2 v^3}.$$

With this, Eq. (7) becomes

$$C_V = 9N k_B \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2}, \quad (8)$$

which is Eq. (2.45). □

6(b) Evaluate the integral at *high* temperature $T \gg \Theta_D$, and therefore determine the high temperature behavior of the specific heat.

Solution. When $\Theta_D \ll T$, $x \ll 1$ in the integrand of Eq. (8), and we can Taylor expand the integrand about $x = 0$ [2, p. 460]. The first term of the expansion, evaluated with Mathematica, is x^2 . Then the specific heat is

$$C_V \sim 9N k_B \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} dx x^2 = 9N k_B \left(\frac{T}{\Theta_D} \right)^3 \left[\frac{x^3}{3} \right]_{\Theta_D/T} = 3N k_B. \quad (9)$$

6(c) Using the formula

$$\int_0^\infty dx \frac{x^4 e^x}{(e^x - 1)^2} = \frac{4\pi^4}{15},$$

determine the low temperature behavior of the Debye specific heat.

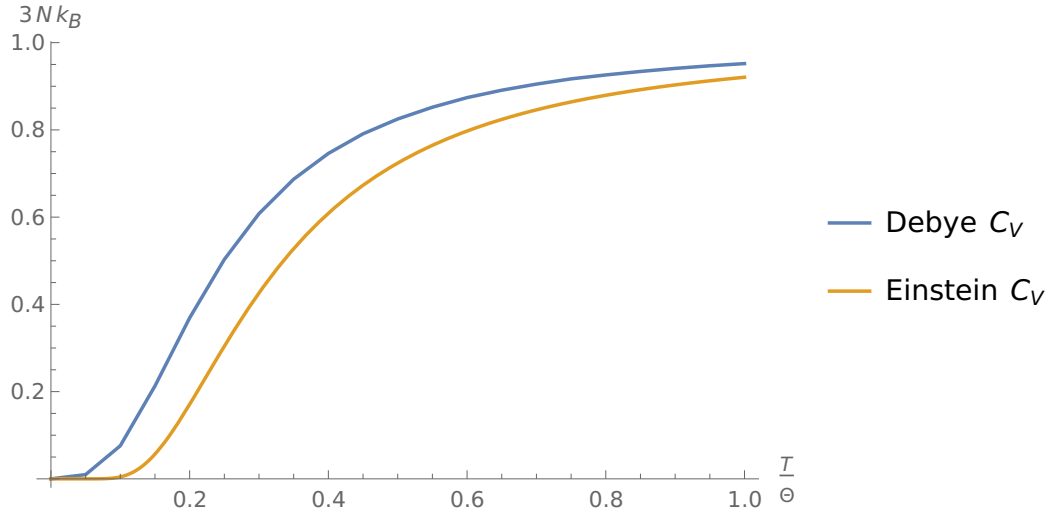


Figure 1: Comparison of the Debye (blue) and Einstein (gold) heat capacity models, where $\Theta = \Theta_D$ or Θ_E as appropriate.

Solution. Substituting the given formula into Eq. (8) where $\Theta_D/T \gg 1$ for small T , we find

$$C_V \approx 9Nk_B \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2} = 9Nk_B \left(\frac{T}{\Theta_D} \right)^3 \frac{4\pi^4}{15} = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta_D} \right)^3.$$

6(d) Sketch the heat capacity formulae from the Debye and Einstein models and compare them.

Solution. From Eqs. (8) and (9), the Debye specific heat goes as $(T/\Theta_D)^3$ at low temperatures and as $3Nk_B$ at high temperatures. So the shape of the curve will be concave up for small T/Θ_D , and the curve will asymptote as T/Θ_D from the left.

As stated on p. 22 of the lecture notes, the specific heat for the Einstein model is given by Eq. (2.43),

$$C_V = 3Nk_B \left(\frac{\Theta_E}{T} \right)^2 \frac{e^{\Theta_E/T}}{(e^{\Theta_E/T} - 1)^2}$$

where $\Theta_E = \hbar\omega_0/k_B$, and goes as $3e^{-\Theta_E/T}$ at low temperatures and as $3Nk_B$ at high temperatures. So the qualitative shape of the curve will be the same as for the Debye model. However, the Debye curve will rise much more rapidly since it has an extra factor of $4\pi^4/5$. Hence, the Einstein heat capacity will always be less than the Debye heat capacity.

Figure 1 shows both heat capacity formulae. Here, the Einstein curve is evaluated exactly with Mathematica while the Debye curve is drawn using the numerical data from Ashcroft & Mermin [2, p. 461]. As expected, both curves have the same overall shape, and the Einstein curve is below the Debye one. The difference between the models is largest at low temperatures, where the Debye model is in better agreement with experimental data [3, p. 117].

References

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