Final Exam, SIF4052, Fall 2001
Solutions

Problem 1

a) The force from atom $(n+1)$ on atom n is $K(u_{n+1} - u_n)$ from atom $(n-1)$ it is $K(u_{n-1} - u_n)$. We add the two to get the total force on atom i. Using Newton's 2. law, we equate this total force to the mass times acceleration of atom n. Equation (1.1) follows.

Inserting a harmonic wave, $u_n \propto \exp(ikna - i\omega t)$ in Eq. (1.1) gives

$$-m\omega^2 = K\left(e^{ika} - 1 + e^{-ika} - 1\right) = K\left(e^{ika/2} - e^{-ika/2}\right)^2$$
$$= -4K\sin^2\left(\tfrac{ka}{2}\right) . \tag{1}$$

Hence,

$$\omega = \sqrt{4\frac{K}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| . \tag{2}$$

The group velocity is

$$v_g = \frac{d\omega}{dk} = K\sqrt{\frac{K}{m}}\,\cos\left(\frac{ka}{2}\right) . \tag{3}$$

b) Set $x = na$ so that $u_n(t) = u(x, t)$. Hence, Eq. (1.1) may be written

$$m\frac{\partial^2 u(x,t)}{\partial t^2} = K\left(u(x+a,t) + u(x-a) - 2u(x,t)\right) . \tag{4}$$

At the macroscopic scale, x is essentially a continuous variable, and we may develop $u(x, t)$ is a Taylor series,

$$u(x \pm a, t) = u(x, t) \pm \frac{\partial u(x,t)}{\partial x}\,a + \frac{a^2}{2}\frac{\partial^2 u(x,t)}{\partial^2 x} + \cdots . \tag{5}$$

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Inserting this expression into Eq. (4) gives

$$m\frac{\partial^2 u(x,t)}{\partial t^2} = Ka^2 \frac{\partial^2 u(x,t)}{\partial^2 x} + \cdots . \qquad (6)$$

Comparing with Eq. (1.2) shows that $c = Ka^2/m$.

c) Counting the number of running waves of a chain with N atoms and with periodic boundary conditions proceeds as follows: The allowed k values are 0, $\pm j(2\pi/N)$, where $0 < j < N$ and $N\pi/N$. The distance between each allowed k value is $2\pi/N$. Hence, the density is $N/(2\pi)$. However, since there are both positive and negative k values, the density with respect to $|k|$ is N/π.

The possible k values for standing waves are $j\pi/N$, where $0 \leq j \leq N$. Hence, the density is N/π — the same result as when using running waves.

The density of states is given by

$$g(\omega)\,\frac{d\omega}{dk} = \frac{N}{\pi} . \qquad (7)$$

Combining Eqs. (2) and (3), we may write $d\omega/k$ as a function of ω. However, from Eq. (2) we note that $\omega < \sqrt{4K/m}$. Hence, the density of states is given by

$$g(\omega) = \begin{cases} \frac{2N}{\pi\sqrt{\frac{4K}{m}-\omega^2}} & \text{for } \omega \leq \sqrt{\frac{4K}{m}} \\ 0 & \text{for } \omega > \sqrt{\frac{4K}{m}} \end{cases} . \qquad (8)$$

Problem 2 The reciprocal lattice consists of all vectors $\vec{G}$ such that

$$e^{i\vec{G}\cdot\vec{R}} = 1 , \qquad (9)$$

where $\vec{R}$ are the Bravais lattice vectors.

We have that

$$\vec{R} = u\vec{a} + v\vec{b} + w\vec{c} , \qquad (10)$$

where u, v and w are integers. Likwise, we have that

$$\vec{G} = k\vec{a}^* + \vec{b}^* + m\vec{c}^* . \qquad (11)$$

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As
$$\vec{a}^* \cdot \vec{a} = \vec{b}^* \cdot \vec{b} = \vec{c}^* \cdot \vec{c} = 2\pi , \qquad (12)$$

and the product of all other combinations of promitive vectors are zero, we have that
$$\vec{G} \cdot \vec{R} = 2\pi (ku + lv + mw) . \qquad (13)$$

Hence, Eq. (9) is fulfilled and Eqs. (2.1), (2.2) and (2.3) are primitive vectors for reciprocal space.

b) The reciprocal of a reciprocal lattice is the Bravais lattice itself. This can be shown by constructing

$$\vec{a}^{**} = 2\pi \; \frac{\vec{a}^* \times \vec{b}^*}{\vec{a}^* \cdot \vec{b}^* \times \vec{c}^*} , \qquad (14)$$

and corresponding expressions for $\vec{b}^{**}$ and $\vec{c}^{**}$. By construction, the same orthogonality rules between the set $\{\vec{a}^*, \vec{b}^*, \vec{c}^*\}$ and $\{\vec{a}^{**}, \vec{b}^{**}, \vec{c}^{**}\}$ as between $\{\vec{a}^*, \vec{b}^*, \vec{c}^*\}$ and $\{\vec{a}, \vec{b}, \vec{c}\}$. Hence, $\{\vec{a}^{**}, \vec{b}^{**}, \vec{c}^{**}\}$ and $\{\vec{a}, \vec{b}, \vec{c}\}$must be the same set. This can also be shown by directly constructing the vectors $\vec{a}^{**}$, $\vec{b}^{**}$ and $\vec{c}^{**}$ — but this is somewhat messy.

c) A primitive cell is a an area that covers completely without overlap space when translated through all Bravais vectors $\vec{R}$. The Wigner-Seitz cell is the primitive cell consisting of all points closer to a given node in the Bravais lattice than any other node. The 1st Brillouin zone is the Wigner-Seitz cell in reciprocal space.

Problem 3 a) The number of electrons in the conduction band is

$$\int_{E_c}^{\infty} dE \, g(E) f(E) , \qquad (15)$$

where $g(E)$ is the density of states and $f(E)$ is the Fermi-Dirac distribution. Hence, the electron density is

$$n = \int_{E_c}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_e{}^*}{\hbar^2} \right)^{3/2} (E - E_c)^{1/2} \; \frac{dE}{e^{(E-\mu)/k_B T} + 1} . \qquad (16)$$

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When f is small, the "plus one" in its denominator is unimportant. Hence, we find

$$
\begin{aligned}
n &= \quad \frac{1}{2\pi^2}\left(\frac{2m_e{}^*}{\hbar^2}\right)^{3/2}\int_{E_c}^{\infty}(E-E_c)^{1/2}\ e^{-(E-\mu)/k_BT}dE \\
&= \frac{1}{2\pi^2}\left(\frac{2m_e{}^*}{\hbar^2}\right)^{3/2}e^{(\mu-E_c)/k_BT}(k_BT)^{3/2}\ \int_0^{\infty}x^{1/2}e^{-x}dx\ ,
\end{aligned}
\tag{17}
$$

where $E = E_c + k_BTx$. The integral is $\sqrt{\pi}/2$, and we have

$$
n = \frac{1}{4}\left(\frac{2m_e{}^*k_BT}{\pi\hbar^2}\right)^{3/2}e^{(\mu-E_c)/k_BT} = N_c e^{(\mu-E_c)/k_BT}\ .
\tag{18}
$$

b) The relative probability that the donor is neutral is

$$
1 + e^{(\mu-E_d)/b_BT} + e^{(\mu-E_d)/k_BT} = 1 + 2e^{(\mu-\mathcal{E})/k_BT}\ .
\tag{19}
$$

The factor two comes from the electron *either* being in a spin-up or a spin-down state. The mean number of valence electrons on the donors is then

$$
N_d - n_d = \frac{0\cdot 1 + 1\cdot e^{(\mu-E_d)/k_BT} + 1\cdot e^{(\mu-E_d)/k_BT}}{1 + 2e^{(\mu-E_d)/k_BT}}\ .
\tag{20}
$$

Hence,

$$
n_d = \frac{N_d}{1 + 2e^{(\mu-E_d)/k_BT}}\ .
\tag{21}
$$

At $T = 0$, the system is in the ground state with filled donor levels and empty conduction band. Hence,

$$
E_d < \mu < E_c
\tag{22}
$$

in this case.

Charge balance dictates

$$
n = n_d + p\ .
\tag{23}
$$

When the valence band is fully occupied, $p = 0$, and we have that

$$
n = n_d\ .
\tag{24}
$$

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Hence,

$$N_c e^{(\mu - E_c)k_B T} = \frac{N_d}{1 + 2e^{(\mu - E_d)/k_B T}} \ . \tag{25}$$

Solving this equation with respect to μ gives

$$\mu = E_d + k_B T \log\left[\frac{1}{4}\sqrt{1 + \frac{8N_d}{N_c}e^{(E_c - E_d)/k_B T}} - \frac{1}{4}\right] \ . \tag{26}$$

At low temperatures, the term $8N_d/N_c \exp[(E_c - E_d)/k_B T]$ dominates and

$$\mu \approx E_d + \frac{1}{2}k_B T \log\left[\frac{8N_d}{N_c}e^{(E_c - E_d)/2k_b T}\right] = E_d + \frac{E_c - E_d}{2} + \frac{1}{2}k_B T \log\left[\frac{8N_d}{N_c}\right] \ . \tag{27}$$

Since $N_c \propto T^{3/2}$, the last term in Eq. (27) is proportional to $T \log T \to 0$ as $T \to 0$. Hence,

$$\mu = \frac{E_c + E_d}{2} \ , \tag{28}$$

at $T = 0$.

c) Inserting the expression for μ, Eq. (3.7) in Eq. (3.6), using $n = n_d$, Eq. (24), we find the sought-after result, Eq. (3.8).

d) At high temperature, it is no longer possible to ignore thermal excitation of electrons in the valence band. When the majority of electrons in the conduction band come from the valence band, i.e., when $p >> n_d$, the semiconductor is *intrinsic*. We have seen in the lectures that in the high-temperature limit of an intrinsic semiconductor, the chemical potential approaches the halfway point between E_v — the top of the valence band and E_c, $\mu \to (E_v + E_c)/2$. The number of electrons in the conduction band will reach a plateau — the saturation range — when the donors are all ionized but the electrons in the valence band still are not excited. In the intrinsic range, n increases boundlessly. This is sketched in Fig. 6.53 in the texbook by Elliott.