# Solutions for Homework Set 4 

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1. Kittel Problem 5.3

## Solution

(a) We are given that

$$
\left\langle R^{2}\right\rangle=\frac{\hbar}{2 \rho V} \sum \omega^{-1}
$$

where the sum is over all independent phonon modes. We may replace this summation by an integral over the density of states in the Debye approximation, and account for the 3 -fold degeneracy in the modes (we are in an isotropic medium, so polarisation is independent of velocity). Also the density of states is given by

$$
\mathcal{D}(\omega)=\frac{V \omega^{2}}{2 \pi^{2} v^{3}} .
$$

Hence,

$$
\begin{align*}
\left\langle R^{2}\right\rangle & =\frac{3 \hbar}{2 \rho V} \int_{0}^{\omega_{D}} \mathcal{D}(\omega) \omega^{-1} \mathrm{~d} \omega \\
& =\frac{3 \hbar \omega_{D}^{2}}{8 \pi^{2} v^{3} \rho} \tag{1}
\end{align*}
$$

(b) In one dimension we have

$$
\left\langle R^{2}\right\rangle \propto \sum \omega^{-1}
$$

so we show that the sum over modes diverges. One approach is to note that the allowed wavevectors take the form $K=2 \pi n / L$, with $n$ an integer. In the Debye approximation we have $\omega=K v$, and so $\omega \propto n$. Hence,

$$
\left\langle R^{2}\right\rangle \propto \sum \omega^{-1} \propto \sum_{n} n^{-1}=\infty
$$

as a harmonic series diverges. Therefore, $\left\langle R^{2}\right\rangle$ and $\sum \omega^{-1}$ both diverge. However, more explicitly

$$
\begin{align*}
\left\langle R^{2}\right\rangle \propto \sum \omega^{-1} & =\int_{0}^{\omega_{D}} \mathcal{D}(\omega) \omega^{-1} \\
& =\int_{0}^{\omega_{D}} \frac{L}{\pi v \omega} \mathrm{~d} \omega \\
& =\infty \tag{2}
\end{align*}
$$

as $\ln 0=\infty$.
The mean square strain is given by $\left\langle(\partial R / \partial x)^{2}\right\rangle=\sum K^{2} u_{0} / 2$ where $u_{0}=\hbar / 2 \rho V \sum \omega^{-1}$.
For a line of $N$ atoms of mass $M$ including only longitudinal modes we convert the sum to an integral giving:

$$
\begin{align*}
\left\langle\left(\frac{\partial R}{\partial x}\right)^{2}\right\rangle & =\int_{0}^{\omega_{D}} \mathcal{D}(\omega) k^{2} \frac{\hbar}{2 \rho V \omega} \\
& =\frac{\hbar}{2 \rho V \omega} \int_{0}^{\omega_{D}} \frac{L}{\pi v} \frac{\omega}{v^{2}} \mathrm{~d} \omega \\
& =\frac{L \hbar \omega_{D}^{2}}{4 M N v^{3}} \tag{3}
\end{align*}
$$

where $\rho L=M N$ is the mass of the lattice, and so the mean square strain is

$$
\begin{equation*}
\frac{L \hbar \omega_{D}^{2}}{4 M N v^{3}} . \tag{4}
\end{equation*}
$$

Note that in this problem there is an ambiguity of a factor of 2 . This originates from a typo in Kittel Equation (4.29) has an extra factor of a $1 / 2$. Try and work it out for yourself!

## Solution

(a) The layers are de-coupled so the problem becomes a $2 D$ one, with modes propagating only in the plane of layers. Hence, the 2D density of states within a plane is given by

$$
\mathcal{D}(\omega)=\frac{L^{2}}{2 \pi} \frac{\omega}{v^{2}}
$$

Then, the energy of the system is given by in the Debye approximation:

$$
\begin{align*}
U & =\int_{0}^{\infty} \mathcal{D}(\omega)\langle n(\omega)\rangle \hbar \omega \mathrm{d} \omega \\
& =\int_{0}^{\omega_{D}} \frac{A \omega}{2 \pi v^{2}} \frac{\hbar \omega}{e^{\hbar \omega / k_{b} T}-1} \mathrm{~d} \omega \\
& =\frac{A k_{b}^{3} T^{3}}{2 \pi \hbar^{2} v^{2}} \int_{0}^{x_{D}} \frac{x^{2}}{e^{x}-1} \tag{5}
\end{align*}
$$

where in the last line we define $x=\hbar \omega /\left(k_{b} T\right)$. In the low temperature limit the integral extends to infinity, and is now independent of temperature. To find the heap capacity, one can then differentiate the resulting expression with respect to $T$, or alternatively differentiate the second line in (5) above for a general temperature. In any case one finds that,

$$
\begin{equation*}
C_{V} \propto T^{2} \tag{6}
\end{equation*}
$$

(b) As the coupling between layers becomes stronger we expect that the heat capacity should go from the $2 D$ result to the $3 D$ result. That is, we expect $C \propto T^{n}$, where $n$ goes from $n=2 \rightarrow 3$.
In $2 D$, at low temperatures $x_{D} \rightarrow \infty$, giving

$$
\begin{equation*}
C_{v} \propto \frac{3 A k_{b}^{2}}{\pi v^{2} \hbar^{2}} \zeta(3) T^{2} \tag{7}
\end{equation*}
$$

where $\zeta(z)$ is the Riemann zeta function. Similarly we know that at low temperatures $C_{v} \propto T^{3}$ for $3 D$, and hence, with weak coupling between layers $C_{V} \propto T^{2}$, as $T^{2}$ dominates $T^{3}$ at low temperatures.

## 3. Kittel Problem 5.4

## Solution

The energy of an arbitrary system is given by

$$
\begin{equation*}
U=\int_{0}^{\infty} \varepsilon n(\varepsilon) \mathcal{D}(\varepsilon) \mathrm{d} \varepsilon \tag{8}
\end{equation*}
$$

which for a free electron gas coincides exactly with the kinetic energy (i.e. no potential energy). Also, $\mathcal{D}(\varepsilon)$ is the density of states for the free electron gas in $3 D$. Explicitly this is given by,

$$
\begin{equation*}
\mathcal{D}(\varepsilon)=\frac{V}{2 \pi^{2}}\left(\frac{2 m}{\hbar^{2}}\right)^{3 / 2} \varepsilon^{1 / 2} \tag{9}
\end{equation*}
$$

Hence, as we are at $T=0$ the Fermi-Dirac distribution is given by the usual step-function giving:

$$
\begin{align*}
U_{0} & =\int_{0}^{\varepsilon_{f}} \frac{V}{2 \pi^{2}}\left(\frac{2 m}{\hbar^{2}}\right)^{3 / 2} \varepsilon^{3 / 2} \mathrm{~d} \varepsilon \\
& =\frac{V}{2 \pi^{2}}\left(\frac{2 m}{\hbar^{2}}\right)^{3 / 2} \frac{2 v e_{f}^{5 / 2}}{5} \\
& =\frac{3}{5} N \varepsilon_{f} \tag{10}
\end{align*}
$$

where in the last line we use

$$
N=\frac{V}{3 \pi^{2}}\left(\frac{2 m \varepsilon}{\hbar^{2}}\right)^{3 / 2}
$$

## Solution

We use the definition of $N$ in terms of $\mathcal{D}(\varepsilon)$ and the Fermi-Dirac distribution function to determine $\mu$ the chemical potential. In $2 D$ the density of states is a constant given by

$$
\mathcal{D}(\varepsilon)=\frac{m}{\pi \hbar^{2}}
$$

The number density of electrons $n=N / V$ in our system at a temperature $T$ is then,

$$
\begin{align*}
n & =\int_{0}^{\infty} \mathcal{D}(\varepsilon) n(\varepsilon) \\
& =\frac{m}{\pi \hbar^{2}} \int_{0}^{\infty} \frac{\mathrm{d} \varepsilon}{e^{(\varepsilon-\mu) / k_{b} T}+1} \\
& =\frac{m k_{b} T}{\pi \hbar^{2}} \int_{0}^{\infty} \frac{e^{-x}}{e^{-\mu / T}+e^{-x}} \mathrm{~d} x \\
& =\frac{m k_{b} T}{\pi \hbar^{2}} \log \left(1+e^{\mu / T}\right) \tag{11}
\end{align*}
$$

Therefore, rearranging for $\mu$ :

$$
\begin{equation*}
\mu=k_{B} T \log \left(e^{\pi \hbar^{2} n / m k_{b} T}-1\right) \tag{12}
\end{equation*}
$$

