Physics 361 Solutions to Problem Sets 3,4

November 1, 2002

1 Typical Compressibilities and Frequencies

$$\phi(r) \equiv 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

We need to estimate both N, the number of atoms in 1 cm^3 and the change in energy per atom Δu during the compression. For the Lennard-Jones potential, the equilibrium spacing is $r_0 = 2^{1/6}\sigma$. The FCC crystal structure has coordination number 12, $a = r_0\sqrt{2}$, and volume per atom $v = a^3/4$. For $\sigma = 5.40$ A this gives $N = V/v = 2.5 \times 10^{22}$. For the change in potential energy, $\Delta u = \frac{1}{2} \cdot 12 \cdot [\phi(r_0 - \Delta r) - \phi(r_0)]$ with $[(r_0 - \Delta r)/r_0]^3 = 0.99$ for a compression of 1%. The result is $\Delta u = 24\epsilon \times 10^{-3}$. The value $\epsilon = 0.167 \times 10^{-13}$ erg gives $N\Delta u = 0.1$ J.

The bulk modulus B is related to the pressure P and the volume V by

$$\begin{aligned} B &\equiv -V\left(\frac{\partial P}{\partial V}\right) \\ &= -\frac{\partial P}{\partial(\ln V)} \\ P &= B\ln(V_i/V) = B\ln\left(\frac{1}{1-\delta'}\right) \approx B\delta' \end{aligned}$$

where $\delta' \equiv (V_i - V)/V_i$. The work is then

$$\begin{aligned} W &= -\int_{V_i}^{V_f} P\, dV \\ &= V_i \int_0^{\delta} B\delta'\, d(\delta') \\ &= \frac{1}{2} B V_i \delta^2 \end{aligned}$$

where $\delta \equiv (V_i - V_f)/V_i = 0.01$. The bulk modulus of iron is 160 GPa, so the energy required to compress one cubic centimeter by one percent is $\frac{1}{2}(160\times10^9 \text{ Pa})(10^{-6} \text{ m}^2)\times10^{-4} = 8.0$ J.

The bulk modulus of water is 2.2 GPa, giving 0.11 J. This is to be compared to 0.10 J for argon.

For small displacements, $\phi(r_0 + \Delta r) - \phi(r_0) = 36\epsilon(\Delta r/r_0)^2$ to leading order in $\Delta r/r_0$. This means the effective spring constant between nearest neighbors is $k = 72\epsilon/r_0^2 = 0.824$ N/m for argon. Using the atomic mass 40 for argon, as well as the assumption that the net restoring force for the 12 nearest neighbors is roughly 12 times the single-neighbor restoring force, $\omega = \sqrt{12k/m} = 1.22 \times 10^{13}$ s^{-1} for the angular frequency. This corresponds to a photon wavelength $\lambda = 155\,\mu$ and energy 8 meV $= 1.28 \times 10^{-21}$ J. At room temperature, $k_B T = 4.14 \times 10^{-21}$ J, which is comparable. The energy of a spin flip is given by the Bohr magneton $\mu_B = 9.27 \times 10^{-24}$ J/Tesla which, in a field of 1 Tesla, is smaller by 2 orders of magnitude.

The diamond structure is given on page 76. It has coordination number 4, $r_0 = a\sqrt{3}/4$, $v = a^3/8$. With the values $\epsilon = 3$ eV and $\sigma = 0.168$ nm, we find $\hbar\omega = 300$ meV, about 40 times the vibration frequency of argon.

2 Lennard-Jones chain

The equilibrium length of the entire chain is Nr_0. If the chain is stretched by a factor γ, then the nearest neighbor spacing becomes $\tilde{r} = r_0 + \Delta r = (1+\gamma)r_0$. The force per atom f required to stretch the chain is given by the first derivative of the potential:

$$f = -\phi'(\tilde{r}) = 4\frac{\epsilon}{r_0}\left[-3(1+\gamma)^{-13} + 3(1+\gamma)^{-7}\right] \approx -72\gamma\epsilon/r_0$$

To find the dispersion of compressional waves, note that the second derivative of ϕ gives the effective spring constant at the new equilibrium position:

$$k_L = \phi''(\tilde{r}) = \frac{4\epsilon}{r_0^2}\left[39(1+\gamma)^{-14} - 21(1+\gamma)^{-8}\right] \approx 72\frac{\epsilon}{r_0^2}(1 - 21\gamma)$$

Then the dispersion for small oscillations becomes $\omega(p) = 2\omega_L|\sin(p\tilde{r}/2)|$ where $\omega_L = \sqrt{k_L/m}$. In the long wavelength limit, $\omega(p) \to p\omega_L\tilde{r}$, which gives the velocity

$$c_L = \omega_L\tilde{r} \approx \omega_L|_{\gamma=0}\, r_0\left(1 - \frac{21}{2}\gamma\right)(1+\gamma) \approx \omega_L|_{\gamma=0}\, r_0\left(1 - \frac{19}{2}\gamma\right)$$

and the speed of waves decreases as the chain is stretched.

The potential for tranverse motion of atom i is

$$U(y_i) = \phi(\sqrt{\tilde{r}^2 + (\Delta y_i)^2}) + \phi(\sqrt{\tilde{r}^2 + (\Delta y_{i+1})^2})$$

where $\Delta y_i = y_i - y_{i-1}$. The effective spring constant is

$$k_T = \partial_{\Delta y}^2\, \phi(\sqrt{\tilde{r}^2 + (\Delta y)^2})\Big|_{\Delta y=0} = \phi'(\tilde{r})/\tilde{r} \approx 72\gamma\frac{\epsilon}{r_0^2}$$

The long wavelength form of the dispersion applies and $c_T = \omega_T\tilde{r}$. Relative to the longitudinal speed this is $c_T/c_L = \sqrt{k_T/k_L} = \sqrt{\gamma}$.

3 2D Specific Heat

The density of states integral in two dimensions is $\int d^2k/(2\pi)^2 \rightarrow kdk/2\pi$. For a linear dispersion $\omega = ck$, the density of states is $g(\omega) = \omega/(2\pi c^2)$. There is one transverse and one longitudinal mode, so the total density of states (per unit volume) is $g(\omega) = \omega/(2\pi) \cdot (1/c_L^2 + 1/c_T^2)$.

Suppose the longitudinal dispersion has a maximum at k_0 as $\omega_L(k) = \omega_0 - A(k-k_0)^2$. A quadratic dispersion has a constant density of states in two dimensions since $d\omega \propto |k - k_0|\, d|k - k_0|$. Specifically,

$$g(\omega) = \int d^2k/(2\pi)^2 \delta(\omega - \omega_0 - A(\vec{k} - \vec{k}_0)^2)$$

Defining $(\vec{k} - \vec{k}_0)$ as $\vec{x}$,

$$g(\omega) = \int \frac{1}{2}(2\pi dx^2)/(2\pi)^2 \;\; \delta(\omega - \omega_0 - Ax^2) = \pi/(2\pi)^2(1/A) \int d(Ax^2)\; \delta(\omega - \omega_0 - Ax^2).$$

The integral is 1, so that

$$g(\omega) = (4\pi A)^{-1}$$

However, there are no states above the maximum, so the density of states changes discontinuously at ω_0 from $(4\pi A)^{-1}$ below to zero above.

4 Phonon numbers in a mode

The probability of the occuption number of the mode being n is $P_n = e^{-\beta\hbar\omega n}/Z$, so the most probable occupation number is always $n = 0$. For the variance, note that $\langle (n - \langle n \rangle)^2 \rangle = \langle n^2 \rangle - \langle n \rangle^2$.

$$\begin{aligned}
\left\langle n^2 \right\rangle &= \sum_{n=0}^{\infty} P_n n^2 \\
&= \frac{1}{Z} \sum_{n=0}^{\infty} n^2 e^{-\beta\hbar\omega n} \\
&= \frac{1}{Z} \frac{1}{(\hbar\omega)^2} \partial_\beta^2 \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} \\
&= \frac{1}{Z} \frac{1}{(\hbar\omega)^2} \partial_\beta^2 Z(\beta)
\end{aligned}$$

The partition function is $Z(\beta) = (1 - e^{-\beta\hbar\omega})^{-1}$. The result can be simplified using $e^{\beta\hbar\omega} = \langle n \rangle^{-1} + 1$ to give $\langle n^2 \rangle = \langle n \rangle (2 \langle n \rangle + 1)$ and

$$\left\langle n^2 \right\rangle - \langle n \rangle^2 = \langle n \rangle^2 + \langle n \rangle$$

For small $\langle n \rangle$, the variance is of order $\langle n \rangle$. For large $\langle n \rangle$ it is of order $\langle n \rangle^2$.

5 Poor man's localization

From the frequency $\omega^2 = (K+G)/M$ and the dispersion $\omega(k)$ we obtain the condition $K^2 + G^2 + 2KG\cos ka = 0$. The solution is to take $k = \pi/a \pm il$ so that $\cosh(la) = (K^2+G^2)/2KG$. Since the right-hand side is always greater than 1 (by $(K-G)^2 > 0$) there is always a real number l that satisfies this equation. The corresponding modes decay as $(-1)^n e^{-l(na)}$ where (na) is the distance from the end of the chain. The limit $K \to G$ is a long wavelength limit, and we may take $\cosh(la) \approx 1 + (la)^2/2 = (K^2+G^2)/2KG$ with solution $la = |K-G|/\sqrt{KG}$. The penetration depth can be defined as $1/l \to Ka/|K-G|$ in this limit.

6 Inelastic scattering

The amplitude of particles arriving at the detector is

$$\begin{aligned}
\psi(t) &= Ae^{-i\Omega t}\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{r}(\mathbf{R},t)} \\
&= Ae^{-i\Omega t}\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot[\mathbf{R}+\mathbf{u}_0\cos(\mathbf{k}\cdot\mathbf{R}-\omega t)]} \\
&\approx Ae^{-i\Omega t}\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}\left[1 + i\frac{1}{2}(\mathbf{q}\cdot\mathbf{u}_0)\left(e^{i(\mathbf{k}\cdot\mathbf{R}-\omega t)} + e^{-i(\mathbf{k}\cdot\mathbf{R}-\omega t)}\right)\right]
\end{aligned}$$

where we have expanded for $\mathbf{q}\cdot\mathbf{u}_0 \ll 1$. Rearranging,

$$\psi(t) \approx Ae^{-i\Omega t}\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} + i\ A\frac{1}{2}(\mathbf{q}\cdot\mathbf{u}_0)e^{-i(\Omega+\omega)t}\sum_{\mathbf{R}} e^{i(\mathbf{q}+\mathbf{k})\cdot\mathbf{R}} + i\ A\frac{1}{2}(\mathbf{q}\cdot\mathbf{u}_0)e^{-i(\Omega-\omega)t}\sum_{\mathbf{R}} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{R}}$$

At this point, we can see that the scattered beam will contain frequencies $\Omega \pm \omega$.

In this form, we can see that the lattice sums of the form $\exp i\mathbf{K}\cdot\mathbf{R}$ will vanish unless $\mathbf{K}$ is in the reciprocal lattice. Therefore, the strongest peaks will be at $\mathbf{q} = \mathbf{K}$ in the reciprocal lattice, and secondary peaks will appear at $\mathbf{q} = \mathbf{K} \pm \mathbf{k}$ with intensity diminished by a factor $(\mathbf{q}\cdot\mathbf{u}_0)^2/4$.

Since the crystal has no particular alignment, only $\mathbf{K} = 0$ in the reciprocal lattice is guaranteed to backscatter coherently, so that $\mathbf{q} = \pm\mathbf{k}$. Note that the definition of $\psi(t)$ implies $\mathbf{q} = \mathbf{k}_{in} - \mathbf{k}_{out}$. Since the radiation is backscattered ($\mathbf{k}_{in}$ is antiparallel to $\mathbf{k}_{out}$) and the wavevector of the phonon is parallel to $\mathbf{k}_{out}$, then $\mathbf{k}$ is antiparallel to $\mathbf{q}$ and $\mathbf{q} + \mathbf{k} = \mathbf{0}$. Backscattered radiation will add coherently only for the component of $\psi(t)$ which varies as $e^{i(\mathbf{q}+\mathbf{k})\cdot\mathbf{R}}$. This component has time dependence $e^{-i(\Omega+\omega)t}$ implying that its energy is $\Omega + \omega$. Energy is added to the beam, since it is reflected from an approaching wave.