Solid State Physics
Solutions, Homework Set for Chapter 5

This problem deals with the vibrations of the two-dimensional gas-atom surface. A monolayer of gas atoms is deposited on an atomically perfect surface. Consider first a model in which the effect of the surface is simply to constrain the atoms to move in the $z = 0$ plane. The atoms form a square lattice (with $a = 3\mathring{A}$), and for small $\mathbf{k} = (k_x, k_y)$, the equations of motion give

$$-M\omega^2 e_i(\mathbf{k}) = -A(k_x^2 + k_y^2)e_i(\mathbf{k}) \quad i = x, y$$

where $M = 6.7 \times 10^{-23}$ gm, and $A = 6.7 \times 10^{-12}$ gmcm^2/sec^2
a. Find the normalized density of states (frequencies) per unit frequency near $\omega = 0$.

The dynamical matrix in this case is diagonal, and thus there are two degenerate solutions

$$\omega_i = \sqrt{A/M}k = ck$$

Of course, this linear dispersion will only hold for small k (in a more realitic system, the k^2 in the equation of motion comes from expanding $\cos(k_x) + \cos(k_y)$ for small k).

The density of states may be calculated in the usual fashion. First, we must establish the Debye cutoff momentum Since there are two modes,

$$2N = 2a^2 \int \frac{d^2k}{(2\pi)^2}\Theta(k_D - k)$$

or $k_D = \sqrt{4\pi N/a^2}$. Then, the DOS is given by the usual expression

$$\begin{aligned} g_i(\omega) &= a^2 \int \frac{d^2k}{(2\pi)^2}\delta(\omega - \omega_i(k)) \\ &= a^2 \int \frac{d^2k}{(2\pi)^2}\delta(\omega - ck)\Theta(k_D - k) \\ &= \frac{a^2\omega}{2\pi c^2}\Theta(\omega_D - \omega) \end{aligned}$$

b. Give an expression for the low temperature specific heat as a function of temperature. What is the specific heat at 100K?

To calculate the specific heat $C = \partial U/\partial T$ we need to first calculate the internal energy U

$$U = \int_0^{\omega_D} d\omega g(\omega) < n(\omega) > \hbar\omega = \int_0^{\omega_D} d\omega \frac{ML^2\omega}{2\pi A}\frac{1}{e^{\beta\hbar\omega} - 1}\hbar\omega = \frac{ML^2\hbar}{2\pi A}\int_0^{\omega_D} d\omega \frac{\omega^2}{e^{\beta\hbar\omega} - 1}$$

In the low T limit it is safe to let $\omega_D \to \infty$ since the integrand will be zero long before we reach $\omega = \omega_D$. We can then solve the integral, by substituting $x = \beta\hbar\omega$ the above integral can be reduced to

$$\frac{d\omega}{dx}\int_0^\infty dx \frac{x^2}{e^x - 1} = \frac{1}{\beta\hbar}\sum_{s=1}^{\infty}\int_0^\infty dx x^2 e^{-sx} = \frac{\Gamma(3)}{\beta\hbar}\sum_{s=1}^{\infty}\frac{1}{s^3} = \frac{\zeta(3)\Gamma(3)}{\beta\hbar} = \frac{2.0404}{\beta\hbar}$$

where $\Gamma(3) = \Gamma(2+1) = 2! = 2$ and $\zeta(3) == 1.202$. Then the U can be written as

$$U = \frac{2.0404 M L^2 k_B^3 T^3}{2\pi A \hbar^2} \Rightarrow C = \frac{7.212 M L^2 k_B^3 T^2}{2\pi A \hbar^2}$$

c. Is the Debye-Waller factor finite or zero and why?

Debye-Waller factor is

$$f(T) = e^{-\left\langle \sum_s <n_s|(k.u)^2|n_s> \right\rangle_T}$$

Assuming that k of the gamma ray is uncorrelated with $\bar{U}(0)$

$$< (k.u)^2 >= \frac{1}{2} k^2 < u^2 > \ \ since \ \frac{1}{2\pi} \int d\theta cos^2\theta = 1/2$$

Then

$$< u^2(0) >= \sum_s \frac{\hbar}{2MN\omega_s} \left(\frac{2}{e^{\beta\omega} - 1} + 1 \right) \sim \int d\omega \left(\frac{2}{e^{\beta\omega} - 1} + 1 \right)$$

For small ω the integrand is $\frac{1}{\beta\omega} + 1$, thus the integral diverges logarithmically and $f(T)$ is then zero.

d. Now account for the potential of the surface, ie. allow for the corrugation of the surface by adding a potential energy

$$\phi = \frac{K}{2} \sum_{n,i} s_{ni}^2$$

where s is, as usual, the displacement from equilibrium, and $K = 6.7 \times 10^4$ gm/sec^2. The wave solutions are of the form

$$s_{ni} = e_{ni} e^{(i\mathbf{k}\cdot\mathbf{r}_n - \omega t)}$$

What are the new frequencies for $\mathbf{k} = 0$?

Corrugation potential

$$\Phi = \frac{k}{2} \sum_{\alpha,\beta r,r'} u_\alpha(r) \frac{\partial^2 \Phi}{\partial r^\alpha \partial r'^\beta} u_\beta(r')$$

If we substitute in the given form for the corrigation potential, then we see that it contributes a term

$$\frac{\partial^2 \Phi}{\partial r^\alpha \partial r'^\beta} = \delta_{\alpha\beta} \delta_{rr'} K$$

thus D is modified as

$$D_{\alpha\beta}(k) = \sum_r e^{-ik.r} D_{\alpha\beta}(r) \Rightarrow \begin{cases} D_{11}(k) = \frac{A}{M}(k_x^2 + k_y^2) + \frac{K}{M} \\ D_{22}(k) = \frac{A}{M}(k_x^2 + k_y^2) + \frac{K}{M} \\ D_{33}(k) = \frac{K}{M} \end{cases}$$

Thus clearly for $k = 0$ $\omega = \sqrt{K/M}$

e. What is the form of the temperature dependence of the specific heat neat $T = 0$?

For $T \to 0$ only low frequency modes $\hbar\omega \sim kT$ are excited thus the dominant mode will be $\omega = \sqrt{K/M}$ and we will have an Einstein specific heat

$$\begin{cases} U = N \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} \\ \omega = \sqrt{K/M} \end{cases} \Rightarrow C = Nk\left(\hbar\omega/kT\right)^2 \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2} \simeq e^{-\hbar\omega/kT}/T^2 \simeq e^{-\hbar\omega/kT}$$

f. Is the Debye-Waller factor finite or zero and why?

Here the Debye Waller factor is finite as the oscillations are limited by the corrugation potential. Again considering the low-T limit where only the lowest energy modes are excited

$$U = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} =< T > + < V >= 2 < T >= K < x^2 >$$

where we used Virial theorem

$$< x^2 >= \frac{\hbar}{\sqrt{kM}(e^{\hbar\omega/kT} - 1)}$$

which is finite.