1 PS1–4

(a) ***Problem:*** *Consider $\omega = \omega_0 \sin \left|\frac{ka_0}{2}\right|$ a phonon dispersion relation in 1D. Compute the resulting density of states.*

We know that the density of states $\mathcal{D}(\omega)$ is the phase space density in momentum space that produces frequency ω under the dispersion relation. Thus, with s indexing the number of types of phonons,

$$\mathcal{D}(\omega) = \sum_s \int \frac{1}{2\pi}\delta(\omega - \omega(k))\mathrm{d}k \tag{1}$$

$$= \sum_s \int \frac{1}{2\pi}\frac{1}{\omega'(k_0)}\delta(k - k_0)\mathrm{d}k \tag{2}$$

where $\omega(k_0) = \omega$, or $k_0 = \frac{2}{a_0}\arcsin\frac{\omega}{\omega_0}$. Thus,

$$\omega'(k_0) = \frac{a_0\omega_0}{2}\cos\left|\arcsin\frac{\omega}{\omega_0}\right| \tag{3}$$

$$= \frac{a_0\omega_0}{2}\sqrt{1 - \frac{\omega^2}{\omega_0^2}} \tag{4}$$

$$= \frac{a_0}{2}\sqrt{\omega_0^2 - \omega^2} \tag{5}$$

$$\mathcal{D}(\omega) = \sum_s \int \frac{1}{2\pi}\frac{2}{a_0}\left(\omega_0^2 - \omega^2\right)^{-1/2}\delta(k - k_0)\,\mathrm{d}k \tag{6}$$

$$= \frac{2}{\pi a_0}\left(\omega_0^2 - \omega^2\right)^{-1/2} \tag{7}$$

(b) ***Problem:*** *Consider now an arbitrary dispersion relation in three dimensions $\omega(\vec{k})$. Compute the dependence of the density of states near a maximum of ω.*

Returning to our earlier expression

$$\mathcal{D}(\omega) = \sum_s \int \frac{1}{2\pi}\delta(\omega - \omega(\vec{k}))\mathrm{d}\vec{k} \tag{8}$$

Ignoring the $\sum\limits_s$ for now, we note that the δ function constrains us to a 2-dimensional subspace. What subspace? Let's expand $\omega(\vec{k})$ about its maximum

$$\omega(\vec{k}) = \omega_{\max} - \sum_{i=1}^{3} a_i\xi_i^2 \tag{9}$$

for positive a_i, $\xi_i = k_i - k_{\max}$. Then, the subspace of $\mathrm{d}\vec{k}$ that we are constrained to is that satisfying

$$\omega - \omega_{\max} + a_i\xi_i^2 = 0 \tag{10}$$

$$a_i\xi_i^2 = \Delta\omega \tag{11}$$

where we define $\Delta\omega > 0 = \omega_{\max} - \omega$. This is clearly an ellipse; call the set of points satisfying (11) S_W, then (8) becomes

$$\mathcal{D}(\omega) = \sum_s \int \frac{1}{2\pi}\frac{1}{v_g}\mathrm{d}S_\omega \tag{12}$$

with $v_g = \dfrac{\mathrm{d}\omega(k)}{\mathrm{d}k}$ the normal derivative to S_ω, generalizing from the 1-D property $\delta(f(a)) = \dfrac{1}{f'(a_0)}\delta(a-a_0)$.

If we follow up to here, then let's switch to polar coordinates to evaluate the integral. S_ω becomes $r^2\mathrm{d}\theta\mathrm{d}\phi$ and we obtain

$$\int \frac{\mathrm{d}S_\omega}{v_g} = \int_0^{2\pi}\int_0^{\pi}\frac{r^2(\theta,\phi)\mathrm{d}\theta\mathrm{d}\phi}{v_g(\theta,\phi)} \tag{13}$$

But then it's clear that $r^2 \propto \Delta\omega$, since $r^2 = \sum\limits_{i=1}^{3}\xi_i^2$. At the same time, $v_g(\theta,\phi)$ is a linear combination of the ξ_i and so scales like $\sqrt{\Delta\omega}$. Thus, the above integral scales like $\sqrt{\Delta\omega} = \sqrt{\omega_{\max} - \omega}$.

I know this ending is a bit shaky; can probably come up with something better by explicitly finding $r^2(\theta,\phi)$, which will depend on the a_i coefficients.

(c) ***Problem:*** *Consider now a 2D dispersion relation. Compute $\mathcal{D}$ near a saddle point of $\omega(\vec{k})$.*

Following our above reasoning, we want to know what shape S_ω takes on. Near a saddle point in ω, a plane of constant ω forms a hyperbolic cross section. Thus, if we follow the same sort of dimensional analysis as before, we'd expect $S_\omega \propto r \propto \sqrt{\Delta\omega}$, and still $v_g \propto \sqrt{\Delta\omega}$ and obtain a constant dependence on $\Delta\omega$. This is indeed correct for $\vec{k}$ near an extremum of ω, but not quite correct for a saddle point.

We err in our analysis because we can only consider a finitely large range of k, and with a hyperbolic cross section, a change in $\Delta\omega$ not only changes the S_w we are looking at but also the k at which we cut off our cross section. This should be a pretty small correction, but the correct dependence which is $\log\Delta\omega/\omega$ is also pretty small so I'm satisfied for now.