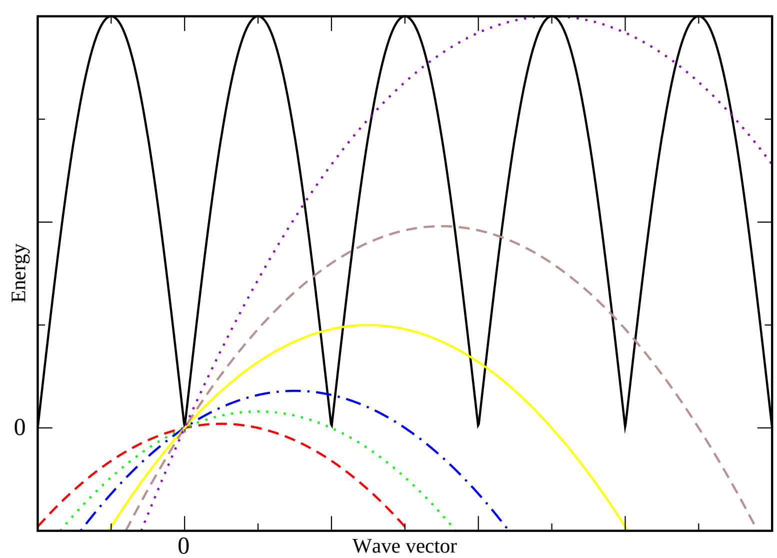
Answer Set 7
Physics 240B

1. a) Energy conservation is $E_i = E_f + \hbar\omega(k)$, or $\frac{p_i^2}{2M} = \frac{p_f^2}{2M} + \hbar\omega(k)$, where p's represent neutron momenta and M is the neutron mass. Using momentum conservation, we can rewrite this as $\frac{p_i^2}{2M} - \frac{(p_i - \hbar k)^2}{2M} = \hbar\omega(k)$. To solve graphically, plot both the right-hand side (the phonon dispersion relation) and the left-hand side as functions of k on the same graph. The conservation laws are satisfied at all intersection points. The neutron energy change turns out to be a downward parabola with vertex $(\frac{p_i}{\hbar}, \frac{p_i^2}{2M})$. With reasonable values for a (e.g., 3Å) and the spring constant K (e.g., $2\sqrt{K/M} = 5 \times 10^{-5}$), the neutron parabola is shallower than the phonon dispersion curve near $k = 0$.

b) As k increases from 0, one might think that the first intersection point will be on the left side of the neutron parabola. If the neutron curve passes through zero at positive k, there is no intersection. In fact, setting the neutron energy difference to zero shows that the left zero of the neutron curve is always at at $k = 0$, which is not really a phonon at all. So we need to think about the right zero, which is at $k = 2p_i/\hbar$. This starts to intersect the dispersion curve for $k = 2\pi/a$ (the next zero of $\omega(k)$), or $p_i = \hbar\pi/a$. As p_i increases even further, there will be non-zero intersections near this dispersion relation minimum.

c) None at low energy, then two after the threshold in b). The number continues to increase in steps (e.g., after $p_i = 2\hbar\pi/a$ there are four intersection points, and six after $p_i = 3\hbar\pi/a$) until the vertex of the neutron parabola is at $2\hbar\sqrt{K/M_{atom}}$, the max of $\hbar\omega(k)$ in the 1D monatomic chain model. Then it gradually decreases back to two, the spots where the neutron curve passes through the phonon energy range.



The above graph illustrates parts of question 3. The "phonon" spectrum I've plotted (solid black line) is the exact answer for the monatomic mass-spring chain. I've also plotted neutron curves for six different initial energies. In order of increasing energy, these are dashed (red online), dotted (green online), dash-dotted (blue online), solid (yellow online), dahsed (brown online), and dotted (violet online). The second curve (dotted green) represents the lowest initial energy required for emission, since it is the first neutron curve that intersects the phonon curve away from $k = 0$. The next three curves have 2, 4, and 6 intersections, respectively. As initial energy continues to increase past my last curve, the neutron curve gets steeper and the number of intersection points goes back down.

2. a) Assume the same sound speed for all three modes, so the sum over ν becomes just $\sum_\nu(\epsilon_{\mathbf{k}\nu}\cdot\mathbf{q})^2$. For any given $\mathbf{k}$, the three vectors $\epsilon_{\mathbf{k}\nu}$ are orthogonal unit vectors, so the sum gives exactly q^2. The sum over $\mathbf{k}$ can be rewritten as an integral, $2W = V\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{N}\frac{\hbar^2q^2}{2M\hbar ck} = \frac{V}{N}\frac{\hbar^2q^2}{4\pi^2M\hbar c}\int_0^{k_D} kdk = \frac{6\pi^2c^3}{\omega_D^3}\frac{\hbar^2q^2}{4\pi^2M\hbar c}\frac{k_D^2}{2} = \frac{3}{4}\frac{\hbar^2q^2}{M\hbar cK_D}$.

b) Now look at the $n_{\mathbf{k}\nu}$ term. The k-integral in 2D for this term is $\int_0^{k_D}\frac{dk}{e^{\hbar ck/k_BT}-1}$. If you go close enough to $k=0$, the exponent becomes small and the integrand looks like $\frac{k_BT}{\hbar ck}$, which gives a divergent integral. By contrast, in 3D you get $\int_0^{k_D}\frac{kdk}{e^{\hbar ck/k_BT}-1}$, and the integrand approaches a constant as $k\to 0$. In fact, you can substitute $y = 1-e^{-\hbar ck/k_BT}$. According to the CRC, $\int_0^1 dw\frac{\ln(1-w)}{w} = -\frac{\pi^2}{6}$. Keeping track of all the constant factors gives an extra contribution to $2W$ of magnitude $\frac{2\pi^2}{3}(\frac{T}{\Theta_D})^2$ times the zero-point contribution calculated in a).

3. Assuming that the displacement is small compared to the length of a side, a displacement d creates "planes" of charge density nde (in units of charge/length^2). Actually, I really want the thing not to be a cube at all, but something a finite-thickness, infinite cross-section slab. Then the charge distribution creates a constant field $4\pi nde$ (cgs units) inside the sample. The field acts to pull the charges back together, and since it's linear in d it's a nice harmonic oscillator situation; the equation of motion is $m\ddot{d} = -4\pi nde^2$, which has a solution $d(t) = \sin\omega t$ with $\omega = \sqrt{4ne^2\pi/m}$.

4. a) This is just dimensional analysis. The matrix element $g_{\mathbf{kk}'}$ is a Fourier component of the potential. In real space, the potential is proportional to the electric field. Hence for the deformation potential interaction, the real-space potential is proportional to df/dx, where f is a function representing the atomic displacements, and the Fourier components go as $|\mathbf{k}-\mathbf{k}'|^{\mathbf{1/2}}$. Since the piezo-electric interaction goes as f in real space, its Fourier components should go as $|\mathbf{k}-\mathbf{k}'|^{\mathbf{-1/2}}$. (Recall that taking taking derivatives in real space acts like multiplying by k in Fourier space.) This means $|g_{\mathbf{kk}'}|^2 \propto |\mathbf{k}-\mathbf{k}'|^{\mathbf{-1}} = \mathbf{1/q}$.

b) At high T, the form of the matrix element is irrelevant to the temperature dependence, since the relative scattering of different parts of the allowed shell of phonons remains constant. Resistivity goes as T, just as for the deformation potential interaction. At low T, there is a T^2 term for how much of the shell remains practical (thanks to the requirement that the phonon energy must be of order kT or less), and $|g_{\mathbf{kk}'}|^2$ contributes a factor $1/T$ to resistivity. The meaning of this second factor is that the long-wavelength (low-q) phonons have the biggest scattering cross-section, so eliminating the shorter-wavelength phonons as T decreases doesn't matter as much as one might expect at first. Together this means $\rho\propto T$ for $T << \Theta_D$. As T falls even further there is an additional T^2 factor because primarily forward collisions don't degrade momentum effectively; then $\rho\propto T^3$. There's actually yet another regime that we didn't discuss in class; at even lower temperatures it turns out that the screening gets more effective, reducing the potential felt by the electrons and giving $\rho\propto T^5$.

c) In a piezo-electric crystal, electrons scatter off phonons by both mechanisms. The dominant one is whichever has more events. At high temperature ($T >> \Theta_D$), all the temperature-dependence contributions are linear, so even with both mechanisms $\rho\propto T$. At sufficiently low temperature, the piezo mechanism *must* give more scattering. For example, $\tau\propto T^{-3}$, as opposed to $\tau\propto T^{-5}$ for deformation potential, if we include momentum non-degradation but not improved screening. Thus $\rho\propto T^3$, with only a small correction from the deformation potential scattering. At intermediate temperatures there can be a more complicated T-dependence.