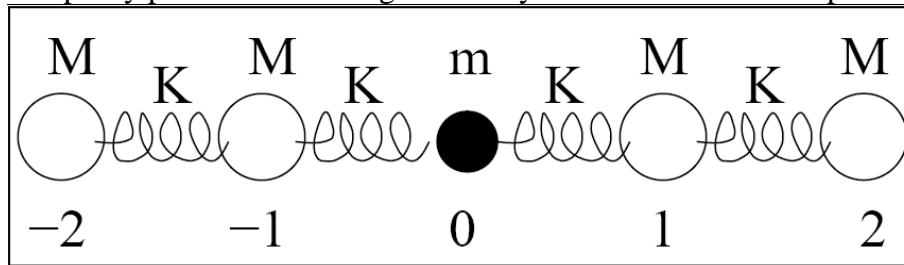


Due Wed. Oct. 3

A technical comment. In Ziman's treatment of the diatomic chain, he has made the substitutions $u_{n1}=U_1(t)\exp(iq(2n)a)$ and $u_{n2}=U_2(t)\exp(iq(2n+1)a)$ into Newton's laws (Bloch wave substitution.) If he had instead used $u_{n1}=U_1(t)\exp(iq(2n)a)$ and $u_{n2}=U_2(t)\exp(iq(2n)a)$, the resulting matrix equation would look a little different, and the eigenvector U_2' would differ from U_2 by the phase factor $\exp(iqa/2)$. The eigenvalues would be unchanged, of course. Either method is a valid Bloch wave transformation. They correspond to different choices of how to split u into "polarization vector" (U) and Bloch phase factor. The second method is more mathematically logical, but for simple diatomic crystals, Ziman's choice may be nicer. In the classic book by Born & Huang (*Dynamical Theory of Crystal Lattices*, Oxford, 1954, p. 55) they use the second method. One thing this illustrates is that for more than 1 atom per cell, **it is not always possible to make the matrix D be real or choose the eigenvectors (polarization vectors) to be real numbers.** Ziman's choice for this problem does allow the eigenvectors to be real.

1. **Impurity vibrations – localized mode.** The picture illustrates the simplest $1d$ model of lattice dynamics with a mass impurity. The chain is infinitely long, and has a mass m at the origin, while all other atoms have mass M . Ziman discusses the impurity problem in a nice general way. Here is an alternate specific case.



- a. The Bloch-wave normal modes of the perfect lattice no longer provide exact solutions for the imperfect lattice. However, a particular solution $u_\ell = A \sin(Q\ell) \exp(-i\omega t)$ (the "odd" superposition of two Bloch states Q and $-Q$) is still a normal mode, with its frequency unperturbed from the perfect chain value. Prove this. Ziman's method shows how most of the modes ($N-1$ in an N -atom chain) are essentially unshifted in frequency. The result above shows that $N/2$ normal modes are completely unaffected. Another $N/2-1$ are locally altered (near the defect) but not globally. I don't know an easy way to find the eigenvectors, but the eigenvalues do not shift except to order $1/L$. One mode is greatly altered – as shown in part b.
- b. Try to find a solution which is localized around the mass defect. Specifically, you can try $u_\ell = A(-1)^\ell \exp(-\alpha|\ell|) \exp(-i\omega t)$. Show that exactly one such solution exists (and only when $m < M$). Find the values of the frequency ω and decay constant α in terms of m/M . Show that the frequency lies above the top of the spectrum of the perfect chain. This agrees with Ziman's result, and illustrates the important fact that localized

modes can bind at impurities, and occur **only** in gaps in the unperturbed spectrum.

2. Impurity vibrations – scattering amplitudes. For the same model, and for arbitrary values of m/M , find the reflection and transmission amplitudes r and t , of Bloch waves. As in problem 1, this issue is classical, and quantum mechanics does not introduce important changes, except for a probabilistic reinterpretation. Specifically, let $|Q\rangle$ denote a Bloch state with $u_\ell = \langle \ell | Q \rangle = \exp(iQ\ell)$. A Bloch state $|Q\rangle$ is assumed to be incident from the left on a mass impurity m at $\ell = 0$. The wave component reflected (to the left) is $r|-Q\rangle$, and the wave transmitted (to the right) is $t|Q\rangle$. Thus the candidate vibrational state has the form $|\lambda\rangle = |Q\rangle + r|-Q\rangle$ for sites ℓ to the left of $\ell = 0$, and $|\lambda\rangle = t|Q\rangle$ for sites to the right. To match smoothly at $\ell = 0$, we can choose $u_0 = \langle 0 | \lambda \rangle = 1 + r = t$. Find formulas for r and t in terms of m/M and Q or ω_Q . Show that the transmitted amplitude goes to 0 at the top of the spectrum $\omega = \omega_{max} = 4K/M$. That is, the wave totally reflects, unless $m=M$. Show also that energy conservation $|r|^2 + |t|^2 = 1$ holds.

3. Velocity correlation function (classical limit). Evaluate the Fourier transform of the velocity correlation function:

$$G(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{\vec{\ell}, \alpha} \langle v(\vec{\ell}, \alpha, t) v(\vec{\ell}, \alpha, 0) \rangle$$

for a harmonic crystal in $d=3$. You may use the methods explained in the “phonon notes” posted on the course web page, and you may use the classical approximation. The brackets $\langle \rangle$ mean a statistical average. Show that the result for $G(\omega)$ has something to do with the density of phonon states. You may use the identity

$$\delta(\omega - \omega_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i(\omega - \omega_0)t}$$