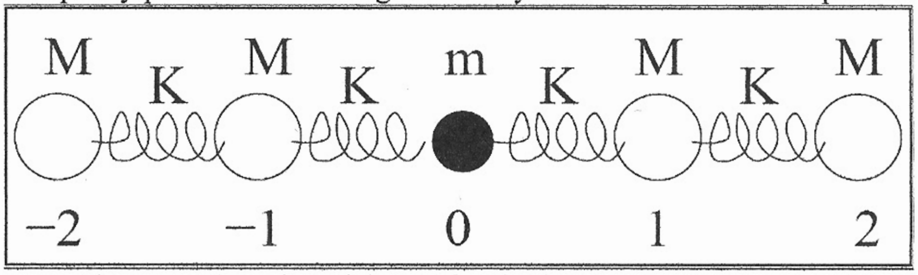
PHY 555 Fall 2007 HW #3

Answers

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 normal modes of the perfect lattice are no longer exact solutions. However, a particular solution $u_\ell = A\sin(Q\ell)\exp(-i\omega t)$ (formed as 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. This result shows that *N/2* are completely unaffected.

   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.

(a) Newton's Law for atom 0 and atom 1

$$m\ddot{u}_0 = -K(2u_0 - u_1 - u_{-1})$$

$$M\ddot{u}_1 = -K(2u_1 - u_2 - u_0)$$

Let $u_\ell = A\sin(Q\ell)e^{-i\omega t}$

For $\ell \neq 0$: $+M\omega^2 \sin(Q\ell) = K\{2\sin Q\ell - [\underbrace{\sin(Q\ell+Q) + \sin(Q\ell - Q)}_{2\sin Q\ell\cos Q}]\}$

$$\Rightarrow \omega^2 = \frac{2K}{M}(1-\cos Q) = \frac{4K}{M}\sin^2\frac{Q}{2}$$

This is the perfect chain result.

For $\ell = 0$ $\quad +m\omega^2 \sin(0) = K[2\sin(0) - \underbrace{\sin(Q) - \sin(-Q)}]$

$$0 = K[0 + 0]$$

$\therefore$ the solution works for $\omega = 2\sqrt{\frac{K}{M}}\left|\sin\frac{Q}{2}\right|$.

(b) The candidate state $u_\ell = A(-1)^\ell e^{-\alpha|\ell|} e^{-i\omega t}$ obeys Newton's law for $|\ell| \geq 2$ if

$$-M\omega^2 A e^{-\alpha|\ell|} = -K\left(2Ae^{-\alpha|\ell|} + Ae^{-\alpha|\ell|}e^{-\alpha} + Ae^{-\alpha|\ell|}e^{\alpha}\right)$$

or if $\omega^2 = \frac{2K}{M}(1+\cosh\alpha)$

which is higher than $\omega_{max}^2 = \frac{4K}{M}$.

It is easily verified that the same requirement occurs on the sites $\ell = \pm 1$. However, $\ell = 0$ is different, which will constrain α:

$$-m\omega^2 A = -K\left(2A + Ae^{-\alpha} + Ae^{-\alpha}\right)$$

Let $x = e^\alpha$. $x > 1$ is required because the state has to decay ($\alpha > 0$) away from $\ell = 0$.

$$m\omega^2 = K(2 + 2/x)$$

$$M\omega^2 = K(2 + x + 1/x)$$

$$(M-m)\omega^2 = K(x - 1/x)$$

$$\frac{M-m}{M} = \frac{x - 1/x}{2 + x + 1/x} = 1 - \frac{m}{M} \equiv \gamma < 1$$

$$\gamma = \frac{x^2-1}{(x+1)^2} = \frac{x-1}{x+1} > 0 \quad \text{since } x > 1$$

a solution only exists if $0 < 1 - \frac{m}{M} < 1$ $(0 < \gamma < 1)$ or $m < M$.

$$x = \frac{1+\gamma}{1-\gamma} = 2\frac{M}{m} - 1 = \boxed{\alpha = \log\left(2\frac{M}{m} - 1\right) > 0}$$

$$2 + 2\cosh\alpha = 2 + x + 1/x = \frac{(x+1)^2}{x} = \frac{4(M/m)^2}{2\frac{M}{m} - 1}$$

$$\boxed{\omega^2 = \frac{K}{M}(2 + 2\cosh\alpha) = \frac{4K}{M}\left(\frac{M/m}{2 - m/M}\right) > \frac{4K}{M}}$$

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. 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 $\omega_Q = \omega_{max} = 4K/M$, that is, there is complete reflection, unless $m=M$. Show also that energy conservation $|r|^2+|t|^2=1$ holds.

It is easy to show that

$$M\ddot{u}_\ell = -K(2u_\ell - u_{\ell+1} - u_{\ell-1}) \quad \text{holds (if } \omega^2 = \tfrac{2K}{m}(1-\cos Q))$$

for $u_\ell = \langle \ell | \lambda \rangle$ when $\ell \neq 0$. When $\ell = 0$, Newton's law is

$$-m\omega^2(1+r) = -K\left[2(1+r) - e^{-iQ} - re^{iQ} - te^{iQ}\right]$$

$$2\frac{m}{M}\cancel{K}(1-\cos Q)(1+r) = 2\cancel{K}(1+r) - \cancel{2K}\cos Q - 2\cancel{K}re^{iQ}$$

where $t = 1+r$ was used and $\omega^2 = 2\frac{K}{M}(1-\cos Q)$

$$r\left\{\frac{m}{M}(1-\cos Q) + e^{iQ} - 1\right\} = (1-\cos Q)\left(1-\frac{m}{M}\right)$$

$$\boxed{r = \frac{(1-\cos Q)\left(1-\frac{m}{M}\right)}{i\sin Q - (1-\cos Q)\left(1-\frac{m}{M}\right)} \qquad t = 1+r = \frac{i\sin Q}{i\sin Q - (1-\cos Q)\left(1-\frac{m}{M}\right)}}$$

From these formulas it is clear that

(1) at $Q = \pi$ (top of the spectrum, $\omega_Q = \frac{4K}{M}$)

$r = -1$, $|r|^2 = 1$, $t = 0$

(2) $|r|^2 + |t|^2 = 1$

Many equivalent forms can be found

For example

$$r = \frac{\left(1-\frac{m}{M}\right) 2\sin^2\frac{\theta}{2}}{i\sin\theta - \left(1-\frac{m}{M}\right) 2\sin^2\frac{\theta}{2}}$$

$$2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

$$r = \frac{\left(1-\frac{m}{M}\right)\sin\frac{\theta}{2}}{i\cos\frac{\theta}{2} + \left(1-\frac{m}{M}\right)\sin\frac{\theta}{2}}$$

$$= \frac{-\tan\theta/2}{\tan\frac{\theta}{2} - i\left(1-\frac{m}{M}\right)^{-1}}$$

Now for $\theta_0 < \theta < \pi$, $\tan\frac{\theta}{2} = \sqrt{\frac{\omega_\theta^2}{\omega_M^2 - \omega_\theta^2}}$

$$r = \frac{-1}{1 - i\frac{\sqrt{\omega_M^2 - \omega_\theta^2}}{\omega_\theta(1-m/M)}}$$

etc.

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

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

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 <> mean a statistical average. Show that the result for *G(ω)* has something to do with the density of phonon states. You may use the identity

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

The "general solution" for $v(\ell\alpha,t)$ is

$$v(\ell\alpha t) = \sqrt{\frac{1}{M_\alpha N}} \sum_{Qj} A_{Qj}\hat{\epsilon}_\alpha(Qj)\omega(Qj)\sin\left(Q\cdot\ell+\gamma_\alpha(Qj)-\omega(Qj)t+\phi(Qj)\right)$$

The average

$$\langle \sin(X+\phi(Qj))\sin(Y+\phi(Q'j'))\rangle$$

$$=\frac{1}{2}\langle -\cos(X+Y+\phi(Q_j)+\phi(Q'j'))\rangle + \langle \cos(X-Y+\phi(Qj)-\phi(Q'j'))\rangle$$

The phases $\phi(Qj)$ are random and average the cos's to zero except when $Qj=Q'j'$, the second part has no phase left

$$\langle \sin(X+\phi(Q_j))\sin(Y+\phi(Q'j'))\rangle$$

$$=\frac{1}{2}\cos(X-Y)\,\delta_{QQ'}\,\delta_{jj'}$$

Therefore

$$\langle v(\ell\alpha t)v(\ell\alpha 0)\rangle = \frac{1}{M_\alpha N}\sum_{Qj}\omega_{Qj}^2\langle A_{Qj}^2\rangle\epsilon_\alpha^2(Q_j)\cos(\omega(Q_j)t)$$

also $\frac{1}{2\pi}\int dt\, e^{i\omega t}\cos(\omega(Q_j)t) = \frac{1}{2}\delta(\omega-\omega_{Q_j})+\frac{1}{2}\delta(\omega+\omega_{Q_j})$

and $\omega_{Qj}^2\langle A_{Qj}^2\rangle = 2k_BT$

so $\frac{1}{2\pi}\int_{-\infty}^{\infty} dw\, e^{i\omega t}\sum_{\ell\alpha}\langle v(\ell\alpha t)V(\ell\alpha 0)\rangle = k_BT\sum_\alpha\sum_{Qj}\frac{\epsilon_\alpha(Qj)^2}{M_\alpha}\left[\delta(\omega-\omega_{Qj})+\delta(\omega+\omega_{Qj})\right]$

That is, it is a "mass-weighted" density of states.

(The $\frac{1}{N}\sum_\ell$ just gives 1)