Localized vibrational mode

The linear chain (mass $M$, spring constant $K$) has propagating normal modes $u_r = A \exp[i(Qt - \omega_r t)]$, where $-\pi < Q < \pi$ and $\omega_r = \omega_0 |\sin(Q/2)|$ and $\omega_0 = 2\sqrt{K/M}$. These are solutions of Newton’s laws, and can be quantized if desired.

According to problem set 3, if there is a mass $m < M$ located at the site $\ell = 0$, then there is also a localized solution $u_r = (-1)^\ell A \exp(-\alpha|\ell|) \exp(-i\omega_r t)$, where the decay constant $\alpha$ is positive and the localized mode frequency $\omega_r$ lies above the top of the continuous spectrum of modes of the perfect chain, $\omega_r > \omega_0$. The values of $\alpha$ and $\omega_r$ can be found by direct substitution into Newton’s laws: $\alpha = \log(2M/m - 1)$ and $\omega_r^2 = \omega_0^2 [(M/m)/(2 - m/M)]$.

The same answers are easily found by the Lippmann-Schwinger approach used by Ziman. This is an alternate formulation of the Newtonian equations. Start by assuming the time-dependence $u_r \propto \exp(-i\omega_r t)$. Then $(\hat{M} + \hat{M}_1)\omega^2 |u\rangle = \hat{K}|u\rangle$ is the equation of motion, where the mass matrix $\hat{M}$ is just the mass $M$ times the unit matrix in atom location space, and the perturbation $\hat{M}_1 = (m - M)|0\rangle\langle 0|$ is spatially localized in this space. The Green’s function is $\hat{G}(\omega) = (\omega^2 - \hat{K}/\hat{M})^{-1}$. The Lippmann-Schwinger equation is $|s\rangle = \hat{G}(\omega)\hat{A}|s\rangle$, where the perturbation is $\hat{A} = (1 - m/M)\omega^2 |0\rangle\langle 0|$. We look for a solution at a split off frequency $\omega_L > \omega_0$, where the solution $u_r = \langle \ell | s \rangle$ is spatially decaying. The Green’s function has an explicit representation in terms of the eigenstates

$$\hat{G}(\omega) = \sum_Q |Q\rangle (\omega^2 - \omega_Q^2)^{-1} |\langle Q|.$$ 

The Lippman-Schwinger equation for the localized solution is then

$$\frac{u_\ell}{u_0} = \left[1 - \frac{m}{M}\right] \sum_Q \left[\frac{\omega_Q^2}{\omega_Q^2 - \omega_0^2}\right] e^{i\omega_Q t} = \left[1 - \frac{m}{M}\right] \frac{1}{2\pi} \int_0^{\pi} dQ \frac{1}{1 - \frac{\gamma}{\sin^2(\omega_Q/2)}} e^{i\omega_Q t},$$

where $0 < \gamma = \omega_0^2/\omega_L^2 < 1$. To evaluate the integral, it is convenient to switch the variable of integration from the real number $Q$ to the complex number $z = e^{iQ}$. As $Q$ cycles once in the Brillouin zone, $z$ cycles once around the unit circle.

$$\frac{u_\ell}{u_0} = \left[1 - \frac{m}{M}\right] \frac{4}{\gamma 2m} \int dz \frac{z'}{z^2 + (4/\gamma - 2)z + 1} = \left[1 - \frac{m}{M}\right] \frac{4}{\gamma 2m} \int dz \frac{z'}{(z-z_+)(z-z_-)} = \left[1 - \frac{m}{M}\right] \frac{4}{\gamma} \frac{z'}{z_+-z_-},$$

The roots of the denominator are $z_{\pm} = \beta \pm \sqrt{\beta^2 - 1}$, where $\beta = 2/\gamma - 1 > 1$. The roots are both real, with $z_+$ lying inside the unit circle and $z_-$ lying outside. Now evaluate at $\ell = 0$, and at $\ell \neq 0$:

$$\frac{u_0}{u_0} = \left[1 - \frac{m}{M}\right] \frac{4}{\gamma z_+ - z_-} = \left[1 - \frac{m}{M}\right] \frac{4}{\gamma 2\sqrt{\beta^2 - 1}}$$

and $u_\ell/\ell = (-1)^\ell e^{-\alpha}$.

After some manipulations, the previous formulas for $\omega_L$ and $\alpha$ are retrieved.