Localized vibrational mode

The linear chain (mass M, spring constant K) has propagating normal modes $u_\ell = A\exp[i(Q\ell - \omega_Q t)]$, where $-\pi<Q<\pi$ and $\omega_Q = \omega_0|\sin(Q/2)|$ 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 $u_\ell = (-1)^\ell A\exp(-\alpha|\ell|)\exp(-i\omega_L t)$, where the decay constant α is positive and the localized mode frequency ω_L lies above the top of the continuous spectrum of modes of the perfect chain, $\omega_L > \omega_0$. The values of α and ω_L can be found by direct substitution into Newton's laws: $\alpha = \log(2M/m - 1)$ and $\omega_L{}^2 = \omega_0^2[(M/m)/(2 - m/M)]$.

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 $u_\ell \propto \exp(-i\omega_L t)$. 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 $\hat{G}(\omega) = \left(\omega^2 - \hat{K}/\hat{M}\right)^{-1}$. The Lippmann-Schwinger equation is $|s\rangle = \hat{G}(\omega)\hat{\Delta}|s\rangle$, where the perturbation is $\hat{\Delta} = (1 - m/M)\omega^2|0\rangle\langle 0|$. We look for a solution at a split off frequency $\omega_L > \omega_0$, where the solution $u_\ell = \langle \ell|s\rangle$ is spatially decaying. The Green's function has an explicit representation in terms of the eigenstates

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

The Lippman-Schwinger equation for the localized solution is then

$$\frac{u_\ell}{u_0} = \left(1 - \frac{m}{M}\right)\sum_Q\left[\frac{\omega^2}{\omega_L^2 - \omega_Q^2}\right]e^{iQ\ell} = \left(1 - \frac{m}{M}\right)\frac{1}{2\pi}\int_{-\pi}^{\pi} dQ\,\frac{1}{1 - \gamma\sin^2(Q/2)}e^{iQ\ell}$$

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.

$$\frac{u_\ell}{u_0} = \left(1 - \frac{m}{M}\right)\frac{4}{\gamma}\frac{1}{2\pi i}\oint dz\,\frac{z^\ell}{z^2 + (4/\gamma - 2)z + 1} = \left(1 - \frac{m}{M}\right)\frac{4}{\gamma}\frac{1}{2\pi i}\oint dz\,\frac{z^\ell}{(z - z_+)(z - z_-)} = \left(1 - \frac{m}{M}\right)\frac{4}{\gamma}\frac{z_+^\ell}{z_+ - z_-}$$

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 $\ell \neq 0$:

$$\frac{u_0}{u_0} = 1 = \left(1 - \frac{m}{M}\right)\frac{4}{\gamma}\frac{1}{z_+ - z_-} = \left(1 - \frac{m}{M}\right)\frac{4}{\gamma}\frac{1}{2\sqrt{\beta^2 - 1}} \quad \text{and} \quad \frac{u_\ell}{u_0} = (-1)^\ell e^{-\alpha\ell}$$

After some manipulations, the previous formulas for ω_L and α are retrieved.