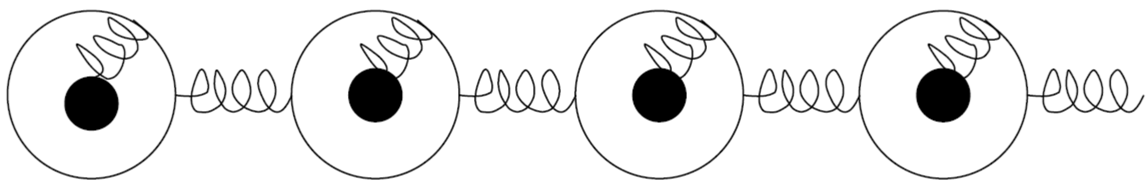
PHY 555 Fall 2007

Long range forces from a short range model with internal freedom

The "shell model" is a way of enlarging the classical point mass model of lattice dynamics to include an internal degree of freedom which is intended to capture some of the reality of the true quantum picture with rich electronic internal degrees of freedom. Just as in the quantum picture, the classical shell model ends up treating the shell as a variable which follows nuclear displacements adiabatically. The figure below illustrates it in 1d. [The most common 3d implementations assign negative and positive charges to the shell and nucleus, and include Coulomb interactions, which are omitted here.]



The Hamiltonian for this is

$$H = \sum_\ell \left[P_\ell^2 / 2M + p_\ell^{\,2} / 2m + K(s_\ell - s_{\ell+1})^2 / 2 + k\left(s_\ell - u_\ell\right)^2 / 2 \right] \qquad (1)$$

where P_ℓ and p_ℓ are the nuclear and shell momenta, M and m are the nuclear and shell masses, and u_ℓ and s_ℓ are the nuclear and shell displacements. As usual, the system repeats periodically after N units. The shell masses m are essentially zero, because these represent electronic degrees of freedom. The adiabatic approximation consists of assuming that at any instant, the shells have adopted displacements s_ℓ that minimize the energy ($\partial H / \partial s_\ell = 0$). The spectrum of normal modes can then be derived. This is a homework problem.

To see the effective long range force, consider what happens if one nucleus (which can be taken to be the one at $\ell = 0$) is given a non-zero displacement $u_0=u$. All other nuclei are undisplaced. The shells adopt new positions, and because they couple to each other, the shell displacement propagates away from $\ell = 0$. Minimizing the energy by shell displacement, we get

$$\partial H / \partial s_\ell = K(2s_\ell - s_{\ell+1} - s_{\ell-1}) + k(s_\ell - u\delta_{\ell,0}) = 0 \qquad (2)$$

This shows each shell coupled to neighbors which ultimately couple to the $\ell = 0$ shell and thus to the displaced nucleus. Explicit formulas for the first few shells are

$$K(2s_0 - s_{+1} - s_{-1}) + k(s_0 - u) = 0$$
$$K(2s_1 - s_2 - s_0) + ks_1 = 0$$
$$K(2s_2 - s_3 - s_1) + ks_2 = 0$$

These can be solved under the approximation $K << k$. The zeroth shell equation then implies that $s_0 \approx u$, the first that $s_1 \approx (K/k)s_0 \approx (K/k)u$, and the second that $s_2 \approx (K/k)s_1 \approx (K/k)^2 u$. By induction, $s_\ell \approx (K/k)^\ell u$. Thus there is a long range force which decays exponentially. The ℓ^{th} nucleus experiences a force $F_\ell \approx k(K/k)^\ell u$.

It is a nice mathematical exercise to solve this problem exactly, and then to verify that the exact solution for s_ℓ approaches the approximate solution in the appropriate limit. To do that, it is necessary to use the Fourier relations

$$s_Q = \sum_\ell s_\ell e^{iQ\ell a} \tag{3}$$

$$s_\ell = \frac{1}{N}\sum_Q s_Q e^{-iQ\ell a} = \frac{a}{2\pi}\int_0^{2\pi/a} dQ s_Q e^{-iQ\ell a} \tag{4}$$

The exactness of these relations is a consequence of the cyclic boundary conditions with N shells and N nuclei in a cycle. Multiplying Eq.(2) by $e^{iQ\ell a}$ and summing over ℓ, one obtains the formula $s_Q\left[k + 2K(1-\cos(Qa))\right] = ku$. Then using Eq.(4) , and defining the new complex variable $z = e^{iQa}$, we obtain

$$s_\ell = \frac{ku}{2\pi i}\oint dz \frac{z^{\ell-1}}{k + 2K - K(z + z^{-1})} = -\frac{ku/K}{2\pi i}\oint dz \frac{z^\ell}{(z - z_-)(z - z_+)} \tag{5}$$

The path of integration is the unit circle in complex *z* space. The poles are at $z_\pm = \alpha \pm \sqrt{\alpha^2 - 1}$, where $\alpha = 1 + k/2K$. The pole at z_- lies inside the contour, and the pole at z_+ lies outside. Therefore the answer is

$$s_\ell = u\sqrt{\frac{\alpha+1}{\alpha-1}}\left(\alpha - \sqrt{\alpha^2-1}\right)^\ell \to u\left(\frac{K}{k}\right)^\ell \tag{6}$$

where the arrow denotes the limit when $K<<k$.