Electron Phonon interaction Derivation

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1 electron phonon interaction, g(k)

We define $g(k)$ as the deformation of an electron band gap by a phonon of wavevector k in a lattice.

$g(k) = \int \psi(x) \cdot dv_k(x)dx$

Where dv is proportional to the change in bond length, which is proportional to deformation of the lattice, and $\psi(x)$ is the wavevector of the electron. In the discrete numerical model, this is taken as a sum over all lattice points' individual contribution, but here this is taken as an integral over all space instead. The electron is assumed to be of a gaussian centred at x = 0; the periodic boundary conditions employed mean that this location isn't particularly important, and in the numerical simulation the electron is also placed atop a lattice point.

$\psi(x) = Ae^{-1/2(\frac{x}{r})^2}$

2 transfer to continuous form for dv_k

Previously, in the discrete model, we defined dv_k for a given point as:

$dv_k(p) = \sum_{nn(p)}(\underline{r}(p) - \underline{r}(nn(p))) \cdot (\underline{v}_k(p) - \underline{v}_k(nn(p))$

where $v(p)$ is the eigenvector oscillation value at the point p and r is its location. In the 1D example, this is summing over the two nearest neighbours, with the same bond length b on each side (with a sign change).

$dv_k(p) = b(\underline{v}_k(p), \underline{v}_k(p+1)) - b(\underline{v}_k(p), \underline{v}_k(p-1))$

$= b(\underline{v}_k(p+1) - \underline{v}_k(p-1))$

Therefore, for the continuous case, $dv_k(x)$ is taken to be:

$dv_k(x) = v_k(x+b) - v_k(x-b)$

3 1D Chain phonons

The following is presented without proof as the known properties of a 1D periodic chain's phonons and dispersion.

$w(k) = \sqrt{\frac{1-cos(ka)}{2m}}$

$v_k(x) = Ae^{i(kx-wt)}$

4 substitution of into $g(k)$

$g(k) = \int \psi(x)(v_k(x+b) - v_k(x-b))dx$
$= \int Ae^{-1/2(\frac{x}{r})^2}(e^{i(k(x+b)-wt)} - e^{i(k(x-b)-wt)})dx$
$= Ae^{-iwt}(e^{ikb} - e^{-ikb}) \int e^{-1/2(\frac{x}{r})^2}(e^{ikx})dx$
$= Ae^{-iwt}(e^{ikb} - e^{-ikb}) \int e^{-1/2(\frac{x}{r})^2}(e^{ikx})dx$
$= Ae^{-iwt}(e^{ikb} - e^{-ikb}) \int e^{-1/2(\frac{x}{r})^2}(e^{ikx})dx$
$= Be^{-iwt}sin(ikb) \int e^{-1/2(\frac{x}{r})^2+ikx}dx$
Complete the square for integral exponent.
$-1/4(\frac{x}{r})^2 + ikx = -\frac{1}{2r^2}(x^2 - 2ikr^2x)$
$= -\frac{1}{2r^2}((x - ikr^2)^2 - (ikr^2)^2)$
$= -\frac{1}{2r^2}((x - 2ikr^2)^2 - (ikr^2)^2)$
$= -\frac{1}{2r^2}(x - 2ikr^2)^2) - \frac{1}{2}k^2r^2$
$g(k) = Be^{-iwt}sin(ikb)e^{-\frac{1}{2}k^2r^2} * \int e^{-\frac{1}{2r^2}(x-2ikr^2)^2)}dx$
$= Ce^{-iwt}sin(ikb)e^{-\frac{1}{2}k^2r^2}$
$\therefore |g(k)|^2 \propto sin(ikb)^2e^{k^2r^2}$