Self-Energy of Phonons in Anharmonic One-Dimensional Crystals

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Using the expression obtained by Green’s function methods the self-energy of phonons, interacting through anharmonic terms of third and fourth order in the expansion of the potential energy, is calculated for a linear chain without further approximations. The phonon energy shift and width show strong dependence on the frequency and the wave-vector.

The evaluation of the lifetime and the shift in energy of phonons in a crystal due to anharmonic terms in the expansion of the potential energy presents great computational difficulties. Maradudin [1] calculated the damping of a phonon in the high-temperature limit for a monatomic linear chain with nearest neighbour interactions. He obtained the lifetime varying as the inverse temperature and being independent of the wavelength of the phonon. This latter result is rather strange as one expects that with decreasing energy of the phonon its damping should decrease, too. Otherwise the anharmonic energy of phonons of long wavelengths would be greater than their harmonic energy.

We report here on an extension of the calculations of Maradudin using the field-theoretic expression for the self-energy which is obtained by Green’s function methods [2, 3, 4] and which is a function of both the energy $\omega$ and the wave-vector $k$. The relation between $\omega$ and $k$ is provided by the spectral function $\chi(k, \omega)$ which is essentially the Fourier transform of the thermal average of the commutator of two displacements. In the notation used in [4], $\omega \chi(k, \omega)$ corresponds to the probability that a phonon with wave-vector $k$ has the energy $\omega$. In the harmonic approximation this probability equals $\delta(\omega - \omega_k)$ and in [1] the lifetime was evaluated for $\omega = \omega_k$ only. In this special case, which has also been treated by Conway [8] and Pathak [9], the lifetime is independent of $k$. The self-energy, considered as a function of both $\omega$ and $k$, however, shows indeed a strong dependence on the wave-vector.

If the potential energy of a linear chain with nearest neighbour interactions and with periodic boundary conditions is expanded up to the fourth order in the
displacements $u_l$, one gets \[ V = \frac{1}{2} \sum_l (u_{l+1} - u_l)^2 + \frac{g}{6} \sum_l (u_{l+1} - u_l)^3 + \frac{\hbar}{24} \sum_l (u_{l+1} - u_l)^4 \] (1)

where $f$ is the spring constant and $g$ and $\hbar$ denote the cubic and quartic coupling parameters. Using the same notation as in [4] we obtain for the relevant anharmonic coefficients

\[ |V^{(3)}(k, k', k'')|^2 = \frac{g^2}{4N\beta^3} \omega_k^2 \omega_{k'}^2 \omega_{k''}^2 \Delta(k + k' + k'') \] (2)

and

\[ V^{(4)}(k, k', k'', k') = \frac{\hbar}{6N\beta^3} \omega_k^2 \omega_k'^2 \omega_k'' \omega_k''. \] (3)

The dispersion law is given by

\[ \omega_k = \sqrt{\frac{4f}{M} \sin \left| \frac{ak}{2} \right|} = \omega_D \sin \left| \frac{ak}{2} \right| \] (4)

where $a$ denotes the lattice constant. Neglecting the contribution from the term proportional to $|V^{(6)}|^2$ the expression for the imaginary part of the self-energy (Eq. (3.11) in [4]) simplifies to

\[ \gamma_1(k, \omega) = \frac{\pi g^2}{4N\beta^3} \omega_k^2 \sum_{k', k''} \Delta(k + k' + k'') \omega_{k'} \omega_{k''} \ \text{Ctgh} \frac{\beta \omega_{k'}}{2} \cdot \left[ \delta(\omega + \omega_{k'} - \omega_{k''}) - \delta(\omega - \omega_{k'} + \omega_{k''}) \right. \] (5)

\[ + \delta(\omega - \omega_{k'} - \omega_{k''}) - \delta(\omega + \omega_{k'} + \omega_{k''}) \right]. \]

We introduce the quantity

\[ \gamma_1(k, \omega) = \frac{1}{4 \omega_k} I_1(k, \omega) \] (6)

which has the dimension of a frequency and whose inverse determines the lifetime of the phonon (see Eq. (6.2) in [4]). Passing to the limit $N \to \infty$ we get for the damping $\gamma_1$ as a function of the continuous variable

\[ \kappa = \frac{ak}{2} \] (7)

the expression

\[ \gamma_1(\kappa, \omega) = \frac{g^2}{16\beta^3} \omega_D \omega(\kappa) \frac{\pi^2}{2} \int \sin |\kappa| \sin |\kappa + \kappa| \ \text{Ctgh} \left( \frac{\beta \omega_D}{2} \sin |\kappa| \right) \] (8)

\[ \cdot \left[ \delta(\omega/\omega_D + \sin |\kappa - \sin |\kappa + \kappa|) - \delta(\omega/\omega_D - \sin |\kappa + \kappa|) \right. \]

\[ + \delta(\omega/\omega_D - \sin |\kappa - \sin |\kappa + \kappa|) - \delta(\omega/\omega_D + \sin |\kappa + \kappa|) \] (9)

If $k$ lies in the first Brillouin zone the above integral from $-\pi/2$ to $\pi/2 - \kappa$ corresponds to contributions from normal processes while the rest stems from Umklapp processes. The evaluation of the integral is straightforward but somewhat cumbersome due to the moduli. The result is

\[ \gamma_1(\kappa, \lambda) = \frac{g^2}{8\beta^3} \omega_D^2 (\lambda^2 - 1) \sinh \left( \frac{\beta}{2} \omega_D \lambda \sin \kappa \right) \] (9)

\[ \cdot \left\{ \frac{\sin^2 \lambda \sqrt{2}}{\sqrt{1 - \lambda^2 \sin^2 \kappa / 2}} \left[ \cosh \left( \frac{\beta}{2} \omega_D \lambda \sin \kappa \right) \right. \right. \]

\[ - \cosh \left( \frac{\beta}{2} \omega_D \sin \kappa / 2 \sqrt{1 - \lambda^2 \sin^2 \kappa / 2} \right) \left[ 1 - \lambda^2 \sin^2 \kappa / 2 \right]^{-1} \cdot \left[ \cosh \left( \frac{\beta}{2} \omega_D \cos \kappa / 2 \sqrt{1 - \lambda^2 \cos^2 \kappa / 2} \right) \right]^{-1} \] (9)

\[ \left. \cdot \left\{ \cosh \left( \frac{\beta}{2} \omega_D \lambda \sin \kappa \right) - \cosh \left( \frac{\beta}{2} \omega_D \cos \kappa / 2 \sqrt{1 - \lambda^2 \cos^2 \kappa / 2} \right) \right) \right\}. \]