Lifetimes of Long Wavelength Longitudinal Phonons in Impure Metals

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Abstract. The standard Green function theory of electron-phonon interaction in metals is extended to include the effect of impurities moving with the lattice. The importance of various diagrams in the perturbation expansion of the phonon Green function is discussed in the light of the accepted theories of ultrasonic absorption in impure metals. The screened impurity potential is treated as arbitrary function of the scattering angle.

Introduction

The absorption of ultrasound in impure metals is well understood in terms of semiclassical theories [1, 2] as well as microscopic theories based on linear response theory (Kubo-formula) [3]. With, to our knowledge, only two exceptions [4, 5] the microscopic treatments employ a transformation to a frame of reference moving with the local lattice velocity, which tends to obscure the physical significance of the quantities involved.

It is the purpose of this paper to extend the standard theory of the electron-phonon interaction [6] to include impurities. It does not seem feasible to base this theory on the Fröhlich Hamiltonian [7] which implicitly takes account of the electron-electron interaction by assuming an acoustic dispersion law for the phonons and a screened electron-phonon interaction, because the screening is modified by the presence of impurities. Furthermore, Schmid [8] has shown that, by extending the Fröhlich Hamiltonian to include the motion of impurities, one obtains an expression for the phonon lifetime that is independent of the phonon wave vector $k$ for small $k$ in contradiction to experiment. Apart from these difficulties, the Fröhlich Hamiltonian fails to give a reasonable result for the velocity of the phonons.

We shall, therefore, treat the Coulomb interaction between electrons explicitly and discuss the screening in some detail (Section 2).

In Section 3 the diagrams which are most important for the electron-phonon interaction in the presence of moving impurities are discussed. The impurities, which act as scattering centers for the electrons, are represented by a potential $v(\Theta)$, where no restriction is imposed on the dependence of $v$ on the scattering angle $\Theta$. For such an impurity potential we derive in Appendix A expressions for the density-density, density-current and the current-current correlation function in terms of continued fractions.

In his treatment of sound absorption in impure jellium, which is essentially based on linear response theory, Eisenriegler [5] shows that the Pippard formula can be derived from diagrams $\Pi_1 + \Pi_3/2$ (9), (B.2). This approximation has also been used by Osaka [4], who includes $p$-wave scattering, while Eisenriegler includes only $s$-wave scattering. Eisenriegler [5] also proves, that $i \text{Im} \Pi_2 + \Pi_3/2 + \Pi_4 + \Pi_5$ is negligible, though each individual term is quite large as can be seen from (B.1) to (B.4).

In Appendix B the calculation of the various contributions to the phonon self energy is presented. It is shown that from our model Hamiltonian we can derive a diagram, that for $k \rightarrow 0$ exactly cancels the diagram discussed by Schmid.

In the concluding section it is shown that the remaining diagrams yield a result for the absorption
coefficient of longitudinal ultrasound, which on specializing \( v(\Theta) \) reduces to well-known expressions \([1, 2, 4, 9]\).

### 1. Model Hamiltonian

We start from the model Hamiltonian of Schultz \([6]\), describing a system of \( N \) electrons and \( N' \) ions:

\[
H = \sum_{i} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} v(r_i - r_j) + \sum_{a} \frac{P_a^2}{2M_a} \left[ \delta_{a,0} + \frac{1}{2} \sum_{a \neq a'} V_{aa'}(R_a - R_{a'}) \right] + \sum_{\alpha} u_\alpha(r_\alpha - R_\alpha).
\]

Here \( p_i \) and \( R_a \) refer to the ion on the lattice site \( \alpha \), while \( p_i \) and \( r_\alpha \) refer to the \( i \)-th conduction electron, the other electrons together with the nuclei are assumed to form rigid ions.

For simplicity we consider only one type of impurity so that \( M_\alpha \) can take two values. \( V_{aa'} \) represents three potentials \( V_1, V_{1'}, V_{1''} \), corresponding to the host ion-host ion, host ion-impurity, and impurity-impurity interactions, respectively. \( u_\alpha \) represents two different functions: the interaction potentials \( u \) between electron and host ion and \( u_{\text{IMP}} \) between electron and impurity ion.

If there are \( N_{\text{IMP}} \) impurities of valence \( Z_{\text{IMP}} \) and \( N_{\text{ION}} \) ions of the host lattice, charge neutrality requires

\[
N = Z_{\text{ION}} N_{\text{ION}} + Z_{\text{IMP}} N_{\text{IMP}} = (N_{\text{ION}} + N_{\text{IMP}}) Z = N' \tilde{Z}
\]

where \( Z \) is the average charge per lattice site.

To show the changes introduced into the system by the impurities more clearly, we write the Hamiltonian in the form

\[
H = \sum_{i} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} v(r_i - r_j) + \sum_{\alpha} \frac{P_{\alpha}^2}{2M_\alpha} \left[ \delta_{\alpha,0} + \frac{1}{2} \sum_{a \neq a'} V_{a\alpha}(R_{a\alpha} - R_{a'a'}) \right] + \sum_{\alpha} u_\alpha(r_\alpha - R_\alpha)
\]

where \( \mu = \frac{M \cdot M_{\text{IMP}}}{M - M_{\text{IMP}}} \).

The sums over \( \beta \) and \( \beta' \) are extended only over lattice sites occupied by impurities.

The first term in the second line, due to different masses of impurity and host ions, leads to the well known Rayleigh scattering of phonons, appreciable only for phonons with wave vectors in the vicinity of the Debye wave vector \( q_D \) \([10]\).

The next two terms represent force constant changes. Their influence on the velocity and lifetimes of phonons have been the object of recent investigation \([11]\).

We shall neglect these two sources of phonon damping because it seems to be safe to assume that in a metal they are dominated by electron-phonon interaction with a modification by impurities given by the last term in (2). The spatial average of \( V_1 \) and \( V_{1'} \) has to be retained, however, to guarantee charge neutrality.

Next, we assume that the ions vibrate around their equilibrium positions \( R_{\alpha} \) and expand the potentials in powers of the displacements \( \delta R_\alpha \). The interaction of the electrons with the periodic lattice given by \( \sum_{i} u(r_i - R_\alpha) \), which leads to band structure effects, will be ignored, i.e. we confine ourselves to the free electron model.

Writing the Hamiltonian in second quantization, with the electron field operator expanded in plane wave states, expressing \( \delta R_\alpha \) in phonon coordinates and Fouriertransforming the potentials we obtain

\[
H = H_{\text{EL}} + H_{\text{PH}} + H_{\text{INT}}
\]

where

\[
H_{\text{EL}} = \frac{1}{2m} \sum_{k\sigma} \frac{k^2}{2} c_{k\sigma}^+ c_{k\sigma}
\]

\[
H_{\text{PH}} = \frac{1}{2} \sum_{k\sigma} \sum_{q=0} \omega_\sigma^2(k) \left[ b_{k\sigma}^+ b_{k\sigma} + 1 \right]
\]

\[
H_{\text{INT}} = \frac{1}{2} \sum_{p,s \neq q=0} \sum_{k=0} v(p,s, q,s') c_{p,s}^+ c_{p',s'} c_{p'-q,s} c_{p-q,s}
\]

\[
+ \frac{1}{2} \sum_{p,s \neq q=0} \sum_{k=0} v(p,IMP(q), q,s) c_{p,s}^+ c_{p'-q,s} \sum_{q'=0} e^{-\frac{i(q-q') k_R^2}{2}}
\]

\[
+ \frac{1}{2} \sum_{p,s \neq q=0} \sum_{k=0} v(IMP(q), q,s) c_{p,s}^+ c_{p'-q,s} \sum_{q'=0} e^{-\frac{i(q-q') k_R^2}{2}}
\]

\[
+ \frac{1}{2} \sum_{p,s \neq q=0} \sum_{k=0} v(IMP(q), q,s) c_{p,s}^+ c_{p'-q,s} \sum_{q'=0} e^{-\frac{i(q-q') k_R^2}{2}}
\]

\[
\text{with } \omega_\sigma^2(k) = \sqrt{\frac{N'}{M \omega_\sigma^2(k)}} k u(k)
\]

\[
\phi_{k\sigma} = \frac{h_{k\sigma}^+ + h_{k\sigma}^-}{\sqrt{2}}
\]

Z. Physik (1974)