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Thermal conductivity of an imperfect anharmonic crystal

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The thermal conductivity of an anharmonic crystal containing randomly distributed substitutional defects due to impurity-phonon scattering is theoretically investigated with the use of the method of double-time thermal Green's functions and the Kubo formalism considering all the terms, i.e., diagonal, nondiagonal, cubic anharmonic, and imperfection terms in the energy-flux operator as propounded by Hardy. The study uses cubic, quartic anharmonic, and defect terms in the Hamiltonian. Mass changes as well as force-constant changes between impurity and host-lattice atoms are taken into account explicitly. It is shown that the total conductivity can be written as a sum of contributions, namely diagonal, nondiagonal, anharmonic, and imperfection contributions. For phonons of small halfwidth, the diagonal contribution has precisely the same form which is obtained from Boltzmann's transport equation for impurity scattering in the relaxation-time approximation. The present study shows that there is a finite contribution of the nondiagonal term, cubic anharmonic term, and the term due to lattice imperfections in the energy-flux operator to the thermal conductivity although the contribution is small compared with that from the diagonal part. We have also discussed the feasibility of numerical evaluation of the various contributions to the thermal conductivity.

I. INTRODUCTION

There has been considerable interest in past theoretical studies of the lattice conductivity of solids doped with impurities. These studies are generally based on the Boltzmann equation for phonons first presented by Peierls[1] and are discussed extensively in review articles by Klemens[2] and Caruthers.[3] These theories suffer from the usual shortcomings of kinetic theories as enumerated by Hardy.[4] The latest theories on phonon transport in solids express the thermal conductivity in terms of a correlation function of the energy-flux operator on the dynamical variables of the system, i.e., the creation and annihilation operators for phonons in the case of a lattice. Hardy[5] has given a systematic derivation of the energy-flux operator for a three-dimensional lattice in terms of the phonon variables, which is valid for all phases of matter. It is shown that even in the harmonic approximations the total energy-flux operator contains the nondiagonal terms in addition to the usual diagonal term. The contributions to the average energy flux for the anharmonic forces and from lattice imperfections are also included.

Within the last few years a large number of workers[6–15] have investigated the behavior of the thermal conductivity of crystals containing substitutional defects using the correlation function formalism of Kubo[16] and various other techniques. In all these studies the effect of lattice imperfections on the average heat-flux operator of the crystal is not taken into account, which becomes significant at low temperature. Goyal and Sharma[17] have considered the influence of lattice imperfection term in the energy-flux operator on the transport of heat in harmonic crystals.

The aim of the present study is to derive an expression for the thermal conductivity of an anharmonic Bravais crystal containing randomly distributed substitutional defects using the double-time thermal Green's-function technique,[18] and the Kubo formalism taking into account both mass and force-constant changes and considering the contributions of lattice imperfections and cubic anharmonic forces to the energy-flux operator as propounded by Hardy.[5] In Sec. II, a general formulation of the Kubo formula for the thermal conductivity is given and the thermal conductivity is separated into terms contributed by diagonal, nondiagonal, anharmonic forces, and imperfection terms in the energy flux. Section III describes the Hamiltonian used and deals with the evaluation of necessary double-time Green's functions with the help of the Dyson equation. In Sec. IV we derive an expression for the diagonal, nondiagonal, anharmonic-force, and lattice-imperfection contributions to the lattice thermal conductivity of the system. In Sec. V we summarize the various results and also discuss the feasibility of numerical evaluation of the various contributions to thermal conductivity.

II. GENERAL FORMULATION

We start with the Kubo correlation formula for the thermal conductivity,[16,19]

$$K=\lim_{\epsilon\to 0}\frac{k_B\beta^2}{3V}\int_0^\infty dt\, e^{-\epsilon t}\mathrm{Re}\langle\vec{Q}(0)\cdot\vec{Q}(t)\rangle\ , \quad (1)$$

where $\beta=(k_BT)^{-1}$, k_B is the Boltzmann constant, V and T are the volume and the temperature of the crystal, $\vec{Q}(t)$ is the heat-flux operator for the lattice in the Heisenberg representation, and the angular brackets denote the canonical ensemble average of the expectation value of the operator and Re stands for the real part of the quantity.

Taking into account the contributions to the average energy flux due to cubic anharmonic forces and from perturbations characterizing lattice imperfections, Hardy[5] has shown that the total heat-flux operator can be written as

$$\vec{Q}(t)=\vec{Q}_0(t)+\vec{Q}'(t)+\vec{Q}''(t)\ , \quad (2)$$

where $\vec{Q}_0(t)$ is independent of perturbation and describes the heat-flux operator of an ideal lattice in the harmonic approximation, $\vec{Q}'(t)$ describes the contribution to the heat-flux operator from the cubic anharmonic forces, and $\vec{Q}''(t)$ represents the contribution to the heat-flux operator due to the lattice imperfection. The detailed expressions for these quantities are given by Hardy.[5]

When Eq. (2), with the expressions of the different quantities involved in it,[5] are substituted into Eq. (1), the thermal conductivity can be written as

$$K=K_d+K_{\mathrm{nd}}+K_c+K_{\mathrm{anh}}+K_{\mathrm{imp}}\ , \quad (3)$$

where

$$K_d=\lim_{\epsilon\to 0}\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s}\sum_{\vec{k}',s'}\omega_{\vec{k}s}\omega_{\vec{k}'s'}\vec{v}_{\vec{k}s}\cdot\vec{v}_{\vec{k}'s'}\,\mathrm{Re}\int_0^\infty dt\, e^{-\epsilon t}R_{\vec{k}s\vec{k}'s'}(t)\ , \quad (4)$$

$$K_{\mathrm{nd}}=\lim_{\epsilon\to 0}\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,s'}\sum_{\vec{k}_1,s_1,s_1'}(\omega_{\vec{k}s}\omega_{\vec{k}s'})^{1/2}(\omega_{\vec{k}_1s_1}\omega_{\vec{k}_1s_1'})^{1/2}\ \vec{v}_{\vec{k}ss'}\cdot\vec{v}_{\vec{k}_1s_1s_1'}\,\mathrm{Re}\int_0^\infty dt\, e^{-\epsilon t}R_{\vec{k}ss'\,\vec{k}_1s_1s_1'}(t)\ , \quad (5)$$

$$K_c=K_c^{(1)}+K_c^{(2)}+K_c^{(3)}\ , \quad (6)$$

$$K_{\mathrm{anh}}=K_1+K_2\ , \quad (7)$$

with

$$K_c^{(1)}=\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\,\vec{k}',s',\,\vec{k}'',s''}\ \sum_{\vec{k}_1,s_1,\,\vec{k}'_1,s'_1,\,\vec{k}''_1,s''_1}\vec{X}_{\vec{k}s,\,\vec{k}'s'\,\vec{k}''s''}\cdot\vec{X}^*_{\vec{k}_1s_1,\,\vec{k}'_1s'_1\,\vec{k}''_1s''_1}$$
$$\times\int_0^\infty dt\, e^{-\epsilon t}R_{\vec{k}s\,\vec{k}'s'\,\vec{k}''s''\,\vec{k}_1s_1\,\vec{k}'_1s'_1\,\vec{k}''_1s''_1}(t)\ , \quad (8a)$$

$$K_c^{(2)}=\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\,\vec{k}',s',\,\vec{k}'',s''}\ \sum_{\vec{k}_1,s_1,\,\vec{k}'_1,s'_1,\,\vec{k}''_1,s''_1}\vec{Y}_{\vec{k}s,\,\vec{k}'s',\,\vec{k}''s''}\cdot\vec{Y}^*_{\vec{k}_1s_1,\,\vec{k}'_1s'_1,\,\vec{k}''_1s''_1}$$
$$\times\int_0^\infty dt\, e^{-\epsilon t}L_{\vec{k}s\,\vec{k}'s'\,\vec{k}''s''\,\vec{k}_1s_1\,\vec{k}'_1s'_1\,\vec{k}''_1s''_1}(t)\ , \quad (8b)$$

$$K_c^{(3)}=\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\,\vec{k}',s',\,\vec{k}'',s''}\ \sum_{\vec{k}_1,s_1,\,\vec{k}'_1s'_1,\,\vec{k}''_1,s''_1}\vec{Z}_{\vec{k}s,\,\vec{k}'s'\,\vec{k}''s''}\cdot\vec{Z}^*_{\vec{k}_1s_1,\,\vec{k}'_1s'_1\,\vec{k}''_1s''_1}$$
$$\times\int_0^\infty dt\, e^{-\epsilon t}L_{\vec{k}''s''\,\vec{k}s\,\vec{k}'s'\,\vec{k}''_1s''_1\,\vec{k}_1s_1\,\vec{k}'_1s'_1}(t)\ , \quad (8c)$$

$$K_1=\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s''}\;\sum_{\vec{k}_1,s_1,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1}\vec{J}_{\vec{k}s,\vec{k}'s'\vec{k}''s''}\cdot\vec{J}^{*}_{\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1}\times\int_0^\infty dt\,e^{-\epsilon t}L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1}(t)\;, \tag{9a}$$

$$K_2=\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s'',\vec{k}''',s'''}\;\sum_{\vec{k}_1,s_1,\vec{k}'_1s'_1,\vec{k}''_1,s''_1,\vec{k}'''_1,s'''_1}\vec{J}_{\vec{k}s,\vec{k}'s',\vec{k}''s'',\vec{k}'''s'''}\cdot\vec{J}^{*}_{\vec{k}_1s_1,\vec{k}'_1s'_1\,\vec{k}''_1s''_1\vec{k}'''_1s'''_1}\times\int_0^\infty dt\,e^{-\epsilon t}L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}'''s'''\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1\vec{k}'''_1s'''_1}(t)\;, \tag{9b}$$

and

$$K_{\text{imp}}=\lim_{\epsilon\to 0}\frac{\hbar^2k_B\beta^2}{12V}\sum_{\vec{k},s,\vec{k}',s'}\;\sum_{\vec{k}_1,s_1,\vec{k}'_1s'_1}\vec{J}_{\vec{k}s,\vec{k}'s'}\cdot\vec{J}^{*}_{\vec{k}_1s_1\vec{k}'_1s'_1}\,\mathrm{Re}\int_0^\infty dt\,e^{-\epsilon t}L_{\vec{k}s\vec{k}'s'\vec{k}_1s_1\vec{k}'_1s'_1}(t)\;, \tag{10}$$

where the asterisk indicates the complex conjugation and expressions for $\vec{X}_{\vec{k}s,\vec{k}'s'\vec{k}''s''}$, $\vec{Y}_{\vec{k}s\vec{k}'s'\vec{k}''s''}$, $\vec{Z}_{\vec{k}s\vec{k}'s'\vec{k}''s''}$, $\vec{J}_{\vec{k}s\vec{k}'s'\vec{k}''s''}$, and $\vec{J}_{\vec{k}s\vec{k}'s'}$ are given by Hardy.[5] Equations (4)—(6) describe the contributions of the diagonal, nondiagonal, and cubic parts of the average heat-flux operator to the thermal conductivity. Equation (7) along with Eqs. (9a) and (9b) gives contribution due to anharmonic forces as correction terms to the thermal conductivity. Equation (10) describes the contribution of the lattice imperfection of the average heat-flux operator to the thermal conductivity.

The correlation functions R and L appearing in the above equations are given by

$$R_{\vec{k}s\vec{k}'s'}(t)=\langle A_{\vec{k}s}(0)B^{\dagger}_{\vec{k}s}(0)A^{\dagger}_{\vec{k}'s'}(t)B_{\vec{k}'s'}(t)\rangle\;, \tag{11}$$

$$R_{\vec{k}ss'\vec{k}_1s_1s'_1}(t)=\langle A_{\vec{k}s}(0)B^{\dagger}_{\vec{k}s'}(0)A^{\dagger}_{\vec{k}_1s_1}(t)B_{\vec{k}_1s'_1}(t)\rangle\;, \tag{12}$$

$$R_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1}(t)=\langle A_{\vec{k}s}(0)A_{\vec{k}'s'}(0)A_{\vec{k}''s''}(0)A^{\dagger}_{\vec{k}_1s_1}(t)A^{\dagger}_{\vec{k}'_1s'_1}(t)A^{\dagger}_{\vec{k}''_1s''_1}(t)\rangle\;, \tag{13}$$

$$\begin{aligned}L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1}(t)=&\langle A_{\vec{k}s}(0)B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)A^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}''_1s''_1}(t)\rangle\\&+\langle B_{\vec{k}''s''}(0)B_{\vec{k}'s'}(0)A_{\vec{k}s}(0)B^{\dagger}_{\vec{k}''_1s''_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\\&+\langle A_{\vec{k}s}(0)B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}''_1s''_1}(t)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\\&+\langle B_{\vec{k}''s''}(0)B_{\vec{k}'s'}(0)A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}''_1s''_1}(t)\rangle\;,\end{aligned} \tag{14}$$

$$\begin{aligned}&L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}'''s'''\vec{k}_1s_1\vec{k}'_1s'_1\,\vec{k}''_1s''_1\vec{k}'''_1s'''_1}(t)\\&\quad=\langle B_{\vec{k}s}(0)B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)A_{\vec{k}'''s'''}(0)B^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}''_1s''_1}A^{\dagger}_{\vec{k}'''_1s'''_1}(t)\rangle\\&\qquad+\langle A_{\vec{k}'''s'''}(0)B_{\vec{k}''s''}(0)B_{\vec{k}'s'}(0)A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}'''_1s'''_1}B^{\dagger}_{\vec{k}''_1s''_1}B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}_1s_1}(t)\rangle\\&\qquad+\langle A_{\vec{k}'''s'''}(0)B_{\vec{k}''s''}(0)B_{\vec{k}'s'}(0)B_{\vec{k}s}(0)B^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}''_1s''_1}(t)A^{\dagger}_{\vec{k}'''_1s'''_1}(t)\rangle\\&\qquad+\langle B_{\vec{k}s}(0)B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)A_{\vec{k}'''s'''}(0)A^{\dagger}_{\vec{k}'''_1s'''_1}B^{\dagger}_{\vec{k}''_1s''_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)B^{\dagger}_{\vec{k}_1s_1}(t)\rangle\;,\end{aligned} \tag{15}$$

and

$$L_{\vec{k}s\vec{k}'s'\vec{k}_1s_1\vec{k}'_1s'_1}(t)=\langle A_{\vec{k}s}(0)B_{\vec{k}'s'}(0)A^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}'_1s'_1}(t)\rangle\;. \tag{16}$$

Thus we notice that the problem of evaluating the lattice thermal conductivity of doped crystals is reduced to that of the calculation of two-time correlation function on a suitable model for the crystal Hamiltonian. These correlation functions can be evaluated by different techniques. Here we use the thermodynamic Green's-function[18] method which is well suited for this purpose. The calculation of the canonical average in Eqs. (4), (5), and (8)–(10) is considerably simplified if the correlation functions are factorized according to a decoupling scheme.[20–22] Thus for the average of a four-operator product *abcd*, we write

$$\langle abcd\rangle=\langle ab\rangle\langle cd\rangle+\langle ac\rangle\langle bd\rangle+\langle ad\rangle\langle bc\rangle\ . \tag{17}$$

With the use of the above decoupling scheme the correlation functions (11)–(16) can be written as

$$R_{\vec{k}s\vec{k}'s'}(t)=\langle A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}'s'}(t)\langle B^{\dagger}_{\vec{k}s}(0)B_{\vec{k}'s'}(t)\rangle+\langle A_{\vec{k}s}(0)B_{\vec{k}'s'}(t)\rangle\langle B^{\dagger}_{\vec{k}s}(0)A^{\dagger}_{\vec{k}'s'}(t)\rangle\ , \tag{18}$$

$$R_{\vec{k}ss'\vec{k}_1s_1s_1'}(t)=\langle A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\langle B^{\dagger}_{\vec{k}s'}(0)B_{\vec{k}_1s_1'}(0)\rangle+\langle A_{\vec{k}s}(0)B_{\vec{k}_1s_1'}(t)\rangle\langle B^{\dagger}_{\vec{k}s'}(0)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\ , \tag{19}$$

$$R_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}_1s_1\vec{k}_1's_1'\vec{k}_1''s_1''}(t)=\langle A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\langle A_{\vec{k}'s'}(0)A_{\vec{k}''s''}(0)A^{\dagger}_{\vec{k}_1's_1'}(t)A^{\dagger}_{\vec{k}_1''s_1''}(t)\rangle\ , \tag{20}$$

$$L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}_1s_1\vec{k}_1's_1'\vec{k}_1''s_1''}(t)=4[\langle A_{\vec{k}s}(0)A_{\vec{k}_1s_1}(t)\rangle\langle B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)B^{\dagger}_{\vec{k}_1's_1'}(t)B^{\dagger}_{\vec{k}_1''s_1''}(t)\rangle]\ , \tag{21}$$

$$\begin{aligned}&L_{\vec{k}s\vec{k}'s'\vec{k}''s''\vec{k}'''s'''\vec{k}_1's_1'\vec{k}_1''s_1''\vec{k}_1'''s_1'''}(t)\\&\qquad=4[\langle A_{\vec{k}'''s'''}(0)A^{\dagger}_{\vec{k}_1'''s_1'''}(t)\rangle\langle B_{\vec{k}s}(0)B_{\vec{k}'s'}(0)B_{\vec{k}''s''}(0)B^{\dagger}_{\vec{k}_1s_1}(t)B^{\dagger}_{\vec{k}_1's_1'}(t)B^{\dagger}_{\vec{k}_1''s_1''}(t)\rangle]\ ,\end{aligned} \tag{22}$$

and

$$L_{\vec{k}s\vec{k}'s'\vec{k}_1s_1\vec{k}_1's_1'}(t)=\langle A_{\vec{k}s}(0)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\langle B_{\vec{k}'s'}(0)B^{\dagger}_{\vec{k}_1's_1'}(t)\rangle+\langle A_{\vec{k}s}(0)B^{\dagger}_{\vec{k}_1's_1'}(t)\rangle\langle B_{\vec{k}'s'}(0)A^{\dagger}_{\vec{k}_1s_1}(t)\rangle\ . \tag{23}$$

In writing Eqs. (19)–(23) we have neglected the correlation functions of the operators with the same time arguments because they do not contribute to the thermal conductivity, which follows from the fact that there is no heat flow in equilibrium.

III. HAMILTONIAN AND GREEN'S FUNCTIONS

For further analysis, an explicit expression for the Hamiltonian is needed. Here we consider a three-dimensional cubic Bravais anharmonic crystal with total number of N atoms whose n lattice sites are occupied by randomly distributed substitutional defects each of mass M', while the remaining $(N-n)$ lattice sites are occupied by host atoms of mass M. The introduction of defects modifies the force constants between the host and impurity atoms around the defect sites in addition to the change in mass. If the defect contribution (n/N) is quite small, one can assume that the distance between any two defect atoms is too large so that the impurity-impurity interaction can be neglected. The force-constant changes associated with defect and host atoms may be assumed to be restricted only to nearest neighbors. It is assumed that the defect causes changes only in the harmonic forces and anharmonic forces remains unchanged. Thus the total Hamiltonian of such a defect anharmonic crystal in second quantized notation can be written as

$$H=H_0+H'+H_A\ , \tag{24}$$

where H_0 is the harmonic Hamiltonian of an unperturbed lattice given by

$$H_0=\sum_k \hbar\omega_k(a_k^{\dagger}a_k+\tfrac{1}{2})=\tfrac{1}{4}\sum_k \hbar\omega_k(A_k^{\dagger}A_k+B_k^{\dagger}B_k)\ . \tag{25}$$

For brevity and convenience in what follows we use index k as a short form for $\vec{k}s$. The perturbation part H' arises because of the substitutional defects in the crystal and can be written as

$$H'=-\hbar\sum_{k_1,k_2}C(k_1k_2)B_{k_1}B_{k_2}+\hbar\sum_{k_1,k_2}D(k_1,k_2)A_{k_1}A_{k_2}\ . \tag{26}$$

The parameters $C(k_1,k_2)$ and $D(k_1,k_2)$ depend upon changes in mass and force constant due to the introduction of impurities and are given in Ref. 11.

The anharmonic contribution H_A which contains dominant cubic and quartic terms in the expansion of the lattice potential energy in powers of atomic displacements can be written as

$$H_A=\hbar \sum_{k_1,k_2,k_3} V^{(3)}(k_1,k_2,k_3)A_{k_1}A_{k_2}A_{k_3}+\hbar \sum_{k_1,k_2,k_3,k_4} V^{(4)}(k_1,k_2,k_3,k_4)A_{k_1}A_{k_2}A_{k_3}A_{k_4} , \tag{27}$$

where the coefficients $V^{(3)}$ and $V^{(4)}$ are the Fourier transforms of third- and fourth-order atomic force constants. They are symmetric with respect to pair of indices k and are given by Maradudin and Fein.[23]

In order to evaluate the correlation functions appearing in Eqs. (18), (20), and (23), we introduce the following one-phonon retarded Green's functions:

$$G^{(1)}_{kk'}(t-t)=\langle\langle A_k(t);A^{\dagger}_{k'}(t')\rangle\rangle=-i\Theta(t-t')\langle [A_k(t),A^{\dagger}_{k'}(t')]\rangle , \tag{28a}$$

$$G^{(2)}_{kk'}(t-t')=\langle\langle A_k(t);B^{\dagger}_{k'}(t')\rangle\rangle , \tag{28b}$$

$$G^{(3)}_{kk'}(t-t')=\langle\langle B_k(t);B^{\dagger}_{k'}(t')\rangle\rangle , \tag{28c}$$

and also for the evaluation of the correlation functions appearing in Eqs. (20)—(22), we introduce the following two-phonon and three-phonon retarded Green's functions:

$$g^{(1)}(t-t')=\langle\langle A_{k_1}(t)A_{k_2}(t);A^{\dagger}_{k'_1}(t')A^{\dagger}_{k'_2}(t')\rangle\rangle , \tag{29a}$$

$$g^{(2)}(t-t')=\langle\langle B_{k_1}(t)B_{k_2}(t);B^{\dagger}_{k'_1}(t')B^{\dagger}_{k'_2}(t')\rangle\rangle , \tag{29b}$$

$$g^{(3)}(t-t')=\langle\langle B_{k_1}(t)B_{k_2}(t)B_{k_3}(t);B^{\dagger}_{k_1}(t')B^{\dagger}_{k_2}(t')B^{\dagger}_{k_3}(t')\rangle\rangle , \tag{29c}$$

where $\Theta(t)$ is the usual Heaviside step function and is equal to 1 for $t>0$ and is 0 for $t<0$.

For the evaluation of the Green's function we apply an approach in which we first develop an expression in terms of Dyson equation using the equation-of-motion method and then to obtain an expression for the polarization operator of the system.

Differentiating Eq. (28a) twice with respect to the time argument t and using the commutation relation for the Hamiltonian (24), we obtain the following equation for the Fourier transform of the Green's function:

$$(\omega^2-\omega_k^2)G^{(1)}_{kk'}(\omega)=\frac{\omega_k}{\pi}\delta_{kk'}+\frac{4}{\pi}C(-k,k')+\frac{\omega_k}{\pi}\langle\langle F^{(1)}_k(t);A^{\dagger}_{k'}(t')\rangle\rangle_{\omega} , \tag{30}$$

where $\delta_{kk'}$ is the Kronecker δ, the suffix ω on the right-hand side indicates the Fourier transformation, and

$$\begin{aligned} F^{(1)}_k(t)=4\pi\sum_{k_1}\left[D(-k,k_1)A_{k_1}(t)+\frac{\omega_{k_1}}{\omega_k}C(-k,k_1)A_{k_1}(t)\right]+\frac{16\pi}{\omega_k}\sum_{k_1,k_2}[C(-k,k_1)D(-k_2,k_1)]A_{k_1}(t) \\ +2\pi\left[3\sum_{k_1,k_2}V^{(3)}(k_1,k_2,-k)A_{k_1}A_{k_2}+4\sum_{k_1,k_2,k_3}V^{(4)}(k_1,k_2,k_3,-k)A_{k_1}A_{k_2}A_{k_3}\right] . \end{aligned} \tag{31}$$

Considering the equation of motion for the Green's function that appears on the right-hand side of Eq. (31) with respect to the time argument t' and substituting the Fourier transform of the resulting expression into Eq. (30), the equation of motion for the Green's function $G^{(1)}_{kk'}(\omega)$ can be written in the form of the Dyson equation,

$$G^{(1)}_{kk'}(\omega)=G^0_k(\omega)\delta_{kk'}+G^0_k(\omega)\widetilde{P}^{(1)}_{kk'}(\omega)G^0_{k'}(\omega)=G^0_k(\omega)\delta_{kk'}+G^0_k(\omega)\Pi^{(1)}_k(\omega)G^{(1)}_{kk'}(\omega) , \tag{32}$$

where

$$G^0_k(\omega)=\frac{\omega_k}{\pi(\omega^2-\omega_k^2)} , \tag{33}$$

and

$$\begin{aligned} \widetilde{P}^{(1)}_{kk'}(\omega)=\frac{1}{2}\left[\langle [F^{(1)}_k(t),B^{\dagger}_{k'}(t')]\rangle+\frac{\omega}{\omega_{k'}}\langle [F^{(1)}_k(t),A^{\dagger}_{k'}(t')]\rangle+\frac{4}{\omega_{k'}}\sum_{k_1}C(k',-k_1)\langle [F^{(1)}_k(t),P_{k_1^{\dagger}}(t')]\rangle\right]_{t=t'} \\ +\langle\langle F^{(1)}_k(t);F^{(1)^{\dagger}}_{k'}(t')\rangle\rangle_{\omega}+4\pi C(-k,k')(\omega_k\omega_{k'})^{-1}(\omega^2-\omega_{k'}^2)^{-1} . \end{aligned} \tag{34}$$

The Dyson equation can be written to give the Green's function as

$$G_{kk'}^{(1)}(\omega)=\frac{\delta_{kk'}}{(G_k^0)^{-1}-\Pi_k^{(1)}(\omega)}\ , \tag{35}$$

where the diagonal polarization operator $\Pi_k^{(1)}(\omega)$ is given by

$$\Pi_k^{(1)}(\omega)=\widetilde{P}_{kk}^{(1)}(\omega)[1+G_k^0(\omega)\widetilde{P}_{kk}^{(1)}(\omega)]^{-1}\ . \tag{36}$$

In the region of frequencies far from the zeros of the denominator in Eq. (36), one may expand the right-hand side in a power series of $\widetilde{P}_{kk}^{(1)}(\omega)$ as

$$\Pi_k^{(1)}(\omega)=\widetilde{P}_{kk}^{(1)}(\omega)[1-G_k^0(\omega)\widetilde{P}_{kk}^{(1)}(\omega)+\cdots]\ . \tag{37}$$

In the above equation [Eq. (37)] only the first term will give the dominating contribution while the remaining terms lead to the corrections of a higher order of smallness. In the lowest approximation, we may write $\Pi_k^{(1)}(\omega)=\widetilde{P}_{kk}^{(1)}(\omega)$, which gives

$$G_{kk'}^{(1)}(\omega)=\frac{\omega_k\delta_{kk'}}{\pi[\omega^2-(\widetilde{\omega}_k^{(1)})^2-2\omega_k P_k^{(1)}(\omega)]}\ , \tag{38}$$

where $\widetilde{\omega}_k^{(1)}$ is the frequency of the renormalized mode k in the lowest approximation of the perturbation theory and is given by

$$(\widetilde{\omega}_k^{(1)})^2=\omega_k^2+\frac{\omega_k}{2\pi}\Bigg[\langle[F_k^{(1)}(t),B_k^{\dagger}(t')]^0\rangle+\frac{\omega}{\omega_k}\langle F_k^{(1)}(t),A_k^{\dagger}(t')]^0\rangle$$
$$+\frac{4}{\omega_k}\sum_{k_1}C(k,-k_1)\langle[F_k^{(1)}(t),B_{k_1}^{\dagger}(t')]^0\rangle+8\frac{(\omega^2-\omega_k^2)}{\omega_k}C(-k,k)\Bigg]_{t=t'} \tag{39}$$

and

$$P_k^{(1)}(\omega)=\frac{1}{2\pi}\langle\langle F_k^{(1)}(t);F_k^{(1)^{\dagger}}(t')\rangle\rangle_\omega\ . \tag{40}$$

The superscript 0 in the Eq. (39) denotes that in the evaluation of the commutators, the phonon occupation number $N_k(=\langle A_k^{\dagger}A_k\rangle)$ is evaluated by means of the zeroth-order Green's function

$$[G_{kk'}^{(1)}(\omega)]^0=\frac{\omega_k\delta_{kk'}}{\pi[\omega^2-(\widetilde{\omega}_k^{(1)})^2]}\ . \tag{41}$$

The response function $P_k^{(1)}(\omega)$ (in the first-order approximation) is obtained by describing the frequency spectrum of the zeroth-order Green's function (41) by an equivalent zeroth-order renormalized Hamiltonian

$$H_{\text{ren}}^0=\frac{\hbar}{4}\sum_k\left[\frac{(\widetilde{\omega}_k)^2}{\omega_k}A_k^{\dagger}A_k+\omega_k B_k^{\dagger}B_k\right]\ . \tag{42}$$

To evaluate the two- and three-phonon Green's functions (29) we use the renormalized Hamiltonian (42). The Fourier transforms of the Green's functions are given by

$$\langle\langle A_{k_1}A_{k_2};A_{k_1'}^{\dagger}A_{k_2'}^{\dagger}\rangle\rangle_\omega=\frac{\delta^{(2)}}{2\pi}\left[\frac{\omega_{k_1}\omega_{k_2}}{\widetilde{\omega}_{k_1}\widetilde{\omega}_{k_2}}\right]\left[(n_{k_1}+n_{k_2})\frac{(\widetilde{\omega}_{k_1}+\widetilde{\omega}_{k_2})}{\omega^2-(\widetilde{\omega}_{k_1}+\widetilde{\omega}_{k_2})^2}+(n_{k_2}-n_{k_1})\frac{(\widetilde{\omega}_{k_1}-\widetilde{\omega}_{k_2})}{\omega^2-(\widetilde{\omega}_{k_1}-\widetilde{\omega}_{k_2})^2}\right]\ , \tag{43}$$

$$\langle\langle B_{k_1}B_{k_2};B_{k_1}^{\dagger}B_{k_2'}^{\dagger}\rangle\rangle_\omega=\frac{\delta^{(2)}}{2\pi}\left[\frac{\widetilde{\omega}_{k_1}\widetilde{\omega}_{k_2}}{\omega_{k_1}\omega_{k_2}}\right]\left[(n_{k_1}+n_{k_2})\frac{(\widetilde{\omega}_{k_1}+\widetilde{\omega}_{k_2})}{\omega^2-(\widetilde{\omega}_{k_1}+\widetilde{\omega}_{k_2})^2}+(n_{k_2}-n_{k_1})\frac{(\widetilde{\omega}_{k_1}-\widetilde{\omega}_{k_2})}{\omega^2-(\widetilde{\omega}_{k_1}-\widetilde{\omega}_{k_2})^2}\right]\ , \tag{44}$$

$$\langle\langle B_{k_1}B_{k_2}B_{k_3};B^{\dagger}_{k'_1},B^{\dagger}_{k'_2},B^{\dagger}_{k'_3}\rangle\rangle_{\omega}=\frac{\delta^{(3)}}{4\pi}\left\{\left[\left(\frac{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k_3}}{\omega_{k_1}\omega_{k_2}\omega_{k_3}}\right)\times(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_1})\frac{(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})^2}\right]+\{\tilde{\omega}_{k_1}\leftrightarrow-\tilde{\omega}_{k_1}\}+\{\tilde{\omega}_{k_2}\leftrightarrow-\tilde{\omega}_{k_2}\}+\{\tilde{\omega}_{k_3}\leftrightarrow-\tilde{\omega}_{k_3}\}\right\}, \tag{45}$$

where

$$\delta^{(2)}=\delta_{k_1k'_1}\delta_{k_2k'_2}+\delta_{k_1k'_2}\delta_{k_2k'_1}, \tag{46a}$$

$$\delta^{(3)}=\delta_{123}+\delta_{213}+\delta_{321}, \tag{46b}$$

with

$$\delta_{123}=\delta_{k_1k'_1}(\delta_{k_2k'_2}\delta_{k_3k'_3}+\delta_{k_2k'_3}\delta_{k_3k'_2}). \tag{46c}$$

In Eq. (45), $\{\tilde{\omega}_{k_1}\leftrightarrow-\tilde{\omega}_{k_1}\}$, $\{\tilde{\omega}_{k_2}\leftrightarrow-\tilde{\omega}_{k_2}\}$, and $\{\tilde{\omega}_{k_3}\leftrightarrow-\tilde{\omega}_{k_3}\}$ indicate three further terms which are obtained by changing $\tilde{\omega}_{k_1}$ to $-\tilde{\omega}_{k_1}$, $\tilde{\omega}_{k_2}$ to $-\tilde{\omega}_{k_2}$, and $\tilde{\omega}_{k_3}$ to $-\tilde{\omega}_{k_3}$ in the first term, respectively.

From Eqs. (31) and (40), after using the expressions (44) and (45) for the two- and three-phonon Green's functions, the response function $P_k^{(1)}(\omega)$ is obtained as

$$\begin{aligned}P_k^{(1)}(\omega)={}&8\sum_{k_1}[\omega_{k_1}S(-k,k_1)S^*(-k,k_1)][\omega^2-(\tilde{\omega}_{k_1}^{(1)})^2]^{-1}\\&+18\sum_{k_1,k_2}|V^{(3)}(k_1,k_2,-k)|^2\frac{\omega_{k_1}\omega_{k_2}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}}\\&\times\left[(n_{k_1}+n_{k_2})\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2})^2}+(n_{k_2}-n_{k_1})\frac{\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}}{\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2})^2}\right]\\&+48\sum_{k_1,k_2,k_3}|V^{(4)}(k_1,k_2,k_3,-k)|^2\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k_3}}\\&\times\left[(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_1})\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})^2}\right.\\&\left.+3(1-n_{k_1}n_{k_2}+n_{k_2}n_{k_3}-n_{k_3}n_{k_1})\frac{\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3}}{\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3})^2}\right],\end{aligned} \tag{47}$$

where

$$S(k_1,k_2)=\left[\frac{\omega_{k_2}}{\omega_{k_1}}C(k_1,k_2)+D(k_1,k_2)\right]+\frac{4}{\omega_{k_1}}\sum_{k'_2}[C(k_1,k'_2)D(-k'_2,k_2)] \tag{48}$$

and

$$n_k=\frac{\tilde{\omega}_k}{\omega_k}\langle A_k^{\dagger}A_k\rangle=\coth\left[\frac{\beta\hbar\tilde{\omega}_k}{2}\right]. \tag{49}$$

For a small quantity $\epsilon \to 0+$, the response function $P_k^{(1)}(\omega)$ can be written as

$$P_k^{(1)}(\omega+i\epsilon)=\Delta_k^{(1)}(\omega)-i\Gamma_k^{(1)}(\omega)\ , \tag{50}$$

where the real part $\Delta_k^{(1)}(\omega)$ represents the shift in the frequency of the kth mode, while the imaginary part $\Gamma_k^{(1)}(\omega)$ gives the halfwidth of the phonons of wave vector $\vec{k}$. The explicit expressions for them are given by

$$\begin{aligned}\Delta_k^{(1)}(\omega)={}&8P\sum_{k_1}[\omega_{k_1}S(-k,k_1)S^*(-k,k_1)][\omega^2-(\tilde{\omega}_k^{(1)})^2]^{-1}\\&+18P\sum_{k_1,k_2}|V^{(3)}(k_1,k_2,-k)|^2\frac{\omega_{k_1}\omega_{k_2}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}}\\&\times\left[(n_{k_1}+n_{k_2})\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2})^2}+(n_{k_2}-n_{k_1})\frac{\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}}{\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2})^2}\right]\\&+48P\sum_{k_1,k_2,k_3}|V^{(4)}(k_1,k_2,k_3-k)|^2\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k_3}}\\&\times\left[(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_1})\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})^2}\right.\\&\left.+\ 3(1-n_{k_1}n_{k_2}+n_{k_2}n_{k_3}-n_{k_3}n_{k_1})\frac{\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3}}{\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3})^2}\right]\end{aligned}\tag{51}$$

and

$$\begin{aligned}\Gamma_k^{(1)}(\omega)={}&8\pi\epsilon(\omega)\sum_{k_1}[\omega_{k_1}S(-k,k_1)S^*(-k,k_1)\delta(\omega^2-(\tilde{\omega}_{k_1}^{(1)})^2)]\\&+18\pi\epsilon(\omega)\sum_{k_1,k_2}|V^{(3)}(k_1,k_2,-k)|^2\frac{\omega_{k_1}\omega_{k_2}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}}\\&\times[(n_{k_1}+n_{k_2})(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2})\delta(\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2})^2)\\&+(n_{k_2}-n_{k_1})(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2})\delta(\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2})^2)]\\&+48\pi\epsilon(\omega)\sum_{k_1,k_2,k_3}|V^{(4)}(k_1,k_2,k_3-k)|^2\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k_3}}\\&\times[(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_1})(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})\delta(\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})^2)\\&+3(1-n_{k_1}n_{k_2}+n_{k_2}n_{k_3}-n_{k_3}n_{k_1})(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3})\delta(\omega^2-(\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3})^2)]\ ,\end{aligned}\tag{52}$$

where P stands for the principal value of the quantity and $\epsilon(\omega)=1$ for $\omega>0$ and $=-1$ for $\omega<0$. With this result, the Green's function (38) can be written as

$$G_{kk'}^{(1)}(\omega+i\epsilon)=\frac{\omega_k\delta_{kk'}}{\pi(\omega^2-\{\nu_k^{(1)}(\omega)\}^2+2i\omega_k\Gamma_k^{(1)}(\omega))}\ , \tag{53}$$

where

$$\{\nu_k^{(1)}(\omega)\}^2=(\tilde{\omega}_k^{(1)})^2+2\omega_k\Delta_k^{(1)}(\omega)\ . \tag{54}$$

Proceeding in a similar manner, with the equations of motion for the Green's function (28b) and (28c) and following the procedure as used above, we obtain the following expressions for the Green's functions:

$$G_{kk'}^{(2)}(\omega+i\epsilon)=\frac{\omega\delta_{kk'}}{\pi(\omega^2-\{\nu_k^{(2)}(\omega)\}^2+2i\omega_k\Gamma_k^{(2)}(\omega))}\ , \tag{55}$$

$$G_{kk'}^{(3)}(\omega+i\epsilon)=\frac{-\omega_k\delta_{kk'}}{\pi(\omega^2-\{\nu_k^{(3)}(\omega)\}^2+2i\omega_k\Gamma_k^{(3)}(\omega))}\ , \tag{56}$$

where

$$\{\nu_k^{(n)}(\omega)\}^2=(\tilde{\omega}_k^{(n)})^2+2\omega_k\Delta_k^{(n)}(\omega),\quad n=2,3\ ,$$

and $\Delta_k^{(n)}(\omega)$ and $\Gamma_k^{(n)}(\omega)$ are the real and imaginary parts of the response function $P_k^{(n)}(\omega)$ occurring in the process of the evaluation of Green's functions (28b) and (28c). The expressions for the renormalized frequencies $\tilde{\omega}_k^{(n)}$ and the response functions $P_k^{(n)}(\omega)$ corresponding to these Green's functions are obtained as

$$\begin{aligned}(\tilde{\omega}_k^{(2)})^2=\omega_k^2+\frac{\omega_k}{2\pi}\Bigg[&\langle[F_k^{(1)}(t),B_k^{\dagger}(t')]^0\rangle+\frac{\omega}{\omega_k}\langle[F_k^{(1)}(t),A_k^{\dagger}(t')]^0\rangle\\&+\frac{4}{\omega_k}\sum_{k_1}D(k,-k_1)\langle[F_k^{(1)}(t);F_k^{(3)}(t)]^0\rangle\Bigg]_{t=t'}\ ,\end{aligned} \tag{57}$$

$$\begin{aligned}(\tilde{\omega}_k^{(3)})^2=\omega_k^2+\frac{\omega_k}{2\pi}\Bigg[&\langle[F_k^{(3)}(t),A_k^{\dagger}(t')]^0\rangle+\frac{\omega}{\omega_k}\langle[F_k^{(3)}(t),B_k^{\dagger}(t')]^0\rangle\\&+\frac{4}{\omega_k}\sum_{k_1}D(-k,k_1)\langle[F_k^{(3)}(t),A_{k_1}^{\dagger}(t')]^0\rangle\Bigg]_{t=t'}\\&+8\pi\frac{(\omega^2-\omega_k^2)}{\omega_k}\left[D(-k,k)+\frac{6}{\omega_k}\sum_{k_1}V^{(4)}(-k,k,k_1,-k_1)N_{k_1}\right]\ ,\end{aligned} \tag{58}$$

$$P_k^{(2)}(\omega)=\frac{1}{2\pi}\langle\langle F_k^{(1)};F_k^{(3)}(t')\rangle\rangle_{\omega}\ , \tag{59}$$

$$P_k^{(3)}(\omega)=\frac{1}{2\pi}\langle\langle F_k^{(3)}(t);F_k^{(3)^{\dagger}}(t')\rangle\rangle_{\omega}\ , \tag{60}$$

with

$$\begin{aligned}F_k^{(3)}(t)=4\pi\sum_{k_1}\Bigg\{&\left[C(-k,k_1)+\frac{\omega_{k_1}}{\omega_k}D(-k,k_1)+\frac{4}{\omega_k}\sum_{k_2}D(-k_2k_2)C(-k_2,k_1)\right]B_{k_1}\\&+2\pi\left[3\sum_{k_1,k_2}V^{(3)}(-k,k_1,k_2)\left[\frac{\omega_{k_1}}{\omega_k}B_{k_1}A_{k_2}A_{k_3}+\frac{\omega_{k_2}}{\omega_k}A_{k_1}B_{k_2}A_{k_3}+\frac{\omega_{k_3}}{\omega_k}A_{k_1}A_{k_2}B_{k_3}\right]\right]\Bigg\}\ .\end{aligned} \tag{61}$$

The response functions $P_k^{(2)}(\omega)$ and $P_k^{(3)}(\omega)$ can easily be obtained from Eqs. (59) and (60) after evaluating the two- and three-phonon Green's functions using the renormalized Hamiltonian (42). It is important to note that we have evaluated the Green's functions (28) in the lowest-order approximation of the polarization operator. However, if the imaginary part of the polarization operator $P_k(\omega)$ in Eqs. (53), (55), and (56) becomes zero for some frequency $\nu_k \neq \tilde{\omega}_k$, its value should be evaluated in the first-order approximation, i.e., by considering higher-order terms in Eq. (36). Having obtained the Green's function we can calculate also the correlation function using the standard relations.

IV. THERMAL CONDUCTIVITY

We separately evaluate the diagonal contribution, nondiagonal contribution, lattice-imperfection contribution, and contribution due to anharmonic forces to the thermal conductivity. Substituting the values of the correlation functions appearing in Eq. (4) with the help of Eqs. (18), (53), (55), and (56) and performing the integration over the time t, the diagonal contribution to the thermal conductivity becomes

$$K_d=\frac{4\hbar^2 k_B\beta^2}{3\pi V}\sum_{\vec{k},s}\omega^4_{\vec{k}s}v^2_{\vec{k}s}\int_{-\infty}^{\infty}d\omega\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\times\left[\frac{\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)][\Gamma^{(3)}_{\vec{k}s}(\omega)]}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)(\{\omega^2-[\nu^{3}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(3)}_{\vec{k}s}(\omega)]^2)}+\frac{\omega^2[\Gamma^{(2)}_{\vec{k}s}(\omega)]^2}{(\{\omega^2-[\nu^{2}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(2)}_{\vec{k}s}(\omega)]^2)^2}\right]. \tag{62}$$

For small values of halfwidths $\Gamma^{(n)}_{\vec{k}s}(\omega)$, the integrands in Eq. (62) are peaked around $\omega=\nu^{(n)}_{\vec{k}s}(\omega)$ and the integrals can be evaluated analytically by replacing the peak distribution by a Dirac δ function. We then obtain the diagonal contribution to the thermal conductivity as

$$K_d=\frac{\hbar^2 k_B\beta^2}{12V}\sum_{\vec{k}s}v^2_{\vec{k}s}\left[\omega^2_{\vec{k}s}\frac{e^{\beta\hbar\nu^{(1)}_{\vec{k}s}(\omega)}}{(e^{\beta\hbar\nu^{(1)}_{\vec{k}s}(\omega)}-1)^2}\frac{1}{\Gamma^{(3)}_{\vec{k}s}(\nu^{(1)}_{\vec{k}s})}+(\nu^{(2)}_{\vec{k}s})^2\frac{e^{\beta\hbar\nu^{(2)}_{\vec{k}s}(\omega)}}{(e^{\beta\hbar\nu^{(2)}_{\vec{k}s}(\omega)}-1)^2}\frac{1}{\Gamma^{(2)}_{\vec{k}s}(\nu^{(2)}_{\vec{k}s})}\right]. \tag{63}$$

Neglecting the shift in the frequency due to anharmonic interactions and the shift in perturbation due to lattice imperfection, the expression has a form similar to the well-known Debye-Peierls expression for the thermal conductivity which is obtained here as a direct consequence of the Kubo formula and the choice of the Hamiltonian.

In a similar manner we can obtain the nondiagonal contribution K_{nd} to the thermal conductivity. Inserting the values of the correlation functions appearing in Eq. (5) with the help of Eqs. (19), (53), (55), and (56) and following the method as used above, the nondiagonal contribution to the thermal conductivity due to the nondiagonal term in the energy-flux operator can be written in the form

$$K_{nd}=\frac{4\hbar^2 k_B\beta^2}{3\pi V}\sum_{\substack{\vec{k},s,s'\\ s\neq s'}}v^2_{\vec{k}ss'}\omega^2_{\vec{k}s}\omega^2_{\vec{k}s'}\int_{-\infty}^{\infty}d\omega\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\times\left[\frac{\omega_{\vec{k}s}\omega_{\vec{k}s'}[\Gamma^{(1)}_{\vec{k}s}(\omega)][\Gamma^{(3)}_{\vec{k}s'}(\omega)]}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)(\{\omega^2-[\nu^{(3)}_{\vec{k}s'}(\omega)]^2\}^2+4\omega^2_{\vec{k}s'}[\Gamma^{(3)}_{\vec{k}s'}(\omega)])}+\frac{\omega^2[\Gamma^{(2)}_{\vec{k}s}(\omega)][\Gamma^{(2)}_{\vec{k}s'}(\omega)]}{(\{\omega^2-[\nu^{(2)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(2)}_{\vec{k}s}(\omega)]^2)(\{\omega^2-[\nu^{(2)}_{\vec{k}s'}(\omega)]^2\}^2+4\omega^2_{\vec{k}s'}[\Gamma^{(2)}_{\vec{k}s'}(\omega)]^2)}\right]. \tag{64}$$

The above expression shows that the nondiagonal contribution due to the nondiagonal part of the energy-flux operator comes from the modes of difference polarization directions and is similar to the diagonal contribution.

We now proceed to evaluate the contribution to the thermal conductivity on account of the terms which are cubic functions of position and momentum operator in the harmonic approximation in the energy-flux operator. Inserting the values of the correlation functions appearing in Eqs. (8) with the help of Eqs. (53), (43), and (44), and performing the integration with respect to time the contribution due to these terms is given by

$$
\begin{aligned}
K_c^{(1)}=\frac{\hbar^2 k_B \beta^2}{3V} \sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s''}\ \sum_{\vec{k},s,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1} \omega^2_{\vec{k}s}\delta^{(2)} \int_{-\infty}^{\infty} d\omega \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}
& \times \frac{\Gamma^{(1)}_{\vec{k}s}(\omega)}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)} \\
& \times \left[\frac{\omega_{\vec{k}'s'}\omega_{\vec{k}''s''}}{\widetilde{\omega}_{\vec{k}'s'}\widetilde{\omega}_{\vec{k}''s''}}\right] \vec{X}_{\vec{k}s,\vec{k}'s',\vec{k}''s''}\cdot\vec{X}^*_{\vec{k}s,\vec{k}'_1s'_1,\vec{k}''_1s''_1} \\
& \times \left[\sum_{l=\pm 1}(n_{\vec{k}''s''}+ln_{\vec{k}'s'})(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''}) \right. \\
& \qquad \left. \times\, \delta(\omega^2-(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''})^2)\right] , \qquad (65a)
\end{aligned}
$$

$$
\begin{aligned}
K_c^{(2)}=\frac{4\hbar^2 k_B \beta^2}{3V} \sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s''}\ \sum_{\vec{k},s,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1} \omega^2_{\vec{k}s}\delta^{(2)} \int_{-\infty}^{\infty} d\omega \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}
& \times \frac{\Gamma^{(1)}_{\vec{k}s}(\omega)}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)} \\
& \times \left[\frac{\widetilde{\omega}_{\vec{k}'s'}\widetilde{\omega}_{\vec{k}''s''}}{\omega_{\vec{k}'s'}\omega_{\vec{k}''s''}}\right] \vec{Y}_{\vec{k}s,\vec{k}',s',\vec{k}''s''}\cdot\vec{Y}^*_{\vec{k}s,\vec{k}'_1s'_1,\vec{k}''_1s''_1} \\
& \times \left[\sum_{l=\pm 1}(n_{\vec{k}''s''}+n_{\vec{k}'s'})(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''}) \right. \\
& \qquad \left. \times\, \delta(\omega^2-(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''})^2)\right] , \qquad (65b)
\end{aligned}
$$

$$
\begin{aligned}
K_c^{(3)}=\frac{4\hbar^2 k_B \beta^2}{3V} \sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s''}\ \sum_{\vec{k},s,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1} \omega^2_{\vec{k}s}\delta^{(2)} \int_{-\infty}^{\infty} d\omega \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}
& \times \frac{\Gamma^{(1)}_{\vec{k}s}(\omega)}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)} \\
& \times \left[\frac{\widetilde{\omega}_{\vec{k}'s'}\widetilde{\omega}_{\vec{k}''s''}}{\omega_{\vec{k}'s'}\omega_{\vec{k}''s''}}\right] \vec{Z}_{\vec{k}''s'',\vec{k}'s',\vec{k}s}\cdot\vec{Z}^*_{k''_1s''_1,\vec{k}'_1s'_1,\vec{k}s} \\
& \times \left[\sum_{l=\pm 1}(n_{\vec{k}''s''}+ln_{\vec{k}'s'})(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''}) \right. \\
& \qquad \left. \times\, \delta(\omega^2-(\widetilde{\omega}_{\vec{k}'s'}+l\widetilde{\omega}_{\vec{k}''s''})^2)\right] , \qquad (65c)
\end{aligned}
$$

We further proceed to evaluate the contribution to the thermal conductivity due to the perturbation terms in the average heat flux arising from cubic anharmonic forces. Substituting for the correlation functions appearing in Eq. (9a) with the help of Eqs. (53) and (44), we obtain the contribution K_1 to the thermal conductivity on account of the term which is a cubic function of position and momentum operators as

$$K_1=\frac{4\hbar^2k_B\beta^2}{3V}\sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s''}\;\sum_{\vec{k},s,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1}\vec{J}_{\vec{k}s,\vec{k}'s',\vec{k}''s''}\cdot\vec{J}^*_{\vec{k}s,\vec{k}'_1s'_1,\vec{k}''_1s''_1}$$

$$\times\omega^2_{\vec{k}s}\delta^{(2)}\int_{-\infty}^{\infty}d\omega\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\left[\frac{\Gamma^{(1)}_{\vec{k}s}(\omega)}{(\{\omega^2-[\nu^{(1)}_{\vec{k}s}(\omega)]^2\}^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)}\right.$$

$$\times\sum_{l=\pm1}\left[\frac{\tilde{\omega}_{\vec{k}'s'}\tilde{\omega}_{\vec{k}''s''}}{\omega_{\vec{k}'s'}\omega_{\vec{k}''s''}}\right](n_{\vec{k}''s''}+ln_{\vec{k}'s'})(\tilde{\omega}_{\vec{k}'s'}+l\tilde{\omega}_{\vec{k}''s''})$$

$$\left.\times\,\delta(\omega^2-(\tilde{\omega}_{\vec{k}'s'}+l\tilde{\omega}_{\vec{k}''s''})^2)\right]. \tag{66a}$$

Similarly, substituting for the correlation functions appearing in Eq. (9b) from Eqs. (53) and (45), the contribution K_2 to the thermal conductivity on account of cubic forces which are quartic functions of position and momentum operators is given by

$$K_2=\frac{2\hbar^2k_B\beta^2}{3V}\sum_{\vec{k},s,\vec{k}',s',\vec{k}'',s'',\vec{k}''',s'''}\;\sum_{\vec{k}_1,s_1,\vec{k}'_1,s'_1,\vec{k}''_1,s''_1}\vec{J}_{\vec{k}s,\vec{k}'s',\vec{k}''s'',\vec{k}'''s'''}\cdot\vec{J}^*_{\vec{k}_1s_1,\vec{k}'_1s'_1\,\vec{k}''_1s''_1,\vec{k}'''s'''}\omega^2_{\vec{k}'''s'''}\delta^{(3)}$$

$$\times\int_{-\infty}^{\infty}d\omega\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\left[\frac{\Gamma^{(1)}_{\vec{k}'''s'''}(\omega)}{(\{\omega^2-[\nu^{(1)}_{\vec{k}'''s'''}(\omega)]^2\}^2+4\omega^2_{\vec{k}'''s'''}[\Gamma^{(1)}_{\vec{k}'''s'''}(\omega)]^2)}\right.$$

$$\times\left\{\left[\left[\frac{\tilde{\omega}_{\vec{k}s}\tilde{\omega}_{\vec{k}'s'}\tilde{\omega}_{\vec{k}''s''}}{\omega_{\vec{k}s}\omega_{\vec{k}'s'}\omega_{\vec{k}''s''}}\right](1+n_{\vec{k}s}n_{\vec{k}'s'}+n_{\vec{k}'s'}n_{\vec{k}''s''}+n_{\vec{k}''s''}n_{\vec{k}s})\right.\right.$$

$$\left.\times\,(\tilde{\omega}_{\vec{k}s}+\tilde{\omega}_{\vec{k}'s'}+\tilde{\omega}_{\vec{k}''s''}\delta(\omega^2-(\tilde{\omega}_{\vec{k}s}+\tilde{\omega}_{\vec{k}'s'}+\tilde{\omega}_{\vec{k}''s''})^2)\right]$$

$$\left.\left.+\;\{\tilde{\omega}_{\vec{k}s}\leftrightarrow-\tilde{\omega}_{\vec{k}s}\}+\{\tilde{\omega}_{\vec{k}'s'}\leftrightarrow-\omega_{\vec{k}'s'}\}+\{\tilde{\omega}_{\vec{k}''s''}\leftrightarrow-\tilde{\omega}_{\vec{k}''s''}\}\right\}\right], \tag{66b}$$

where $\{\tilde{\omega}_{\vec{k}s}\leftrightarrow-\tilde{\omega}_{\vec{k}s}\}$ represents a term which is obtained by replacing $\tilde{\omega}_{\vec{k}s}$ by $-\tilde{\omega}_{\vec{k}s}$ in the first term.

Finally, we come to the evaluation of the contribution K_{imp} due to the thermal conductivity on account of perturbation term in the energy flux due to lattice imperfection. Inserting the values of the correlation function appearing in Eq. (10) with the help of Eqs. (23), (53), and (55) and following the method as used above, we obtain

$$K_{\text{imp}}=\frac{4\hbar^2k_B\beta^2}{3\pi V}\sum_{\vec{k},s,\vec{k}',s'}\omega_{\vec{k}s}\omega_{\vec{k}'s'}\int_{-\infty}^{\infty}d\omega\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

$$\times\left[\frac{\omega_{\vec{k}s}\omega_{\vec{k}'s'}[\Gamma^{(1)}_{\vec{k}s}(\omega)][\Gamma^{(3)}_{\vec{k}'s'}(\omega)](\vec{J}_{\vec{k}s,\vec{k}'s'}\cdot\vec{J}^*_{\vec{k}s,\vec{k}'s'})}{([\omega^2-\{\nu^{(1)}_{\vec{k}s}(\omega)\}^2]^2+4\omega^2_{\vec{k}s}[\Gamma^{(1)}_{\vec{k}s}(\omega)]^2)([\omega^2-\{\nu^{(3)}_{\vec{k}'s'}(\omega)\}^2]^2+4\omega^2_{\vec{k}'s'}[\Gamma^{(3)}_{\vec{k}'s'}(\omega)]^2)}\right.$$

$$\left.+\frac{\omega^2[\Gamma^{(2)}_{\vec{k}s}(\omega)][\Gamma^{(2)}_{\vec{k}'s'}(\omega)](\vec{J}_{\vec{k}s,-\vec{k}'s'}\cdot J^*_{-\vec{k}'s',\vec{k}s})}{([\omega^2\{\nu^{(2)}_{\vec{k}s}(\omega)\}^2]^2+4\omega^2_{\vec{k}s}[\Gamma^{(2)}_{\vec{k}s}(\omega)]^2)([\omega^2-\{\nu^{(2)}_{\vec{k}'s'}(\omega)\}^2]^2+4\omega^2_{\vec{k}'s'}[\Gamma^2_{\vec{k}'s'}(\omega)]^2)}\right]. \tag{67}$$

V. DISCUSSION

In the present paper we have derived an expression for the thermal conductivity of an impure anharmonic Bravais crystal. Equations (63)–(67) give various contributions to the temperature dependence of the thermal conductivity of a doped Bravais anharmonic crystal due to impurity-phonon scattering. The diagonal contribution (63) in the limit of small halfwidth of phonons has essentially the same form as obtained by Klemens[2] and Carruthers[3] using the Boltzmann transport equation. The nondiagonal contributions due to the nondiagonal part of the energy-flux operator, and also due to the term corresponding to lattice imperfections as propounded by Hardy,[5] come from different modes of different polarization directions. Hardy[5] has shown that Q_c is negligible except below 10 K. The contributions of cubic anharmonic forces Q' are significant only when the amplitude of the particle displacements are appreciable compared to spacings between particles such as at temperatures near the melting point. Therefore at low temperatures where only long-wavelength phonons are present, the diagonal contribution gives the major contribution to the thermal conductivity of a defect crystal. However, at high temperatures we should also consider the other remaining contributions. Based on the classical treatment of phonon operators Hardy has pointed out that the nondiagonal part of the energy-flux operator is an oscillating function of terms where frequencies are the sum and difference of the frequencies of different branches and give negligible contribution to thermal conductivity compared to the diagonal one when averaged over a long period of time. The present study shows that there is a finite contribution of the nondiagonal terms, the cubic anharmonic term, and the term due to lattice imperfections in the energy-flux operator of the thermal conductivity. Though the contributions may be much smaller than the diagonal one, the contributions from the cubic anharmonic force term in the energy-flux operator are at least 2 orders of magnitude smaller than the diagonal contribution. The results obtained here are correct for small concentration of impurities and to the lowest nonvanishing order in the anharmonic force constants.

It emerges from the present study that from the Kubo formula and double-time Green's-function technique it is easier to evaluate the thermal conductivity for a suitable model of a doped Bravais anharmonic crystal taking into account the lattice-imperfection term and the effect of cubic anharmonic forces in the energy-flux operator. We have not evaluated numerical values of various contributions to thermal conductivity due to the great complexity of the computation which arises mainly from the wide range of phonon frequencies that must be included and the presence of impurities and anharmonicity in the crystal. Even then, by computing the numerical values of different parameters involved in the various expressions and substituting these in the respective places, one can find the numerical values of the various contributions to thermal conductivity by solving the integrals with the help of a computer.

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