Equation of motion for the Green's function in anharmonic solids

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We discuss the double-time Green's-function approach for the phonon-phonon interaction in anharmonic solids. Using a certain interpretation of the phonon operators, the crystal Hamiltonian may be rewritten in a compact form. The equation of motion for the Green's function is tremendously simplified with this formalism. The self-energy can be obtained in a very simple way, to any desired perturbation order. Our results reproduce the corresponding terms of the available literature results, which are limited to the fourth order in the perturbation parameter.

I. INTRODUCTION

The theoretical interpretation of Raman and infrared spectra in molecular crystals has made effective and extensive use of the methods of many-body quantum field theory.[1-4] The phonon-phonon interactions due to the crystal anharmonicity are responsible for the finite lifetime of the phonon excitations and thus for the line broadening of the optical bands.[2-4] Recently, high-resolution Raman techniques,[5-8] Fourier-transform infrared (FTIR) spectroscopy,[9] and time-resolved coherent anti-Stokes Raman spectroscopy (CARS) (Refs. 10-12) have allowed reliable measurments of the phonon bandwidths in the frequency domain or the direct observation of the time evolution of phonon excitations. Theoretical studies in molecular crystals have been generally carried out by limiting the perturbation expansion of the Green's function to the lowest-order terms.[13,14] In this approximation the computed bandwidths depend linearly on the temperature in the classical limit. Experimentally, the temperature dependence of the bandwidths has been found to be linear only in a few cases, such as some lattice phonons in naphtalene[15] and antracene.[16] In the case of the intramolecular modes, the temperature dependence has turned out to be quadratic in most of the experimental studies.[12,17-19] Recent Raman[5] and infrared measurements[20] on CO_2 crystal have shown that, at high temperature, higher-order processes are important also for lattice phonons. In the case of nitrogen, the bandwidth of the observed lattice modes and intramolecular modes has been found[7] to follow a nonlinear behavior even at relatively low temperatures. Higher-order processes thus appear generally to play a crucial role in determining the spectral properties of molecular solids. An effective tool for evaluating the phonon linewidths at high perturbation orders would be very useful in the interpretation of experiments. The approach used by most authors is based on the Matsubara representation for the temperature-dependent Green's function.[21-23] In this formalism the Green's functions are time independent and are evaluated

by use of a perturbation expansion of the scattering matrix S.[23] The Green's function is given by a summation of terms which are represented as Feynman diagrams. At each perturbation order, one must construct all the topologically distinct diagrams and then evaluate the corresponding Green's function by contour integration, using rules given by Maradudin[2] and Abrikosov, Gorkov, and Dzyaloshinski.[24] The method is involved and becomes rapidly unmanageable with increasing perturbation order. Moreover, for high orders, the construction of all topologically distinct diagrams is far from being a trivial task. Tripathy and Pathak[25] and Monga and Pathak[26] succeeded in deriving most of the terms of order λ^4 contributing to the phonon lifetime. To our knowledge, there has not been a subsequent attempt to extend the Matsubara technique to higher-order corrections of the photon self-energy.

An alternative description of the spectral properties in anharmonic solids is based on the double-time Green's functions. The double-time Green's functions (retarded, advanced, or causal) are explicitly time dependent. Using the Heisenberg equation of motion, one can build up an infinite chain of coupled equations involving a Green's function of increasing complexity. This technique, known as the equation-of-motion method, was used by Zubarev[27] to study electron-phonon interactions in metals. Tyablikov and Bonch-Bruevich[28] developed a perturbation series for the mass operator based on a simple decoupling scheme. Recently, this technique has been used to study phonon-phonon interactions by Bogani, Cardini, and Schettino[29] for the vibrational relaxation of the Fermi doublets in CO_2 crystals, and by Procacci et al.[30] for the relaxation of isolated vibrons in linear chains of polyatomic molecules. The double-time Green's-function method has been reviewed by Parry[23] and more recently by Wallis and Balkanski.[31] The method is, in principle, straightforward, although the results depend on the approximations used in decoupling the infinite chain of equations.[23,31] Furthermore, the algebraic intricacies involved in decoupling even a short chain of equations have deterred many from applying the

method to the phonon-phonon interaction.

In the present study we discuss the double-time Green's-function approach in the case of the phonon-phonon interaction (i.e., for anharmonic crystals). We shall show how the equation-of-motion method may be improved by appropriately redefining the crystal Hamiltonian and the decoupling scheme, in order to evaluate in an extremely straightforward and surprisingly simple way the self-energy to any desired perturbation order. Results up to order λ^4 are found to be equivalent to those obtained by other authors using the standard technique of the temperature Green's function.[24,32] The present paper is organized as follows. In Sec. II we rewrite the crystal Hamiltonian by redefining the phonon operators. In our formalism both positive and negative signs of the branch indices are allowed. The sign of the branch index distinguishes between annihilation and creation operators. With this simple device, the crystal Hamiltonian is rewritten in an extremely compact form. The equation-of-motion method is introduced in Sec. III and developed in Sec. IV, where, in order to build up the infinite chain of coupled equations, we derive an exact equation satisfied by the Green's function. The decoupling scheme for the infinite chain is discussed in Sec. V. The decoupling method allows one to obtain *at once* the complete self-energy expression to any desired perturbation order without drawing all the topologically distinct irreducible diagrams. The latter may be easily identified, *a posteriori*, by decomposing the overall expression for the self-energy. In Sec. VI, finally, we give an explicit example of finite-order expansion by adopting our procedure up to order λ^4. The overall expression for the proper self-energy has been decomposed into the various contributions arising from all the topologically distinct λ^2 and λ^4 diagrams. All the diagrams obtained by Tripathy and Pathak[25] are easily identified. We also report some additional λ^4 contributions to the real part of the proper self-energy.

II. HAMILTONIAN OF THE SYSTEM

The Hamiltonian of an anharmonic crystal in a second-quantization representation may be written as a diagonal harmonic term $\mathcal{H}_2$ plus a series of off-diagonal anharmonic contributions[4,33] $\mathcal{H}_n$, $n \geq 3$:

$$\mathcal{H} = \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4 + \mathcal{H}_5 + \cdots ,\qquad (2.1)$$

where

$$\mathcal{H}_2 = \sum_{\mathbf{k},i} \omega_{\mathbf{k}i}(b_{\mathbf{k}i}^\dagger b_{\mathbf{k}i} + \tfrac{1}{2}) ,\qquad (2.2)$$

$$\mathcal{H}_n = \sum_{\mathbf{k}_1,i_1, \cdots \mathbf{k}_n,i_n} V_{\mathbf{k}_1 i_1 \cdots \mathbf{k}_n i_n}(b_{\mathbf{k}_1 i_1} + b_{-\mathbf{k}_1 i_1}^\dagger)$$
$$\times \cdots (b_{\mathbf{k}_n i_n} + b_{-\mathbf{k}_n i_n}^\dagger) .\qquad (2.3)$$

The operator $b_{\mathbf{k}i}$ and its adjoint $b_{\mathbf{k}i}^\dagger$ annihilate and create phonons with wave vector $\mathbf{k}$ and energy $\omega_{\mathbf{k}i}$ and satisfy the boson commutation rules

$$[b_{\mathbf{k}_a i_a}, b_{\mathbf{k}_b i_b}^\dagger] = \delta_{\mathbf{k}_a \mathbf{k}_b} \delta_{i_a i_b} ,$$
$$[b_{\mathbf{k}_a i_a}, b_{\mathbf{k}_b i_b}] = [b_{\mathbf{k}_a i_a}^\dagger, b_{\mathbf{k}_b i_b}^\dagger] = 0 .\qquad (2.4)$$

The interaction coefficients $V_{\mathbf{k}_1 i_1 \cdots \mathbf{k}_n i_n}$ are multidimensional Fourier transforms of potential derivatives and are symmetric in the indices $\mathbf{k}i$. The label i distinguishes different phonon branches with the same wave vector. We choose *positive* integers as branch labels.

Equations (2.3) and (2.4) are rather complex and cannot be manipulated easily. We will transform them into extremely compact expressions with the device of introducing *negative* indices for the branch labels. For a negative i, we define

$$b_{\mathbf{k}i} \equiv b_{-\mathbf{k}-i}^\dagger \quad \text{(for } i < 0) .\qquad (2.5)$$

In this notation each factor $b_{\mathbf{k}i} + b_{-\mathbf{k}i}^\dagger$ in Eq. (2.3) becomes a sum on both positive and negative signs $b_{\mathbf{k}i} + b_{\mathbf{k}-i}$. Thus, by allowing the sums to run on both positive and negative branch indices and choosing $V_{\mathbf{k}_1 i_1 \cdots \mathbf{k}_n i_n}$ to be independent of the signs of the branch indices, we rewrite Eqs. (2.2) and (2.3) as

$$\mathcal{H}_2 = \sum_{a > 0} \omega_a(b_{-a} b_a + \tfrac{1}{2}) ,\qquad (2.6)$$

$$\mathcal{H}_n = \sum_{1, \ldots, n} V_{1 \cdots n} b_1 \cdots b_n .\qquad (2.7)$$

Here and in the following, in order to make complex expressions more compact, we have replaced each pair of indices $\mathbf{k}, i$ with a single collective index: $a \equiv (\mathbf{k}_a, i_a)$ and $-a \equiv (-\mathbf{k}_a, -i_a)$. By $a > 0$, we mean $i_a > 0$.

The commutators (2.4) may be rewritten as a single equation:

$$[b_a, b_b] = \sigma_a \delta_{a-b} ,\qquad (2.8)$$

where $\sigma_a \equiv \text{sgn}(i_a)$ has been introduced to make Eq. (2.8) valid for all signs of a and b. Equations (2.6)–(2.8) are compact equivalents of (2.2)–(2.4) and constitute the starting point in our derivation by completely defining the phonon system.

III. EQUATION OF MOTION FOR RETARDED GREEN'S FUNCTION

Green's functions in many-body theory are a generalization of correlation functions. Given two operators in the Heisenberg representation, $A(t')$ and $B(t'')$, acting at different times t' and t'', the retarded Green's function $G(A, B; t)$ depends, for a stationary system, only on the time lag[27,34,35] $t = t' - t''$ and is defined by

$$G(A, B; t) \equiv -i\Theta(t)\langle [A(t), B(0)] \rangle ,\qquad (3.1)$$

where $\Theta(t)$ is the unit-step function (1 for $t > 0$ and 0 for $t \leq 0$) and the angular brackets indicate the canonical ensemble average appropriate to the anharmonic Hamiltonian (2.1). By differentiating Eq. (3.1) with respect to the time t, we obtain

$$i\frac{dG(A, B; t)}{dt} = \delta(t)\langle [A(t), B(0)] \rangle$$
$$- i\Theta(t)[\langle [A(t), H], B(0)] \rangle$$
$$= \delta(t)\langle [A(t), B(0)] \rangle + G([A, H], B; t) ,\qquad (3.2)$$

where $\delta(t)=d\Theta(t)/d(t)$ is the Dirac's δ function and we have used the fact that the operator $A(t)$ obeys Heisenberg's equation of motion,

$$i\frac{dA(t)}{dt}=[A(t),H] . \tag{3.3}$$

By taking the Fourier transform of both sides of Eq. (3.2), we obtain

$$\omega G(A,B;\omega)=\langle [A(0),B(0)]\rangle$$
$$+G([A,H],B;\omega) , \tag{3.4}$$

where $G(A,B;\omega)$ is the Fourier transform of the Green's function $G(A,B;t)$, i.e.,

$$G(A,B;\omega)\equiv \int_{-\infty}^{+\infty} e^{i\omega t}G(A,B;t)dt . \tag{3.5}$$

The last term in Eq. (3.4) is a higher-order Green's function involving $[A(t),H]$ instead of $A(t)$. The equation for $G([A,H],B;\omega)$ may be obtained by replacing A with $[A,H]$ in Eq. (3.4), producing the new Green's function $G([[A,H],H],B;\omega)$ on the right-hand side. Repeating this process, we construct an infinite chain of coupled equations involving a hierarchy of Green's function.[27]

IV. GREEN'S FUNCTION HIERARCHY

Our objective is the determination of the phonon spectrum of the crystal, that is, the transition probability of the system under an applied periodic field. Linear-response theory relates the spectrum to the one-phonon Green's function $G(b_q,b_q^\dagger;\omega)$. The distribution of the poles of $G(b_q,b_q^\dagger;\omega)$ is found to correspond to the spectrum of the elementary excitations of the system.[34-37] In our notation $G(b_q,b_q^\dagger;\omega)$ becomes $G(b_q,b_{-q};\omega)$, with $q>0$. As we will see, by repeatedly applying Eq. (3.4),

we obtain a hierarchy of Green's functions of the form $G(A,b_{-q};\omega)$, where A is a product $b_a b_b b_c \cdots b_d b_e$ of operators.

The commutators $[A,b_{-q}]$, $[A,\mathcal{H}_2]$, and $[A,\mathcal{H}_n]$ that are required to use Eq. (3.4) may be evaluated by induction on the number of operators b_j appearing in A, as is shown in the Appendix. The resulting commutators are given here for a generic product A of the form $A=b_a b_b b_c \cdots b_d b_e$. The commutator $[A,\mathcal{H}_2]$ is proportional to A. The proportionality constant is a sum of energies ω_j, one for each operator b_j appearing in A, with the minus sign for $j<0$ (i.e., for a creation operator $b_j=b^\dagger_{-\mathbf{k}_j-i_j}$ and the plus sign for $j>0$ (for an annihilation operator $b_j=b_{\mathbf{k}_j i_j}$:

$$[A,\mathcal{H}_2]=(\omega_a+\omega_b+\omega_c+\cdots+\omega_d+\omega_e)A , \tag{4.1}$$

where, by taking into account the fact that $\omega_{-\mathbf{k}i}=\omega_{\mathbf{k}i}$ (because of the time-reversal symmetry of the phonon Hamiltonian), we have defined the energy as an odd function:

$$\omega_j\equiv -\omega_{-j} . \tag{4.2}$$

The commutator $[A,b_{-q}]$ is a sum of terms, one for each operator b_j in A. The term corresponding to b_j is obtained by replacing b_j with δ_{jq} in A:

$$[A,b_{-q}]=\delta_{aq}b_b b_c \cdots b_d b_e+b_a\delta_{bq}b_c \cdots b_d b_e$$
$$+b_a b_b b_c \cdots \delta_{dq}b_e+\cdots b_a b_b b_c \cdots b_d\delta_{eq} . \tag{4.3}$$

Also, the commutator $[A,\mathcal{H}_n]$ is a sum of terms, one for each operator b_j in A. Each term is a copy of A with b_j replaced by

$$n\sum_{2,3,\ldots,n}\sigma_j V_{-j23\cdots n}b_2 b_3 \cdots b_n :$$

$$[A,\mathcal{H}_n]=n\sum_{2,3,\ldots,n}(\sigma_a V_{-a23\cdots n}b_2 b_3 \cdots b_n)b_b b_c \cdots b_d b_e+n\sum_{2,3,\ldots,n}b_a(\sigma_b V_{-b23\cdots n}b_2 b_3 \cdots b_n)b_c \cdots b_d b_e$$
$$+\cdots+n\sum_{2,3,\ldots,n}b_a b_b b_c \cdots b_d(\sigma_e V_{-e23\cdots n}b_2 b_3 \cdots b_n) . \tag{4.4}$$

We are now in position to apply the equation of motion (3.4) by writing down the starting equation in the hierarchy for $G(b_q,b_{-q};\omega)$:

$$\omega G(b_q,b_{-q};\omega)=\langle [b_q,b_{-q}]\rangle+G([b_q,\mathcal{H}_2],b_{-q};\omega)+\sum_{n\geq 3}G([b_q,\mathcal{H}_n],b_{-q};\omega)$$

$$=1+\omega_q G(b_q,b_{-q};\omega)+\sum_{n\leq 3}n\sum_{2,3,\ldots,n}V_{-q23\cdots n}G(b_2 b_3 \cdots b_n,b_{-q};\omega) , \tag{4.5}$$

where, using Eqs. (4.3), (4.1), and (4.4), with $A=b_q$, we have exploited the linearity of $G(A,B;\omega)$ and the fact that $\sigma_q=1$ (as $q>0$). As we have anticipated, the equation of motion (3.4) for the Green's function $G(b_q,b_{-q};\omega)$ involves higher-order functions of the form $G(b_2 b_3 \cdots b_n,b_{-q};\omega)$. Because of the form of Eqs. (4.1) and (4.4), the equation for $G(b_2 b_3 \cdots b_n,b_{-q};\omega)$ involves more Green's functions of the same form. In our effort to remove all excess baggage from the formalism, we leave as implicit the arguments b_{-q} and ω, which are always present in the Green's functions, and use the shorthand

$$G(abc \cdots d)\equiv G(b_a b_b b_c \cdots b_d,b_{-q};\omega) .$$

Thus we rewrite Eq. (4.5) for $G(q) = G(b_q, b_{-q}; \omega)$ as

$$(\omega - \omega_q) G(q) = 1 + \sum_{n \geq 3} n \sum_{2,3,\ldots,n} V_{-q23\cdots n} G(23 \cdots n) . \tag{4.6}$$

Neglecting the last term in Eq. (4.6), we obtain the Green's function in absence of anharmonic interactions (the "bare" Green's function), $G_0(q)$:

$$G_0(q) \equiv \frac{1}{\omega - \omega_q} . \tag{4.7}$$

$G_0(q)$ has a pole at $\omega = \omega_q$, the unperturbed phonon energy. In order to go beyond this zeroth-order approximation, we need to evaluate the Green's functions $G(23 \cdots n)$ appearing in Eq. (4.6). Thus, using again Eqs. (3.4), (4.1), and (4.4), we write the equation of motion for the generic Green's function $G(abc \cdots de)$ as

$$G(abc \cdots de) = \frac{1}{\omega - (\omega_a + \omega_b + \omega_c + \cdots + \omega_d + \omega_e)}$$

$$\times \left\{ \langle [b_a b_b b_c \cdots b_d b_e, b_{-q}] \rangle + \sum_{n \geq 3} n \sum_{2,3,\ldots,n} \sigma_a V_{-a23\cdots n} G(23 \cdots nbc \cdots de) \right.$$

$$\left. + \sigma_b V_{-b23\cdots n} G(a23 \cdots nc \cdots de) + \cdots + \sigma_e V_{-e23\cdots n} G(abc \cdots d23 \cdots n) \right\} . \tag{4.8}$$

This compact equation, of which Eq. (4.6) is a special case, is the basic equation that will be used in moving up on the hierarchy of coupled equations for the Green's functions. The advantage of using positive and negative branch indices to distinguish annihilation and creation operators is evident in Eq. (4.8), which, for n operators $b_a, b_b, \ldots, b_e$, is equivalent to a set of 2^n equations involving various combinations of the operators $b_a, b_a^\dagger, b_b, b_b^\dagger, \ldots, b_e, b_e^\dagger$. The signs of the energies ω_j [Eq. (4.2)] and of the factors σ_j adjust for the signs of the branch indices j and thus allow a single compact equation to replace several equations. Equation (4.8) is a direct consequence of Heisenberg's equation of motion (3.3) and of the definition of the system [Eqs. (2.6)–(2.8)] and is thus an exact equation.

V. DECOUPLING SCHEME AND DYSON'S EQUATION

The Green's function $G(q)$ may be evaluated by repeatedly substituting Eq. (4.8) in Eq. (4.6). Thus we obtain an expression for $G(q)$ involving the thermal averages $\langle [b_a b_b \cdots b_c, b_{-q}] \rangle$. Because of the structure of Eq. (4.8), all such thermal averages appear in combinations of the form

$$[\omega - (\omega_a + \omega_b + \cdots + \omega_c)]^{-1} \langle [b_a b_b \cdots b_c, b_{-q}] \rangle .$$

This combination is the only nontrivial factor left to evaluate in the expansion for $G(q)$. In order to evaluate it, we use first Eq. (4.3) to reduce the commutator to a combination of simple products $b_a b_b \cdots b_c$ and then approximate the thermal averages $\langle b_a b_b \cdots b_c \rangle$ by performing them over the ensemble appropriate to a purely harmonic Hamiltonian. With this approximation and in the limit of a large sample, Wick's theorem holds.[4,23,24] The average of a product of creation and annihilation operators is nonzero only if there is an even number of operators and these occur in conjugate pairs $b_{-b} b_b$. The

average is equal to the sum of the products of all possible pair averages $\langle b_a b_b \rangle = \delta_{a-b} \langle b_{-b} b_b \rangle$. The operators in each pair are in the same order than in the original product. For a number $2n$ of operators, there are $(2n)!/(2^n n!)$ different possible pairing schemes. Thus

$$\langle b_a b_b \cdots b_c b_d \rangle = \langle b_a b_b \rangle \cdots \langle b_c b_d \rangle$$

$$+ \text{all other pairing schemes}$$

$$= \delta_{ab} \cdots \delta_{cd} n_b \cdots n_d$$

$$+ \text{all other pairing schemes} , \tag{5.1}$$

where, by taking into account the commutator (2.8), we have defined

$$n_b \equiv \langle b_{-b} b_b \rangle$$

$$= \begin{cases} \langle b_b^\dagger b_b \rangle = n(\omega_b) & \text{for } b > 0 , \\ \langle b_{-b} b_{-b}^\dagger \rangle = n(\omega_{-b}) + 1 & \text{for } b < 0 \end{cases} \tag{5.2}$$

and

$$n(\omega) = \frac{1}{(e^{\omega/k_B T} - 1)} \tag{5.3}$$

is the mean phonon occupation number at the temperature T as given by Planck's distribution.

The connection between Wick's theorem [Eq. (5.1)] and the possibility of representing perturbative expansions in terms of sums on diagrams is discussed in many standard texts.[4,21,22,31] Wick's theorem implies that all the arguments of the interaction coefficients occur in conjugate pairs $j, -j$. The Feynman diagram corresponding to a term is obtained by drawing a vertex for each interaction coefficient, with a line for each argument, and then connecting all pairs of lines which correspond to conjugate summation indices $j, -j$. All the diagrams that occur in the expansion for $G(q)$ have two "external" lines (i.e., arguments not subject to summations), labeled

$-q$ and q, which arise, respectively, from Eq. (4.6) and from the δ_{aq} factors in Eq. (4.3).

In the digrammatic treatment of the Green's function $G(q)$,[22–24] the error made in substituting the average using the anharmonic Hamiltonian with that using the unperturbed harmonic Hamiltonian [Eq. (5.1)] is eventually canceled by the contribution of the "disconnected" diagrams, so that Wick's theorem holds without any approximation. As the equation-of-motion treatment is apparently equivalent to the diagrammatic treatment,[28,34] we suspect that an analogous proof could be possible also in our case. We have almost no doubts about the equivalence of the two treatments, as we may recognize, *a posteriori*, which diagram corresponds to which term in our expansion. By examining a large number of terms, we have convinced ourselves that no diagram is missing and that they are properly evaluated. However, we do not know of any formal proof of the equivalence of the two treatments, and we have not attempted such a proof here. Theorems and concepts originally developed in the framework of the diagrammatic treatment will be used without further proof other than the assumed equivalence of these two treatments.

Going back to the combination

$$[\omega-(\omega_a+\omega_b+\cdots+\omega_c)]^{-1}\langle[b_ab_b\cdots b_c,b_{-q}]\rangle \ ,$$

we see that the average is nonzero only if one of indices $a,b,\ldots,c$ is equal to q, as a result of the δ_{aq} factors in Eq. (4.3), while all other indices occur in conjugate pairs $j,-j$, as a result of the δ_{a-b} factors in Eq. (5.1) (Wick's theorem). Thus one of the energies in $(\omega_a+\omega_b+\cdots+\omega_c)$ is ω_q, while all the other energy pairs $\omega_j+\omega_{-j}$ vanish as $\omega_j=-\omega_{-j}$ [Eq. (4.2)]. Hence

$$[\omega-(\omega_a+\omega_b+\omega_c\cdots+\omega_d+\omega_e)]^{-1}$$

$$\times\langle[b_ab_bb_c\cdots b_db_e,b_{-q}]\rangle$$

$$=(\omega-\omega_q)^{-1}(\delta_{aq}\delta_{b-c}\cdots\delta_{d-e}n_c\cdots n_e$$

$$+\text{other terms}) \ , \tag{5.4}$$

where, for $2n+1$ operators, the sum is extended to all $(2n+1)!/(2^n n!)$ terms allowed by Eqs. (4.3) and (5.1).

We now note that the factor $(\omega-\omega_q)^{-1}$ in Eq. (5.4) is the noninteracting, or bare, Green's function $G_0(q)$. Because of the structure of Eq. (4.8), all terms in the expansion for $G(q)$ contain such a factor. Thus we may write Eq. (4.6) as

$$(\omega-\omega_q)G(q)=1+\Sigma_0(\omega)G_0(q) \ , \tag{5.5}$$

where the function $\Sigma_0(\omega)$ contains the complete sum in Eq. (4.6) except for the factor $G_0(q)$. The function $\Sigma_0(\omega)$ may be expressed as a sum on all diagrams. Let us define the auxiliary function $\Sigma(\omega)$ as the same sum restricted to the "irreducible" diagrams. A reducible diagram is a diagram where the connection between the external lines q and $-q$ may be severed by cutting just one internal line. In the diagrammatic treatment it is proved that Eq. (5.5) remains valid if the sum on all diagrams $\Sigma_0(\omega)$ is replaced by the sum on the irreducible diagrams $\Sigma(\omega)$, and simultaneously the bare Green's function $G_0(q)$ is replaced by

the full, or interacting, Green's function $G(q)$:[4,23]

$$(\omega-\omega_q)G(q)=1+\Sigma(\omega)G(q) \ . \tag{5.6}$$

This equation is Dyson's equation, with neglect of "polarization mixing."[2] In order to ensure that the same equation is obtained also in the equation-of-motion treatment, we make exactly the same two steps: (1) discard all terms in the expansion for $G(q)$ that are represented by reducible diagrams and (2) replace $G_0(q)$ by $G(q)$ in Eq. (5.4).

Dyson's equation [Eq. (5.6)] is equivalent to

$$G(q)=[\omega-\omega_q-\Sigma(\omega)]^{-1} \ . \tag{5.7}$$

Thus the full Green's function $G(q)$ is mathematically similar to the bare Green's function $G_0(q)=(\omega-\omega_q)^{-1}$ [Eq. (4.7)], except for an energy change $\Sigma(\omega)$, which is the "self-energy."[1,3,38] The pole of $G_0(q)$, at the unperturbed energy $\omega=\omega_q$, is moved to a pole of $G(q)$, at a new perturbed energy. If $\Sigma(\omega)$ is a small enough and slowly varying function of ω, this perturbed energy is approximately $\omega=\omega_q+\Sigma(\omega_q)$. In general, $\Sigma(\omega_q)$ is complex, with a real part Δ_q, which represent an energy shift, and an imaginary part Γ_q, which may be interpreted in terms of a linewidth Γ_q or a phonon lifetime[4] h/Γ_q.

Some comments about the validity of Eq. (5.7) are in order. In the diagrammatic treatment Dyson's equation [Eq. (5.7)] is obtained[4,23] by proving that Eq. (5.5) may be rewritten as

$$G=G_0+G_0\Sigma_0G_0$$

$$=G_0+G_0\Sigma G_0+G_0\Sigma G_0\Sigma G_0+G_0\Sigma G_0\Sigma G_0\Sigma G_0+\cdots \ , \tag{5.8}$$

where all function arguments have been dropped to hide unessential details and the terms with one, two, etc., Σ functions represent all diagrams made on one, two, etc., irreducible parts. Equation (5.8) is the power-series expansion for $G=(G_0^{-1}-\Sigma)^{-1}$, that is, Eq. (5.7). In our treatment we have found, to a finite order, that the expansion for $G(q)$ may be reorganized in the form of Eq. (5.8). Thus we have further evidence for the equivalence of the two treatments. As a qualitative argument, we note that both in applying Wick's theorem and in discarding the reducible diagrams we are neglecting some correlations induced by the anharmonic interactions between the phonons. Hence it is reasonable to assume that the error in the decoupling is at least partially compensated by the replacement of the bare Green's function $G_0(q)$ with the full interacting Green's function $G(q)$ and that Eq. (5.7) is a good approximation.

VI. FINITE-ORDER EXPANSION

Since the expansion for $G(q)$, which is obtained by repeated substitution of Eq. (4.8) in Eq. (4.6), involves an infinite number of terms, we need a systematic criterion for grouping terms in successive order of approximation. Following Van Hove, Hugenholtz, and Howland,[39] we regard $\mathscr{H}_2,\mathscr{H}_3,\mathscr{H}_4,\ldots,\mathscr{H}_n$ as being of order $\lambda^0,\lambda^1,\lambda^2,\ldots,\lambda^{n-2}$, where λ is some suitably chosen expansion parameter. The Green's function $G(q)$ may be

evaluated to any desired order n in λ by repeatedly substituting Eq. (4.8) in Eq. (4.6), while systematically discarding all terms of order higher than λ^n until no Green's function is left. As the second term of Eq. (4.8) is of order λ, $n+1$ successive substitutions are sufficient to eliminate all the Green's functions of order λ^n or lower. At this stage we evaluate all the thermal averages using Eq. (5.4), discard all terms represented by reducible diagrams, and replace $G_0(q) = (\omega - \omega_q)^{-1}$ by $G(q)$. A finite expression for $G(q)$ is thus obtained in terms of interaction coefficients $V_{123\cdots n}$, factors σ_j and n_j, and resonance factors $[\omega - (\omega_a + \omega_b + \cdots + \omega_c)]^{-1}$.

In order to compute the self-energy $\Sigma(\omega_q)$, we will

eventually replace ω by ω_q in the resonance factors. Thus we introduce the shorthand

$$z_{ab\cdots c} \equiv [-(\omega_a + \omega_b + \cdots + \omega_c)]^{-1} , \tag{6.1}$$

so that

$$[\omega_q - (\omega_a + \omega_b + \cdots + \omega_c)]^{-1} = z_{-qab\cdots c} .$$

We choose this definition so that z has the desirable property of being symmetric in all the indices.

In order to clarify the nature of the expansion for $G(q)$ and to make the discussion more concrete, we report as an example the expansion to order λ^2:

$$(\omega - \omega_q)G(q) = 1 + 3V_{-q23}G(23) + 4V_{-q234}G(234)$$

$$= 1 + 9V_{-q23}[\omega - (\omega_2 + \omega_3)]^{-1}\{\langle [b_2 b_3, b_{-q}]\rangle + \sigma_2 V_{-245}G(453) + \sigma_3 V_{-345}G(253)\}$$

$$+ 4V_{-q234}[\omega - (\omega_2 + \omega_3 + \omega_4)]^{-1}\langle [b_2 b_3 b_4, b_{-q}]\rangle$$

$$= 1 + 9V_{-q23}V_{-245}\sigma_2[\omega - (\omega_2 + \omega_3)]^{-1}G(q)(\delta_{q4}\delta_{5-3}n_3 + \delta_{q5}\delta_{4-3}n_3 + \delta_{q3}\delta_{4-5}n_5)$$

$$+ 9V_{-q23}V_{-345}\sigma_3[\omega - (\omega_2 + \omega_3)]^{-1}G(q)(\delta_{q2}\delta_{4-5}n_5 + \delta_{q4}\delta_{2-5}n_5 + \delta_{q5}\delta_{2-4}n_4)$$

$$+ 4V_{-q234}G(q)(\delta_{q2}\delta_{3-4}n_4 + \delta_{q3}\delta_{2-4}n_4 + \delta_{q4}\delta_{2-3}n_3)$$

$$= 1 + G(q)\{18V_{q-1-2}V_{-q12}z_{-q12}(n_1\sigma_2 + \sigma_1 n_{-2}) + 18V_{q-q1}V_{-12-2}z_1\sigma_1 n_2 + 12V_{q-q1-1}n_1\} . \tag{6.2}$$

Here we have used in sequence Eqs. (4.6), (4.8), and (5.4), discarded all terms of order higher than λ^2, discarded commutator averages involving an odd number of operators, summed away the Kronecker δ's, replaced $(\omega - \omega_q)^{-1}$ by $G(q)$, and renamed the summation indices to collect identical terms. For compactness, the sums on the indices $1, 2, 3, \ldots$ have been left implicit. By comparing Eq. (6.2) with the expected form $(\omega - \omega_q)G(q) = 1 + \Sigma(\omega)G(q)$ [Eq. (5.6)], we recognize the expression in braces as the self-energy $\Sigma(\omega)$. The three terms in braces correspond to diagrams (1), (2) of Fig. 1 and (1) of Fig. 2. If the sums on positive and negative indices are carried out using Eqs. (4.2), (5.2), and (6.1), we obtain the usual expression[4] for $\Sigma(\omega_q) = \Sigma_1(\omega_q) + \Sigma_2 + \Sigma_3$.

$$\Sigma_1(\omega_q) = 18 \sum_{\substack{1>0, \\ 2>0}} |V_{-q12}|^2 \left\{ \frac{n_1 + n_2 + 1}{\omega_q - (\omega_1 + \omega_2)} \right.$$

$$+ \frac{-n_1 + n_2}{\omega_q - (\omega_1 - \omega_2)}$$

$$+ \frac{n_1 - n_2}{\omega_q - (-\omega_1 + \omega_2)}$$

$$\left. + \frac{-n_1 - n_2 - 1}{\omega_q - (-\omega_1 - \omega_2)} \right\} , \tag{6.3a}$$

$$\Sigma_2 = 18 \sum_{\substack{1>0, \\ 2>0}} V_{q-q1}V_{-12-2}\frac{(2n_2 + 1)}{\omega_1} , \tag{6.3b}$$

$$\Sigma_3 = 12 \sum_{1>0} V_{q-q1-1}(2n_1 + 1) . \tag{6.3c}$$

The real and imaginary parts of $\Sigma(\omega_q) = \Delta_q i\Gamma_q$ may be calculated in the standard fashion[2] by setting ω_q equal to $\omega_q - i\varepsilon$ and taking the limit for $\varepsilon \to 0+$.

Making these steps, namely, decomposing the thermal averages, discarding the reducible diagrams, and replacing the bare Green's function with the full Green's func-
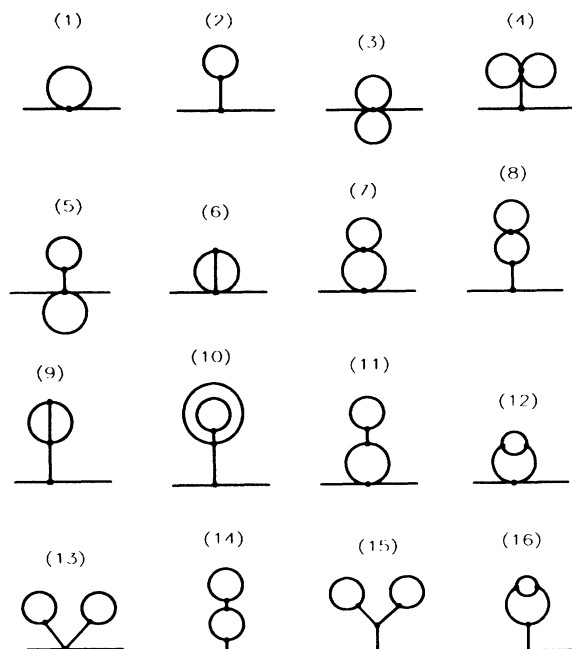

FIG. 1. ω-independent diagrams.

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TABLE I. Self-energy expressions for the ω-independent diagrams.

(1) $12V_{q-q1-1}n_1$

(2) $18V_{q-q1}V_{-12-2}z_1\sigma_1 n_2$

(3) $90V_{q-q1-12-2}n_1 n_2$

(4) $90V_{q-q1}V_{-12-23-3}z_1\sigma_1 n_2 n_3$

(5) $180V_{q-q1-12}V_{-23-3}z_2 n_1\sigma_2 n_3$

(6) $120V_{q-q123}V_{-1-2-3}z_{123}(n_1 n_2\sigma_3+n_1\sigma_2 n_{-3}+\sigma_1 n_{-2}n_{-3})$

(7) $144V_{q-q12}V_{-1-23-3}z_{12}(n_1\sigma_2+\sigma_1 n_{-2})n_3$

(8) $216V_{q-q1}V_{-123}V_{-2-34-4}z_1 z_{23}\sigma_1 n_4(n_2\sigma_3+\sigma_2 n_{-3})$

(9) $144V_{q-q1}V_{-2-3-4}V_{-1234}z_1 z_{234}\sigma_1\sigma_4[n_{-2}(n_{-3}+n_3)+n_2 n_3]$

(10) $216V_{q-q1}V_{-22-3}V_{-13-44}z_1 z_3\sigma_1 n_{-2}\sigma_3 n_{-4}$

(11) $216V_{q-q12}V_{-1-23}V_{-34-4}z_{12}z_3\sigma_1 n_4(n_1\sigma_2+\sigma_1 n_{-2})$

(12) $216V_{q-q12}V_{-134}V_{-2-3-4}z_{12}z_{234}\sigma_1[(n_{-2}+n_2)(n_3\sigma_4+\sigma_3 n_{-4})+\sigma_2(n_3 n_4+n_{-3}n_{-4})]$

(13) $216V_{q-q12}V_{-13-3}V_{-24-4}z_1 z_{12}\sigma_1\sigma_2 n_3 n_4$

(14) $324V_{q-q1}V_{-123}V_{-2-34}V_{-45-5}z_1 z_{23}z_4\sigma_1\sigma_4 n_5(n_2\sigma_3+\sigma_2 n_{-3})$

(15) $324V_{q-q1}V_{-123}V_{-24-4}V_{-35-5}z_1 z_{23}z_3\sigma_1\sigma_2\sigma_3 n_4 n_5$

(16) $324V_{q-q1}V_{-123}V_{-245}V_{-3-4-5}z_1 z_{23}z_{345}\sigma_1\sigma_2[(n_3+n_{-3})(n_4\sigma_5+\sigma_4 n_{-5})+\sigma_3(n_4 n_5+n_{-4}n_{-5})]$

tion, constitutes our decoupling scheme. The extension to orders higher than λ^2 is trivial, although rather tedious and lengthly. In Tables I and II, we list the self-energy $\Sigma(\omega_q)$ for all diagrams of order λ^2 and λ^4, omitting the intermediate steps which, at this stage of the discussion, should be straightforward. The corresponding diagrams are shown in Figs. 1 and 2. The diagrams have been partitioned into two sets: The diagrams in the first set (ω-independent diagrams, Table I, Fig. 1) yield self-energy terms which do not depend on ω_q; they contribute only

TABLE II. Self-energy expressions for the ω-dependent diagrams.

(1) $18V_{q-1-2}V_{-q12}z_{-q12}(n_1\sigma_2+\sigma_1 n_{-2})$

(2) $360V_{q-1-2}V_{-q123-3}z_{-q12}n_3(n_1\sigma_2+\sigma_1 n_{-2})$

(3) $96V_{q-1-2-3}V_{-q123}z_{-q123}(n_1 n_2\sigma_3+n_1\sigma_2 n_{-3}+\sigma_1 n_{-2}n_{-3})$

(4) $432V_{q-1-2}V_{-q13}V_{2-34-4}z_{-q13}n_4[z_{-q12}\sigma_3(n_1\sigma_2+\sigma_1 n_{-2})+z_{-23}\sigma_1(n_2\sigma_3+\sigma_2 n_{-3})]$

(5) $216V_{q-1-2}V_{12-3-4}V_{-q34}z_{-q12}z_{-q34}(n_1\sigma_2+\sigma_1 n_{-2})(n_3\sigma_4+\sigma_3 n_{-4})$

(6) $432V_{q-1-2}V_{-q123}V_{-34-4}z_{-q12}z_3\sigma_3 n_4(n_1\sigma_2+\sigma_1 n_{-2})$

(7) $648V_{q-1-2}V_{-q13}V_{2-34}V_{-45-5}z_{-q13}z_4\sigma_4 n_5[z_{-q12}\sigma_3(n_1\sigma_2+\sigma_1 n_{-2})+z_{23}\sigma_1(n_{-2}\sigma_3+\sigma_{-2}n_{-3})]$

(8) $432V_{q-1-2}V_{-q134}V_{2-3-4}(z_{-q134}[z_{-q12}(n_1\sigma_2+\sigma_1 n_{-2})(n_3\sigma_4+\sigma_3 n_{-4})$

$\qquad +z_{-234}\sigma_1(n_{-2}n_3\sigma_4+n_{-2}\sigma_3 n_{-4}+\sigma_{-2}n_{-3}n_{-4})]$

$\qquad +z_{-q12}\{z_{-q134}\sigma_2(n_1 n_3\sigma_4+n_1\sigma_3 n_{-4}+\sigma_1 n_{-3}n_{-4})$

$\qquad +\tfrac{1}{2}z_{-4-32}[\sigma_1\sigma_{-3}(n_4+n_{-4})(n_2+n_{-2})+\sigma_1\sigma_2(n_3 n_4+n_{-3}n_{-4})]\})$

(9) $648V_{q-1-2}V_{-q13}V_{24-5}V_{-3-45}z_{-q13}\{z_{-q12}z_{-q1-45}\sigma_3\sigma_5(n_1\sigma_2+\sigma_1 n_{-2})(n_4+n_{-4})$

$\qquad +\tfrac{1}{2}z_{-2-45}(z_{-23}+z_{-q1-45})\sigma_1\sigma_3[(\sigma_5(n_4+n_{-4})(n_2+n_{-2})+\sigma_{-2}(n_4 n_{-5}+n_{-4}n_5)]$

$\qquad +z_{-23}z_{34-5}\sigma_1\sigma_2(n_3 n_4\sigma_{-5}+n_3\sigma_4 n_5+\sigma_3 n_{-4}n_5)\}$

(10) $1296V_{q-1-2}V_{-q34}V_{1-3-5}V_{2-45}z_{-q34}z_{-q235}\{z_{-q12}\sigma_4(n_1\sigma_2+\sigma_1 n_{-2})(n_3\sigma_5+\sigma_3 n_{-5})$

$\qquad +z_{-135}\sigma_2\sigma_4(n_{-1}n_3\sigma_5+n_{-1}\sigma_3 n_{-5}+\sigma_{-1}n_{-3}n_{-5})\}$
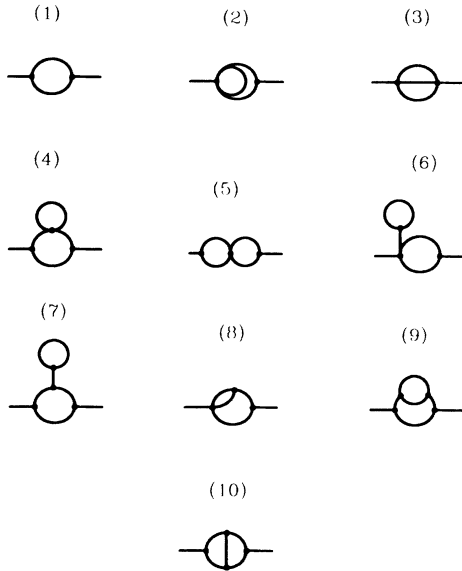
FIG. 2. ω-dependent diagrams.

to the real part Δ of the self-energy,[25,26] resulting in a shift of the phonon energies ω_q. The diagrams of the other set (ω-dependent diagrams, Table II, Fig. 2) introduce an imaginary contribution $i\Gamma$ as well and describe the effect of decay mechanisms. Such diagrams are responsible for the finite lifetime of the phonon excitations. For diagrams 2, 6, and 8, which are not symmetric for exchange of q and $-q$, we have summed the diagram shown and its mirror symmetric.

The analytical expressions for diagrams (4), (5), (8)–(11), (14), and (15) in Table I and (6) and (7) in Table II are also given. All these terms involve "instantaneous" vertices of odd order (third and fifth order), involving anharmonic coefficients of the form V_{q-q1} and $V_{q-q1-12}$. It has been proved[40-42] that these coupling coefficients vanish if each atom in the crystal lies on a center of inversion. For a cubic molecular crystal of small centrosymmetric molecules, such as CO_2 and N_2, it has been found that such contributions are negligible.[14,23] These diagrams cannot be in general neglected for noncentrosymmetric crystals or for centrosymmetric crystals of large molecules.

VII. CONCLUSION

In this study we have discussed the application of the equation-of-motion method to the effect of phonon-phonon interactions on the spectral properties of the system. We have developed a formalism in which the positive or negative sign of the branch indices is used to distinguish between annihilation and creation operators. Using this formalism, we have been able to write the equation of motion [Eq. (4.8)] for a general Green's function in an extremely compact form. A decoupling scheme has been proposed for obtaining the expression for the self-energy to any perturbation order. In this scheme the thermal averages are replaced with those appropriate for a harmonic Hamiltonian, the contributions

represented by reducible diagrams are discarded, and the bare Green's function is replaced by the full Green's function. All the topologically distinct diagrams are naturally included by following the proposed decoupling scheme. The method is parallel to the usual diagrammatic method,[23] and we are convinced that the two treatments are equivalent. As a matter of fact, our results for the self-energy up to order λ^4 are found to be identical to those obtained with the standard diagrammatic treatment. The λ^4 contributions to the phonon self-energy arising from diagrams with instantaneous vertices of odd orders are also reported. The decoupling strategy, due to the compactness of the adopted formalism, is particularly suitable to be implemented on a computer. The description of an algorithm for computing self-energy corrections at higher orders is planned to be the topic of a forthcoming paper, where we will report the expressions to order λ^6 for the ω-dependent diagrams. The compactness of the self-energy expressions is useful in the actual calculations of high-order diagrams. We have numerically evaluated the contributions to the linewidths of selected diagrams up to order λ^{10} in solid nitrogen. The computed linewidths compare well with the experiments. Contributions of order higher than λ^4 have been found to be important for lattice phonons but negligible for vibrons. These results will be presented in a subsequent work.

ACKNOWLEDGMENTS

APPENDIX: EVALUATION OF COMMUTATORS

All the required commutators, $[A, b_{-q}]$, $[A, \mathcal{H}_2]$, and $[A, \mathcal{H}_n]$, may be evaluated by replacing B with b_{-q}, $\mathcal{H}_2$, or $\mathcal{H}_n$ in the identity

$$[b_1 b_2 b_3 \cdots b_m, B] + [b_1, B] b_2 b_3 \cdots b_m$$
$$+ b_1 [b_2, B] b_3 \cdots b_m$$
$$+ b_1 b_2 b_3 \cdots [b_m, B] . \qquad \text{(A1)}$$

We prove this identity by induction on the number m of operators. Equation (A1) is obviously valid for the case of a single operator $A = b_1$. Now, if (A1) is valid for a product $A = b_1 b_2 b_3 \cdots b_m$ of m operators, then, using the identity $[XY, Z] = [X, Z]Y + X[Y, Z]$ we find that a commutator involving a product of $m + 1$ operators also has the stated form

$$[b_1 \cdots b_m b_{m+1}, B] = [b_1 \cdots b_m, B] b_{m+1}$$
$$+ b_1 \cdots b_m [b_{m+1}, B] . \qquad \text{(A2)}$$

Equation (4.3) for $[A, b_{-q}]$ is obtained immediately by substitution of the commutator (2.8) into Eq. (A1) and taking into account that $\sigma_a \delta_{aq} \equiv \delta_{aq}$, as $q > 0$.

Using the commutator (2.8) and the definition of $\mathcal{H}_2$ and ω_{-j} [Eqs. (2.6) and (4.2), we find directly

$$[b_j, \mathcal{H}_2] = \omega_j b_j \ . \tag{A3}$$

Thus Eq. (4.1) is valid for A made of a single b_j operator. Substitution into Eq. (A1) yields Eq. (4.1) for $[A, \mathcal{H}_2]$.

Using Eq. (2.8), we may easily prove by induction on the number of operators $b_1 b_2 \cdots b_n$ that

$$[b_j, b_1 b_2 \cdots b_n] = \sigma_1 \delta_{1-j} b_2 \cdots b_n$$
$$+ b_1 \sigma_2 \delta_{2-j} \cdots b_n$$
$$+ \cdots + b_1 b_2 \cdots \sigma_n \delta_{n-j} \ . \tag{A4}$$

Now, by properly renaming the summation indices $1, 2, \ldots, n$ and exploiting the symmetry of $V_{12\ldots n}$ with respect to exchanges of indices, we prove that Eq. (4.4) for $[A, \mathcal{H}_n]$ is valid for a single operator b_j:

$$[b_j, \mathcal{H}_n] = n \sum_{2,3,\ldots,n} \sigma_j V_{-j23 \cdots n} b_2 b_3 \cdots b_n \ . \tag{A5}$$

Substitution into Eq. (A1) completes the proof of Eq. (4.4).

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