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Computer-Aided Series Expansion for Phonon Self-Energy

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In this paper we discuss an algorithm for calculation of the temperature-dependent anharmonic correction to the phonon spectrum in atomic and molecular crystals. We show how the equation of motion method can be used to compute corrections of arbitrary perturbation order to the phonon self-energy. Complete analytical expressions up to order λ^6 are obtained as an application of the method.

Key Words: anharmonicity; phonon lifetimes; self-energy; single-phonon Green's function; phonon decay; perturbation theory.

1. INTRODUCTION

The decay of vibrational excitations in crystalline solids is due to anharmonic perturbations in which the phonons exchange energy and is most compactly described in terms of Green's functions [1–4]. The poles of the single-particle Green's function for noninteracting phonons (harmonic approximation) correspond to the harmonic frequencies of the crystal. The Green's function for interacting phonons instead has poles in the complex plane. The anharmonic correction to the harmonic frequency is thus a complex quantity, the self-energy, whose real part corresponds to a frequency shift and whose imaginary part is related to the lifetime of the elementary excitation [4–6]. In the framework of perturbation theory [2, 3, 7, 8], the self-energy can be written as a summation of contributions, which are represented as Feynman's diagrams describing specific decay processes and which can be grouped in perturbation orders λ^2, λ^4, λ^6 . . ..

Both experimentally, by investigating the temperature dependence of the phonon lifetimes [9–13], and theoretically, by numerically computing a few high-order contributions [14–18], it has been found that high-order processes can be quite important. All contributions to the self-energy at the two lowest orders, namely λ^2 and λ^4, are completely known

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[19–21]. At higher orders only contributions from a single kind of diagram are normally available [17]. Diagrams for which no expression is known are simply ignored in actual calculations. Though very successful in some cases [14, 17, 22], this is clearly an uncontrolled approximation without a clear justification [17].

In a past study [21], we proposed a general theoretical approach based on the equation of motion method [23–26] for evaluating the self-energy at any order. This approach was applied to the determination of the λ^4 contribution to the self-energy. In the present study, we describe a practical implementation of the method using a computer-aided technique for determining the analytical expression of any connected diagram in terms of the coupling coefficient, resonance factors, and boson occupation numbers. As a nontrivial application and as a step toward better comprehension of the convergence properties of the perturbation series for the Green's function, we have found all contributions at order λ^6.

Recently, Shukla and Cowley [27] proposed an accurate analytical expression for the free energy and the equation of state of anharmonic Lennard–Jones solids near melting, which was tested against Monte Carlo calculations. Those expressions were obtained by summing up infinite subsets of free energy diagrams derived by self-energy insertion of the known λ^2 and λ^4 contributions. The present work, by yielding the complete λ^6 order, also makes available some λ^6 self-energy contributions which cannot be derived by self-energy insertion of lower order diagrams, and hence may provide an opportunity to improve Shukla's and Cowley's result.

The paper is organized as follows. In Section 2 we briefly recall the theoretical foundation of the phonon–antiphonon formalism [21] for the equation of motion method in anharmonic solids. In Section 3 we describe practical implementation of the Green's function expansion leading to the determination at the order λ^6 of the self-energy, chosen as a useful and nontrivial example. We also show how the analytical form of the self-energy arising for the Green's function expansion can be rearranged in terms of Feynman diagrams using a sorting algorithm. Conclusive remarks appear in Section 4.

2. THEORY

The phonon spectrum of a crystal is related [4, 5, 28–31] to the distribution of the poles of the one-phonon causal Green's function $G(q) = G(b_q, b_q^\dagger; \omega)$. Here b_q and $b_q^\dagger$ are the usual boson operators which annihilate and create phonons with unperturbed (harmonic) energy ω_q.

Following Ref. [21], we adopt the phonon–antiphonon formalism, in which the annihilation of a phonon with energy ω is reinterpreted as the creation of an "antiphonon" with negative energy $-\omega$. This prescription is implemented by allowing both positive and negative signs for the phonon labels q. The sign $\sigma_q = \mathrm{sign}(q)$ of the label distinguishes between annihilation and creation operators, b_q and $b_{-q} = b_q^\dagger$, and between positive and negative energies, ω_q and $\omega_{-q} = -\omega_q$. With this notation, all the usual equations involving phonon operators become extremely compact expressions using only a single kind of operators.

Using the equation of motion method and adopting the phonon–antiphonon formalism, it can be shown [21] that a generic Green's function $G(abc..de) = G(b_a b_b b_c..b_d b_e, b_{-q}; \omega)$

obeys an algebraic equation involving still higher order Green's functions:

$$G(abc..de) = [\omega - (\omega_a + \omega_b + \omega_c + \cdots + \omega_d + \omega_e)]^{-1} \Big[\langle [b_a b_b b_c \ldots b_d b_e, b_{-q}] \rangle + \sum_{n\geq 3} n \sum_{2..n} \sigma_a V_{-a2..n} G(2..nbc..de) + \sigma_b V_{-b2..n} G(a2..nc..de) + \cdots + \sigma_e V_{-e2..n} G(abc..d2..n) \Big]. \quad (1)$$

Here $V_{12..n}$ is the nth order anharmonic coupling coefficient [4, 5, 32] (of perturbation order λ^{n-2}); [,] indicates a commutator, which is evaluated directly; and $\langle\ \rangle$ represents a thermal average, which is approximated by performing it over the statistical ensemble appropriate to a purely harmonic Hamiltonian. In this approximation, according to Wick's theorem [1, 3, 33], the average of a product of creation and annihilation operators is nonzero only if there are 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 $\langle b_a b_b \rangle = \delta_{ab} \langle b_{-b} b_b \rangle$, with the operators in each pair left in the same order as in the original product. The average in Eq. (1) is thus rewritten as

$$\begin{aligned} &[\omega - (\omega_a + \omega_b + \omega_c + \cdots + \omega_d + \omega_e)]^{-1} \langle [b_a b_b b_c \ldots b_d b_e, b_{-q}] \rangle \\ &= (\omega - \omega_q)^{-1} (\delta_{aq} \delta_{b-c} n_c \ldots \delta_{d-e} n_e \ldots + \delta_{bq} \delta_{a-c} n_c \ldots \delta_{d-e} n_e \ldots \\ &\quad + \delta_{cq} \delta_{a-b} n_b \ldots \delta_{d-e} n_e \ldots + \text{other terms}), \end{aligned} \quad (2)$$

where, for $2n+1$ operators $b_a b_b b_c \ldots b_d b_e$, the sum is extended to all $(2n+1)!! = 1 \cdot 3 \cdot 5 \ldots (2n+1)$ terms allowed by the basic commutator $[b_a, b_{-q}] = \delta_{aq}$ and by Wick's theorem, and we have defined

$$n_b = \langle b_{-b} b_b \rangle = \begin{cases} \langle b_b^\dagger b_b \rangle = n(\omega_b), & \text{for } b > 0 \\ \langle b_{-b} b_{-b^\dagger} \rangle = n(\omega_{-b}) + 1, & \text{for } b < 0. \end{cases} \quad (3)$$

Here $n(\omega) = [\exp(\omega / k_B T) - 1]^{-1}$ is the mean phonon occupation number at the temperature T. Equation (1) defines an infinite chain of coupled equations involving a hierarchy of Green's function of increasing order. This chain represents a perturbative expansion which we truncate at some high order to obtain a finite expression. The initial equation in the chain, which is Eq. (1) for $G(q) = G(b_q, b_{-q}; \omega)$, is

$$(\omega - \omega_q)\ G(q) = 1 + \sum_{n\geq 3} n \sum_{23..n} V_{-q23\ldots n} G(23..n). \quad (4)$$

Neglecting the last term in Eq. (4), we obtain the "bare" (i.e., harmonic) Green's function in the absence of anharmonic interactions, $G_0(q) = (\omega - \omega_q)^{-1}$. $G_0(q)$ has a pole at $\omega = \omega_q$, the unperturbed phonon energy. To go beyond this 0th order approximation we evaluate the Green's function $G(q)$ by repeatedly substituting Eq. (1) in Eq. (4). Due to the structure of Eqs. (1) and (2), all terms in the resulting expansion for $G(q)$ contain the factor $(\omega - \omega_q)^{-1} = G_0(q)$. Thus, we may write Eq. (4) as

$$(\omega - \omega_q)\ G(q) = 1 + \sum_0 (\omega) G_0(q), \quad (5)$$

where the function $\sum_0(\omega)$ contains the complete sum in Eq. (4) except for the factors $G_0(q)$.

As is clear from the structure of Eqs. (1), (2), and (4), the equation of motion method yields the complete expression of the self-energy at finite order as a sum of "terms" given by the product of coupling coefficients, frequency factors, and occupation numbers. A term can be assigned to a "diagram" according to the topology of the indices within its coupling coefficients $V_{12..n}$, which, due to Wick's theorem, always occur in conjugate pairs $j, -j$: the diagram corresponding to a given term is obtained by drawing a vertex for each coupling coefficient, with a line for each argument, and then connecting all pairs of lines that correspond to conjugate summation indices $j, -j$. All the diagrams that occur in the expansion for $G(q)$ have two "external" lines $-q$ and q (arguments not subject to summations).

The function $\sum_0(\omega)$ can be thus expressed as a sum on all diagrams. We define an auxiliary function $\sum(\omega)$ as the same sum restricted to the "irreducible" diagrams. Diagrams where the connection between the external lines q and $-q$ may be severed by cutting just one internal line are "reducible." It can be shown [1–4, 8] that Eq. (5) remains valid if the sum on all diagrams $\sum_0(\omega)$ is replaced by the sum on the irreducible diagrams $\sum(\omega)$, and simultaneously the bare Green's function $G_0(q)$ is replaced by the full Green's function $G(q)$:

$$(\omega - \omega_q)\, G(q) = 1 + \sum(\omega) G(q). \tag{6}$$

This is Dyson's equation, which may be rewritten as $G(q) = [\omega - \omega_q - \sum(\omega)]^{-1}$. The full Green's function $G(q)$ is thus mathematically similar to the bare Green's function $G_0(q) = (\omega - \omega_q)^{-1}$, except for an energy change $\sum(\omega)$, the self-energy. 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 $\omega \approx \omega_q + \sum(\omega_q)$. In general, $\sum(\omega_q)$ is complex, with a real part Δ_q that represents a frequency shift and an imaginary part $-\Gamma_q$ that may be interpreted in terms of a linewidth Γ_q or a lifetime h/Γ_q [4, 5].

3. ALGORITHM AND CALCULATIONS

Our evaluation strategy for the self-energy, which is based on the previous discussion, has the following steps: (a) expand $G(q)$ to a desired order n in λ by repeatedly substituting Eq. (1) in Eq. (4); (b) discard all terms of order higher than λ^n; (c) evaluate the thermal averages with Eq. (2); (d) discard all terms in the expansion for $G(q)$ that are represented by reducible diagrams; and (e) replace $G_0(q) = (\omega - \omega_q)^{-1}$ by $G(q)$.

Since the second term in the brackets of Eq. (1) is at least of order λ, $n+1$ successive substitutions are sufficient to eliminate all the Green's functions to order λ^n. A finite expression for $G(q)$ is thus obtained in terms of coupling coefficients $V_{12\ldots n}$, σ_j and n_j factors, and frequency factors $[\omega - (\omega_a + \omega_b + \cdots + \omega_c)]^{-1}$. To compute the self-energy $\sum(\omega_q)$, we replace ω by ω_q in the frequency factors.

By analyzing the structure of Eqs. (1), (2), and (4), it can be found that the number of terms of order λ^n in the expansion for $G(q)$ is zero for odd n, and $N_n = (n+1)!!\,(n+1)!/2$ for even n. Since $N_2 = 9$, $N_4 = 900$, and $N_6 = 264600$, the evaluation of $G(q)$ beyond λ^4, though a straightforward task in principle, in practice can be performed only by brute force using a computer. However, since many terms are actually equal and differ only in the

labeling of the dummy summation indices, a considerable simplification of the end result should be possible.

The symbolic algebra program that we used initially, Reduce [34], could perform without any problem the repeated substitution and the thermal averages, but was unable to simplify the output. Identical terms with different choices for the dummy summation indices appeared different to the program, which quickly exhausted all the available storage while climbing up the hierarchy of coupled equations. The Mathematica [35] program also gave the same problem. We have thus abandoned Reduce and Mathematica and adopted a "divide and conquer" strategy by partitioning the complete algorithm into a sequence of simple steps. Several programs have been written to perform the various steps. Each program is designed to read a sum of terms from a file, transform each term into a mathematically equivalent form, and pass the transformed sum to the next program for further processing. All the programs are short and have relatively simple tasks, so that it is easy to prove that they perform mathematically correct transformations.

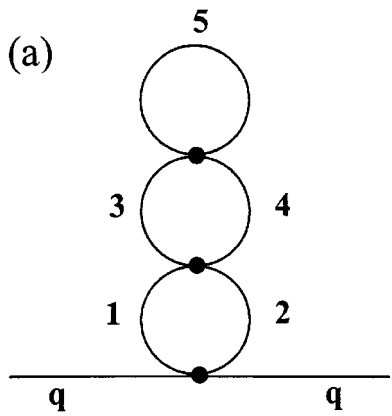
To climb up the hierarchy, Eq. (1), and perform the thermal averages, Eq. (2), we have used two programs written in the pattern scanning and processing language AWK [36]. We start from a file containing only the single term that we want to calculate, namely $G(q)$. Several passes through the program that climbs up the hierarchy, equivalent to applying Eq. (1) repeatedly, are then performed. At each pass all the Green's function $G(\mathrm{ab}\ldots c)$ are replaced by thermal averages $\langle b_a b_b \ldots b_c\rangle$ and higher order Green's functions. All terms of order higher than λ^6 are systematically discarded in the process. After 7 passes no Green's function is left and the file is passed through the program which computes the thermal averages. All terms involving averages over an odd number of b_j operators, which are zero, are discarded, while the averages involving an even number of operators are evaluated according to Eq. (2). We are thus left with an unsimplified expression for $G(q)$ up to order λ^6.

This first part of the algorithm is very straightforward. Overall we had to consider 2957 Green's functions, different for the number or order of the arguments, while climbing the hierarchy. As the thermal averages are performed, 2584 Green's functions give a nonzero contribution, yielding a total of 265509 terms which include all terms of order λ^2, λ^4, and λ^6. To develop an effective simplification method that allows all the terms to be assigned to topologically distinct diagrams and that is thus absolutely necessary to produce an usable result, we have carefully analyzed the reason for the failure of Reduce. At the origin of the failure is the fact that identical terms may appear in many different forms. However, this also implies that we have considerable freedom in choosing the appearance of a given term. We are free to alter the order of the various factors appearing in the term and the order of the arguments of symmetric functions such as $V_{ab\ldots c}$ and $z_{ab\ldots c}$. The dummy summation indices may be renamed freely. Furthermore, as the sums extend on both positive and negative values, we are also free to change the sign of the summation indices. Among all the possible forms in which a term may appear we choose an arbitrary, but unique, canonical form. Two terms are identical if, and only if, they have the same canonical form.

The canonical form has been defined so that it can be obtained efficiently. The definition, which is quite convoluted, is briefly sketched in Appendix A. The implementation is based on a sequence of steps in which the function arguments, the factors in each term, and the labels of the summation indices are sorted according to some arbitrarily defined order. The sort algorithm and the other steps in the reduction to canonical form have been implemented in Pascal [37]. Terms corresponding to reducible diagrams are also recognized and discarded at this stage, as discussed in Appendix B. After the reduction to canonical form, we sort

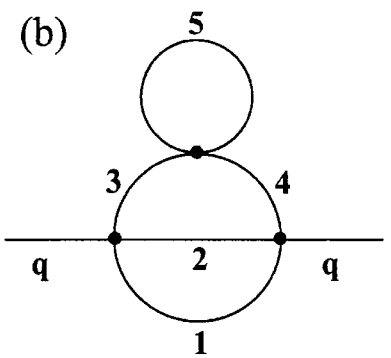
the file of terms. Identical terms, which are adjacent after the sort, are then simply counted. The simplification process is quite effective: 32718 terms, represented by 192 reducible diagrams, are discarded, and we are left with 232791 terms represented by 348 topologically distinct irreducible diagrams which include 3 diagrams of order λ^2, 26 diagrams of order λ^4, and 319 diagrams of order λ^6. All calculations were performed in a few CPU days on a low-end personal computer.

Typical self-energy contributions of order λ^6, chosen to give a feeling for the kind of expressions that are obtained, are shown in Fig. 1 along with the corresponding diagrams. About 40% of the irreducible diagrams represent "instantaneous" processes, such as that shown in Fig. 1a, in which an incoming phonon is annihilated and immediately recreated at the same vertex. These are "ω-independent" diagrams, which yield self-energy terms that



$$27\ V_{\mathbf{q}-\mathbf{q}12}V_{-1-234}V_{-3-45-5}\ \ \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\ \times$$

$$\times\ \ z_{12}z_{34}(n_1+n_2-2)(n_3+n_4-2)(n_5-3)$$



$$27\ V_{\mathbf{q}123}V_{-\mathbf{q}-1-24}V_{-3-45-5}\ \ \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\ \times$$

$$\times\ \ (n_5+1)\{(z_{\mathbf{q}123}+z_{\mathbf{q}12-4})\ z_{34}\ [(n_1+n_2-2)(n_3+n_4-2)]$$

$$-\ \ z_{\mathbf{q}123}z_{\mathbf{q}12-4}[(n_1+n_2-2)(n_3-n_4)+2(n_1-1)(n_2-1)+8]\}$$

FIG. 1. (a) Example of ω-independent irreducible diagrams of order λ^6. Here $z_{ab\ldots c}=[-(\omega_a+\omega_b+\cdots+\omega_c)]^{-1}$. (b) Example ω-dependent irreducible diagrams of order λ^6.

TABLE I

Number of Terms and of Connected Diagrams at Various Perturbation Orders, Classified According to the Dictionary Order of the Coupling Coefficients

		ω-dependent		ω-independent		Reducible	
Order	Coefficients	Terms	Diagrams	Terms	Diagrams	Terms	Diagrams
2	V_4	.	.	3	1	.	.
	V_3V_3	4	1	2	1	.	.
4	V_6	.	.	15	1	.	.
	V_3V_5	48	2	42	3	.	.
	V_4V_4	18	1	18	1	9	1
	$V_3V_3V_4$	264	6	84	6	42	4
	$V_3V_3V_3V_3$	264	3	36	3	60	4
6	V_8	.	.	105	1	.	.
	V_3V_7	360	2	480	3	.	.
	V_4V_6	360	2	390	3	90	2
	V_5V_5	240	2	180	2	.	.
	$V_3V_3V_6$	3120	8	1710	8	210	4
	$V_3V_4V_5$	6444	22	2550	16	666	10
	$V_4V_4V_4$	918	2	360	3	297	5
	$V_3V_3V_3V_5$	18576	27	4680	19	1944	20
	$V_3V_3V_4V_4$	26460	42	5280	25	3960	38
	$V_3V_3V_3V_3V_4$	85920	62	10020	36	13680	72
	$V_3V_3V_3V_3V_3V_3$	60240	22	3600	12	11760	32

Note. Entries in columns 3–6 refer to irreducible diagrams.

do not depend on ω_q and contribute only to the real part Δ_q of the self-energy, resulting in a shift of the phonon energies. The remaining "ω-dependent" diagrams, such as that shown in Fig. 1b, introduce also an imaginary contribution $i\Gamma_q$ and describe decay processes.

In Table I, we report the number of terms and of diagrams found for each combination of coupling coefficients $V_n = V_{12\ldots n}$, classified as ω-dependent, ω-independent, and reducible. The reducible diagrams are of no interest and are counted only to monitor the efficiency of the simplification process and to verify that no term is lost.

4. CONCLUSION

In this paper we have presented a computer-aided technique for evaluating the analytical expression of the phonon self-energy in anharmonic solids, based on the equation of motion of method combined with the phonon–antiphonon formalism. As an application of the method, the complete self-energy expression up to order λ^6 has been obtained and then rearranged, using a sorting reduction scheme, in terms of the Feynmann diagrams commonly used in the representation of the perturbation series.

The analytical expressions of the self-energy contribution of order λ^2 and λ^4 have been published elsewhere [21]. Examples of λ^6 diagrams are given in Section 3. The complete self-energy up to order λ^6 is part of the supplementary material available from the authors upon request and also available via the Internet [38]. Since the programs are not portable, they are not made available. The present implementation of the equation of motion method is found to be a powerful device for counting, classifying, and determining

the diagrammatic contributions at orders that are hardly within the reach of conventional techniques in perturbation theory. However, for practical application, we must remark that the extremely rapid increase in the number of diagrams with perturbation order (see Table I) makes a comprehensive calculation at finite orders extremely difficult, if not impossible. Nevertheless, we hope that the knowledge of an extra order for the series will provide useful clues for the development of more reasonable approximations or more efficient computational schemes [27].

APPENDIX A

Canonical Form of a Term

As discussed in the text, the canonical form for a term is defined by choosing (1) the labels and the signs of the summation indices, (2) the order of the function arguments, and (3) the order of the factors.

This definition is made in several steps. We initially assign arbitrary labels 1, 2, 3... and arbitrary signs to the summation indices. The order $q, -q, 1, -1, 2, -2 \ldots$ is then chosen for the function arguments. The order of the factors in the term, which are V, z, n and σ functions, is defined by the dictionary order of their arguments. The dictionary order of two lists of arguments is found in the usual way, by comparing in sequence corresponding elements of the two lists. Equal elements are ignored, and the first pair of unequal elements determines the order.

Thus, we have completely defined the textual representation of a term, except for arbitrary permutations and sign changes of the summation indices. Among all such permutations and sign changes we chose as canonical the one that yields the minimum textual representation in the dictionary order sense. With this representation, two terms with different canonical form correspond to the same diagram if and only if the canonical form of their coupling coefficients is identical.

APPENDIX B

Identification of Reducible Diagrams

We consider, as described in the text, the diagram corresponding to the term. We add two dummy vertices at the free ends of the "entry" and "exit" lines labeled q and $-q$, so that every line connects exactly two vertices, and then assign arbitrary labels 1, 2, 3... to the vertices. For all pairs i, j of vertices we find the number L_{ij} of lines that connect i and j. Given the incidence matrix L_{ij} we can obtain the diagram and vice versa, so that the matrix constitutes a representation of the diagram. The identification of the reducible diagrams is performed by searching for reducible paths in the incidence matrix L_{ij}. To find out whether a diagram is still connected after a line has been severed (i.e., after a matrix element L_{ij} has been decreased by one), we use a very efficient graph-theoretical algorithm described in Ref. [39].

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