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A modified Lanczos algorithm and the continued-fraction representation of correlation functions. An example: a correlation function of the exciton–phonon system

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Abstract. A modification of the Lanczos algorithm is suggested for calculating the frequency representations of correlation functions, averaging over the canonical ensemble. The problem is reduced to a recursive construction of a set of operators so that the commutator of each operator with the Hamiltonian is equal to a linear combination of three operators: previous, given and subsequent. As an initial operator of the set the one entering the correlation function is used. The coefficients with which the operators enter the linear combinations are equal to the elements of the continued fraction representing the correlation function. On the basis of the developed algorithm formulae are obtained for the correlation function of the system of Frenkel excitons interacting with non-polar optical phonons, which describes the absorption spectrum of a dielectric crystal.

1. Introduction

The recursion method of calculating the matrix elements of the resolvents of Hamiltonians, based on the Lanczos algorithm (Lanczos 1950, Voevodin and Kuznetsov 1984), has been shown to be a powerful tool for solving a number of problems (see Haydock 1980, Kelly 1980 and references therein, Sherman 1985, 1986). The merits of the method are a comparatively small required storage, simplicity and applicability to large sparse matrices. The matrix elements of resolvents may be considered as frequency representations of time correlation functions with averaging over some pure state. It is undoubtedly of interest to generalise this method for the case of averaging over the canonical ensemble, incidentally preserving their positive features. The method of a continued-fraction expansion of such correlation functions has been found by Mori (1965). In this method the continued-fraction elements are calculated with the help of recurrence relations which, however, are rather complicated and demand a lot of intermediate results to be memorised. Therefore the realisation of this calculation scheme encounters a number of difficulties, both in analytical and computer calculations, that prevents a large number of continued-fraction elements from being evaluated.

In this paper, a modification of the Lanczos algorithm is suggested for calculating correlation functions with averaging over the canonical ensemble by a recursion method. This modification preserves the above mentioned positive features of the algorithm and considerably simplifies analytical calculations and computer programs in comparison with the Mori method. The required storage is also essentially reduced. As an example of an application of the developed algorithm formulae are deduced for the correlation function of the exciton-phonon system, describing the absorption spectrum of a dielectric crystal in a wide temperature range.

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2. A modified Lanczos algorithm

Let us consider the Laplace transform

$$R_0(z) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-zt} R_0(t)$$

of the time correlation function $R_0(t) = \langle \mathscr{A}_0(t) \mathscr{A}_0^+ \rangle$, where the angle brackets denote the average over the canonical ensemble with the Hamiltonian H and $\mathscr{A}_0$ is an arbitrary operator, $\mathscr{A}_0(t) = \exp(\mathrm{i}Ht)\mathscr{A}_0 \exp(-\mathrm{i}Ht)$, with $\hbar = 1$. Let us suppose that $\langle \mathscr{A}_0 \mathscr{A}_0^+ \rangle = 1$ (at $\langle \mathscr{A}_0 \mathscr{A}_0^+ \rangle \neq 0, 1$ this may be achieved by multiplying $\mathscr{A}_0$ by the corresponding constant). An operator $\mathscr{A}_1$ is determined by the following equation:

$$[H, \mathscr{A}_0] = c_1^0 \mathscr{A}_1 + c_0^0 \mathscr{A}_0$$

where the coefficients c_1^0 and c_0^0 are determined by conditions $\langle \mathscr{A}_1 \mathscr{A}_0^+ \rangle = 0$ (hence $\langle \mathscr{A}_0 \mathscr{A}_1^+ \rangle = 0$) and $\langle \mathscr{A}_1 \mathscr{A}_1^+ \rangle = 1$. Analogously, operators $\mathscr{A}_n$, $n = 2, 3, \ldots$, are introduced successively according to the equations

$$[H, \mathscr{A}_{n-1}] = \sum_{i=0}^{n} c_i^{n-1} \mathscr{A}_i \tag{1}$$

where $n+1$ coefficients c_i^{n-1} are determined by $n+1$ conditions

$$\langle \mathscr{A}_n \mathscr{A}_i^+ \rangle = \delta_{n,i}. \tag{2}$$

It is easy to see, however, that in the sum (1) only three coefficients, c_n^{n-1}, c_{n-1}^{n-1} and c_{n-2}^{n-1}, are not equal to zero. Indeed,

$$c_k^{n-1} = \langle [H, \mathscr{A}_{n-1}] \mathscr{A}_k^+ \rangle = \langle \mathscr{A}_{n-1} [\mathscr{A}_k^+, H] \rangle = \sum_{i=0}^{k+1} \overset{*}{c}_i^k \langle \mathscr{A}_{n-1} \mathscr{A}_i^+ \rangle$$

from which, according to equations (2), follows the conclusion made above. From this relation it also follows that

$$c_{n-1}^{n-1} = \overset{*}{c}_{n-1}^{n-1} \qquad c_n^{n-1} = \overset{*}{c}_{n-1}^{n}.$$

According to definition (1) the coefficients c_n^{n-1} can always be chosen real and positive. Such choice is assumed in the following. Thus,

$$\begin{aligned} &[H, \mathscr{A}_n] = V_{n+1}\mathscr{A}_{n+1} - E_n \mathscr{A}_n + V_n \mathscr{A}_{n-1} \qquad n = 0, 1, \ldots \\ &V_0 = 0 \qquad E_n = -\langle [H, \mathscr{A}_n] \mathscr{A}_n^+ \rangle \qquad V_n = \langle [H, \mathscr{A}_n] \mathscr{A}_{n-1}^+ \rangle \end{aligned} \tag{3}$$

where the notations $E_n = -c_n^n$, $V_n = c_{n-1}^n$ are introduced.

Let us show, by using the projection operator technique developed by Mori (1965), that the coefficients E_n and V_n are the elements of the continued fraction representing the correlation function $R_0(z)$. The projection operator P_n on the operator $\mathscr{A}_n$ is determined by the equation

$$P_n Q = \langle Q \mathscr{A}_n^+ \rangle \mathscr{A}_n.$$

Time dependences of the operators $\mathscr{A}_n(t)$ are introduced by the equations

$$\begin{aligned} &(\mathrm{d}/\mathrm{d}t)\mathscr{A}_0(t) = \mathrm{i}[H, \mathscr{A}_0(t)] \qquad \mathscr{A}_0(0) = \mathscr{A}_0 \\ &(\mathrm{d}/\mathrm{d}t)\mathscr{A}_n(t) = \mathrm{i} \prod_{k=0}^{n-1} (1 - P_k)[H, \mathscr{A}_n(t)] \qquad \mathscr{A}_n(0) = \mathscr{A}_n \qquad n = 1, 2, \ldots \end{aligned} \tag{4}$$

from which it follows that $\langle \mathscr{A}_n(t)\mathscr{A}_i^+\rangle = 0$ at $i = 0, 1, \ldots, n-1$. $\mathscr{A}_n(t)$ can be presented in the form

$$\mathscr{A}_n(t) = R_n(t)\mathscr{A}_n + \mathscr{A}'_n(t) \tag{5}$$

where $R_n(t) = \langle \mathscr{A}_n(t)\mathscr{A}_n^+\rangle$ and hence $\mathscr{A}'_n(t) = (1 - P_n)\mathscr{A}_n(t)$. An equation determining the time evolution of $\mathscr{A}'_n(t)$ follows from equations (3)-(5):

$$(\mathrm{d}/\mathrm{d}t)\mathscr{A}'_n(t) = \mathrm{i}R_n(t)V_{n+1}\mathscr{A}_{n+1} + \mathrm{i}\prod_{k=0}^{n}(1 - P_k)[H, \mathscr{A}'_n(t)] \qquad \mathscr{A}'_n(0) = 0$$

which gives

$$\mathscr{A}_n(t) = R_n(t)\mathscr{A}_n + \mathrm{i}\int_0^t R_n(s)V_{n+1}\mathscr{A}_{n+1}(t-s)\,\mathrm{d}s. \tag{6}$$

By making use of equations (3), (4) and (6) and conditions (2) we find an equation determining the correlator $R_n(t)$,

$$(\mathrm{d}/\mathrm{d}t)R_n(t) = \mathrm{i}\left\langle\left\{\prod_{k=0}^{n-1}(1 - P_k)[H, \mathscr{A}_n(t)]\right\}\mathscr{A}_n^+\right\rangle$$

$$= \mathrm{i}\langle \mathscr{A}_n(t)[\mathscr{A}_n^+, H]\rangle = -\mathrm{i}E_nR_n(t) - V_{n+1}^2\int_0^t R_n(s)R_{n+1}(t-s)\,\mathrm{d}s.$$

For the Laplace transform $R_n(z)$ this equation is rewritten as

$$R_n(z) = \frac{1}{z + \mathrm{i}E_n + V_{n+1}^2 R_{n+1}(z)}$$

and

$$R_0(z) = \cfrac{1}{z + \mathrm{i}E_0 + \cfrac{V_1^2}{z + \mathrm{i}E_1 + \cfrac{V_2^2}{z + \mathrm{i}E_2 + \cfrac{V_3^2}{\ddots}}}}. \tag{7}$$

Thus the calculation of the correlator $R_0(z)$ has been reduced to a recursive construction of the set of operators $\{\mathscr{A}_n\}$ in accordance with algorithm (3) and to the determination of the coefficients E_n and V_n entering into continued fraction (7). In practical calculations, it is convenient to choose a suitable basis of operators and to decompose the operators $\mathscr{A}_n$ onto this basis. For instance, such a basis may be constructed from creation and annihilation operators (see the next paragraph). The coefficients of such a decomposition may be considered as components of a vector representing the operator $\mathscr{A}_n$. Expressing the Hamiltonian H in terms of the operators of the basis chosen, we represent the commutator in (3) as some procedure accomplished on the nth vector components. In the Lanczos algorithm, this procedure corresponds to the multiplication of a matrix representing H by a vector (Lanczos 1950, Voevodin and Kuznetsov 1984, Haydock 1980). As in the Lanczos algorithm, the sequence of

E_n and V_n calculations is as follows. By using the nth vector components found in the previous calculation step, E_n is determined and this allows us, in accordance to (3), to find the $(n+1)$th vector components multiplied by V_{n+1}. The latter value is determined from the conditions $\langle \mathscr{A}_{n+1}\mathscr{A}_{n+1}^{+}\rangle = 1$ and the cycle is repeated. As follows from (3), the information about only two sets of components describing $\mathscr{A}_n$ and $\mathscr{A}_{n-1}$ must be stored in the computer memory for the next step of computations. An obvious similarity of the two algorithms allows one to call the recurrence procedure (3) a modified Lanczos algorithm.

Algorithm (3) may be slightly changed by giving up the conditions $\langle \mathscr{A}_n\mathscr{A}_n^{+}\rangle = 1$ and leaving only $\langle \mathscr{A}_n\mathscr{A}_i^{+}\rangle = 0$ at $n \neq i$. In this case

$$[H, \mathscr{A}_n] = \mathscr{A}_{n+1} + b_n^n\mathscr{A}_n + b_{n-1}^n\mathscr{A}_{n-1}$$

$$b_{-1}^0 = 0 \qquad b_n^n = \langle [H, \mathscr{A}_n]\mathscr{A}_n^{+}\rangle\langle \mathscr{A}_n\mathscr{A}_n^{+}\rangle^{-1} = b_n^{*n} \tag{3'}$$

$$b_{n-1}^n = \langle \mathscr{A}_n\mathscr{A}_n^{+}\rangle\langle \mathscr{A}_{n-1}\mathscr{A}_{n-1}^{+}\rangle^{-1}.$$

Analogously to the previous case one obtains equation (7) for $R_0'(z) = R_0(z)\langle \mathscr{A}_0\mathscr{A}_0^{+}\rangle^{-1}$, where $E_n = -b_n^n$ and $V_n^2 = b_{n-1}^n$. Recurrent schemes (3) and (3′) naturally give the same results and the choice of one of them is determined by convenience in a definite situation.

In comparison with the Mori algorithm, which can be described by

$$\mathscr{A}_{n+1} = \mathrm{i}\prod_{k=0}^{n}(1 - P_k')[H, \mathscr{A}_n] \qquad P_k'Q = \langle Q\mathscr{A}_k^{+}\rangle\langle \mathscr{A}_k\mathscr{A}_k^{+}\rangle^{-1}\mathscr{A}_k$$

E_n and V_n in (7) being determined by (3′) (Mori 1965), algorithms (3) and (3′) possess two basic advantages. To find the $(n+1)$th operator in the Mori algorithm the information about all $(n+1)$ preceding operators must be stored, while in (3) and (3′), only two operators, the nth and $(n-1)$th, must be memorised. This leads to a considerable economy in the required storage. On the other hand, with the growth of n the recurrence relation of the Mori algorithm becomes rapidly complicated and the number of operations increases. The character of computations in (3) and (3′) is the same on each step and these recurrence relations are simpler, which reduces the number of operations and simplifies the routine in comparison with the Mori algorithm.

Taking advantage of the symmetry in a Hamiltonian, in analogy with the Lanczos algorithm (Haydock 1980, Sherman 1985, 1986), can save time and storage in computation. As follows from (3) and (3′), if the starting operator $\mathscr{A}_0$ belongs to an irreducible representation of the symmetries of H, all the operators $\mathscr{A}_n$ appearing in (3) and (3′) belong to the same row of the same irreducible representation. This imposes some restrictions on vector components representing $\mathscr{A}_n$ (see the next paragraph). The continued-fraction elements E_n and V_n are the same for starting operators corresponding to different rows of the same irreducible representation.

By interrupting the computation on the nth step and equating $R_n(z)$ to zero one approximates continued fraction (7) by the nth convergent which has n simple poles on the imaginary axis. The position of other possible singularities, branch points and essential singularities, is determined by the asymptotic behaviour of the coefficients E_n and V_n at large n (Haydock 1980). For some problems it can be determined on the basis of calculated coefficients or from other physical considerations (Haydock 1980, Sherman 1986). A number of methods of approximating $R_n(z)$ have been considered by Mori (1965).

The algorithm described above can also be used for calculating the Laplace transforms of the correlators $\langle \mathscr{A}(t)\mathscr{B}^+\rangle$, where $\mathscr{A} \neq \mathscr{B}$. Note that

$$\langle \mathscr{A}(t)\mathscr{B}^+\rangle = \tfrac{1}{2}\langle\{\mathscr{A}(t)+\mathscr{B}(t)\}\{\mathscr{A}^+ + \mathscr{B}^+\}\rangle$$
$$+\tfrac{1}{2}\mathrm{i}\langle\{\mathscr{A}(t)+\mathrm{i}\mathscr{B}(t)\}\{\mathscr{A}^+ - \mathrm{i}\mathscr{B}^+\}\rangle - \tfrac{1}{2}(1+\mathrm{i})\{\langle \mathscr{A}(t)\mathscr{A}^+\rangle + \langle \mathscr{B}(t)\mathscr{B}^+\rangle\}$$

and the problem is reduced to the calculation of four correlators of the type $\langle \mathscr{A}(t)\mathscr{A}^+\rangle$.

3. A correlation function of the exciton–phonon system

As an example of an application of the algorithm described above let us consider a calculation of a correlation function for a model system with the Hamiltonian

$$H = \varepsilon_A \sum_n a_n^+ a_n - (B/12)\sum_n \sum_a{}' a_{n+a}^+ a_n + \omega \sum_n b_n^+ b_n + \sqrt{S\omega}\sum_n a_n^+ a_n (b_n + b_n^+) \tag{8}$$

describing the interaction of Frenkel excitons with non-polar optical phonons in a SC crystal. In (8), a_n^+ and b_n^+ are the creation operators of an exciton and a phonon, respectively, on the nth lattice site, ε_A is the energy of the exciton band centre counted from the ground state of the crystal, $B \ll \varepsilon_A$ is the exciton bandwidth, ω is the phonon frequency, and $S \ll \varepsilon_A$, the Stokes shift, is the energy gain achieved at the vibrational relaxation of a localised excitation in case $B = 0$. The prime indicates that the summation over a proceeds over six vectors of the nearest neighbours of the zero site. We are interested in the correlation function

$$R_0(z) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-zt}\langle a_\kappa(t) a_\kappa^+\rangle$$

where $a_\kappa = N^{-1/2}\Sigma_n \exp(\mathrm{i}\kappa n) a_n$ is an exciton annihilation operator with wavevector κ and N is the number of sites of the periodic crystal region. In particular, $\mathscr{A}(\Omega) = \pi^{-1}\,\mathrm{Re}\, R_0(-\mathrm{i}\Omega + \eta)$, $\eta \to +0$, describes an absorption spectrum of an ideal dielectric. Here Ω is the frequency of the absorbing photon, κ, its wavevector, which will hereafter be supposed to be equal to zero.

In the situations common for dielectric crystals, $\exp(-\varepsilon_A/T) \ll 1$, where T is the temperature in energetic units. The terms of the order of or less than this exponent will be neglected below. In this approximation, $\langle a_\kappa a_\kappa^+\rangle = 1$ and the absorption spectrum $\mathscr{A}(\Omega)$ is normalised to unity. Thus we can use algorithm (3), supposing $\mathscr{A}_0 = a_\kappa$. It is easy to see from (3) and (8) that the operators $\mathscr{A}_n$ can be presented in the form

$$\mathscr{A}_n = N^{-1/2} \sum_{\nu=0}^{n} \sum_{\mu=0}^{n-\nu} \sum_{l_1, l_2, \ldots, l_\nu} \sum_{m_1, m_2, \ldots, m_\mu} \sum_L \mathscr{D}_{n,\nu,\mu}(l_1, l_2, \ldots, l_\nu; m_1, m_2, \ldots, m_\mu)$$
$$\times a_L b_{L+l_1}^+ \ldots b_{L+l_\nu}^+ b_{L+m_1} \ldots b_{L+m_\mu}. \tag{9}$$

The commutator in (3) leads to the appearance of terms containing the combinations $a_{m_1}^+ a_{m_2} a_{m_3}$, $a_{m_1}^+ a_{m_2}^+ a_{m_3} a_{m_4} a_{m_5}$, etc, in $\mathscr{A}_n$. On the one hand, these terms give contributions of the order of or less than $\exp(-\varepsilon_A/T)$ into E_n and V_n, and on the other hand, by a commutation with the Hamiltonian, do not give terms of type (9) (containing only one exciton annihilation operator) in $\mathscr{A}_{n+1}$. Therefore these terms are omitted in (9).

Substituting (8) and (9) into (3) one finds a recurrence formula for calculating the vector components determining $\mathscr{A}_n$,

$$V_{n+1}\mathscr{D}_{n+1,\nu,\mu}(\bar{\boldsymbol{l}}_\nu;\bar{\boldsymbol{m}}_\mu)=\theta(n-\nu)\theta(n-\nu-\mu)[(\nu-\mu)\omega+E_n-\varepsilon_A]\mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_\nu;\bar{\boldsymbol{m}}_\mu)$$
$$+\theta(n-\nu)\theta(n-\nu-\mu)\frac{B}{12}\sum_{\boldsymbol{a}}{}'\,\mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_\nu-\boldsymbol{a};\bar{\boldsymbol{m}}_\mu-\boldsymbol{a})$$
$$-\theta(n-\nu)\theta(\mu-1)\frac{\sqrt{S\omega}}{\mu}\sum_{i=1}^{\mu}\mathscr{D}_{n,\nu,\mu-1}(\bar{\boldsymbol{l}}_\nu;\boldsymbol{m}_\mu^i)\delta_{m_i,\mathbf{0}}$$
$$-\theta(n-\nu)\theta(n-\mu-\nu-1)(\mu+1)\sqrt{S\omega}\,\mathscr{D}_{n,\nu,\mu+1}(\bar{\boldsymbol{l}}_\nu;\bar{\boldsymbol{m}}_\mu,\mathbf{0})$$
$$-\theta(\nu-1)\frac{\sqrt{S\omega}}{\nu}\sum_{i=1}^{\nu}\mathscr{D}_{n,\nu-1,\mu}(\boldsymbol{l}_\nu^i;\bar{\boldsymbol{m}}_\mu)\delta_{l_i,\mathbf{0}}$$
$$-\theta(n-\nu-1)\theta(n-\nu-\mu-1)V_n\mathscr{D}_{n-1,\nu,\mu}(\bar{\boldsymbol{l}}_\nu;\bar{\boldsymbol{m}}_\mu). \tag{10}$$

For the sake of brevity we have introduced the following shorthand in (10): $\bar{\boldsymbol{l}}_\nu$ denotes ν arguments $\boldsymbol{l}_1,\boldsymbol{l}_2,\ldots,\boldsymbol{l}_\nu$ in $\mathscr{D}_{n,\nu,\mu}$; analogously $\bar{\boldsymbol{l}}_\nu-\boldsymbol{a}=\boldsymbol{l}_1-\boldsymbol{a},\boldsymbol{l}_2-\boldsymbol{a},\ldots,\boldsymbol{l}_\nu-\boldsymbol{a}$; $\boldsymbol{l}_\nu^i=\boldsymbol{l}_1,\ldots,\boldsymbol{l}_{i-1},\boldsymbol{l}_{i+1},\ldots,\boldsymbol{l}_\nu$; $-\bar{\boldsymbol{l}}_\nu=-\boldsymbol{l}_1,-\boldsymbol{l}_2,\ldots,-\boldsymbol{l}_\nu$. $\theta(l)=0$ at $l<0$ and $\theta(l)=1$ at $l\geqslant 0$.

As follows from (10), the component $\mathscr{D}_{n,\nu,\mu}$ are invariant with respect to the operations of the symmetry group O_h acting simultaneously on all vectors $\boldsymbol{l}_i$ and $\boldsymbol{m}_i$ at the fixed point $\mathbf{0}$. This conclusions results from the symmetry of the Hamiltonian and the initial operator $\mathscr{A}_0$ described by the only components $\mathscr{D}_{0,0,0}=1$, and it illustrates the symmetry considerations of the previous paragraph. In this connection note that with respect to translations operators (9) are characterised by the zero wavevector, as is $\mathscr{A}_0$. In accordance with (9) $\mathscr{D}_{n,\nu,\mu}$ is also invariant with respect to permutations of any pair of vectors $\boldsymbol{l}_i$ as well as of any pair of vectors $\boldsymbol{m}_i$. These symmetry properties allow one to reduce the required storage and the number of operations by memorising only non-equal components and multiplicities of their repetitions.

Using (9), conditions (2) are written in the form

$$\sum_{\nu=0}^{n}\sum_{\nu'=0}^{n'}\sum_{\mu=\mu_1}^{\mu_2}\sum_{\alpha=\alpha_1}^{\alpha_2}\sum_{\bar{\boldsymbol{l}},\bar{\boldsymbol{l}}'}\sum_{\bar{\boldsymbol{m}},\bar{\boldsymbol{m}}'}f\mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha},\bar{\boldsymbol{l}}'_{\nu'-\alpha};\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha},\bar{\boldsymbol{m}}_{\mu'-\alpha})$$
$$\times\mathscr{D}_{n',\nu',\mu'}(\bar{\boldsymbol{m}}'_\alpha,-\bar{\boldsymbol{l}}'_{\nu'-\alpha};\bar{\boldsymbol{m}}'_\alpha,-\bar{\boldsymbol{m}}_{\mu'-\alpha})=\delta_{n,n'}. \tag{11}$$

Here $\mu'=\mu+\nu'-\nu$, $\mu_1=\max(0,\nu-\nu')$, $\mu_2=\min(n'-2\nu'+\nu,n-\nu)$, $\alpha_1=\max(0,\nu'-\nu)$, $\alpha_2=\min(\mu',\nu')$ and

$$f=\frac{\mu'!\,\nu'!\,\mu!\,\nu!}{(\mu'-\alpha)!\,(\nu'-\alpha)!\,(\nu-\nu'+\alpha)!\,\alpha!}(\bar{n}+1)^{\mu'-\alpha}\bar{n}^{\nu+\alpha}$$

with $\bar{n}=[\exp(\omega/T)-1]^{-1}$. On deriving (11) it has been taken into account that, in the accepted approximation,

$$\langle a_{\boldsymbol{L}}b^+_{\boldsymbol{L}+\boldsymbol{l}_1}\ldots b^+_{\boldsymbol{L}+\boldsymbol{l}_\nu}b_{\boldsymbol{L}+\boldsymbol{m}_1}\ldots b_{\boldsymbol{L}+\boldsymbol{m}_\mu}b^+_{\boldsymbol{L}'+\boldsymbol{m}'_{\mu'}}\ldots b^+_{\boldsymbol{L}'+\boldsymbol{m}'_1}b_{\boldsymbol{L}'+\boldsymbol{l}'_{\nu'}}\ldots b_{\boldsymbol{L}'+\boldsymbol{l}'_1}a^+_{\boldsymbol{L}'}\rangle$$
$$=\langle 0|a_{\boldsymbol{L}}a^+_{\boldsymbol{L}'}|0\rangle\langle b^+_{\boldsymbol{L}+\boldsymbol{l}_1}\ldots b^+_{\boldsymbol{L}+\boldsymbol{l}_\nu}b_{\boldsymbol{L}+\boldsymbol{m}_1}\ldots b_{\boldsymbol{L}+\boldsymbol{m}_\mu}$$
$$\times b^+_{\boldsymbol{L}'+\boldsymbol{m}'_{\mu'}}\ldots b^+_{\boldsymbol{L}'+\boldsymbol{m}'_1}b_{\boldsymbol{L}'+\boldsymbol{l}'_{\nu'}}\ldots b_{\boldsymbol{L}'+\boldsymbol{l}'_1}\rangle_{\boldsymbol{L}}$$

where the last brackets denote the averaging with the statistical operator $\exp(-H_{\boldsymbol{L}}/T)/\mathrm{Sp}[\exp(-H_{\boldsymbol{L}}/T)]$, $H_{\boldsymbol{L}}=\omega\sum_{\boldsymbol{n}}b^+_{\boldsymbol{n}}b_{\boldsymbol{n}}$; $|0\rangle$ is the vacuum state of the exciton subsystem. When making use of the Bloch-de Dominicis theorem (Bloch and de

Dominicis 1958, Tyablikov 1975), note that due to the symmetry of $\mathscr{D}_{n,\nu,\mu}$ with respect to permutations of the arguments, all terms arising at the pairing of any α creation operators with primed subscript $(\boldsymbol{L}'+\boldsymbol{m}'_i)$ with any α annihilation operators with primed subscripts $(\boldsymbol{L}'+\boldsymbol{l}'_i$, the remaining operators of such groups are paired with those possessing unprimed subscripts $\boldsymbol{L}+\boldsymbol{l}_i$ and $\boldsymbol{L}+\boldsymbol{m}_i$) are equal. One only has to count the number of such terms. This is easy to do taking into account that there are $\nu![\alpha!(\nu-\alpha)!]^{-1}$ possibilities to select α operators from the ν given and $\alpha!$ possibilities for α annihilation and creation operators to be paired.

By making use of conditions (11) in (10), after some transformations we find

$$
\begin{aligned}
E_n = \varepsilon_A + \sum_{\nu,\nu'=0}^{n} \sum_{\mu=\mu_1}^{\mu_3} \sum_{\alpha=\alpha_1}^{\alpha_2} \sum_{\bar{\boldsymbol{l}},\bar{\boldsymbol{l}}'} \sum_{\bar{\boldsymbol{m}},\bar{\boldsymbol{m}}'} & f\mathscr{D}_{n,\nu',\mu'}(\bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{l}}'_{\nu'-\alpha}; \bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{m}}_{\mu'-\alpha}) \\
\times \Bigg(& \omega(\mu-\nu)\mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{l}}'_{\nu'-\alpha}; \bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{m}}_{\mu'-\alpha}) \\
& - \frac{B}{12} \sum_{\boldsymbol{a}}{}' \mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{l}}'_{\nu'-\alpha} - \boldsymbol{a}; \bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{m}}_{\mu'-\alpha} - \boldsymbol{a}) \Bigg) \\
& + 2(\bar{n}+1)\sqrt{S\omega} \sum_{\nu,\nu'=0}^{n} \sum_{\mu=\mu_1}^{\mu_4} \sum_{\alpha=\alpha_1}^{\alpha_2} \sum_{\bar{\boldsymbol{l}},\bar{\boldsymbol{l}}'} \sum_{\bar{\boldsymbol{m}},\bar{\boldsymbol{m}}'} f(\mu+1) \\
& \times \mathscr{D}_{n,\nu,\mu+1}(\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{l}}'_{\nu'-\alpha}; \bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{m}}_{\mu'-\alpha}, \boldsymbol{0}) \\
& \times \mathscr{D}_{n,\nu',\mu'}(\bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{l}}'_{\nu'-\alpha}; \bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{m}}_{\mu'-\alpha}) \\
& + 2\bar{n}\sqrt{S\omega} \sum_{\nu=0}^{n} \sum_{\nu'=0}^{n-1} \sum_{\mu=\mu_1}^{\mu_5} \sum_{\alpha=\alpha_1}^{\alpha_2} \sum_{\bar{\boldsymbol{l}},\bar{\boldsymbol{l}}'} \sum_{\bar{\boldsymbol{m}},\bar{\boldsymbol{m}}'} f(\nu'+1) \\
& \times \mathscr{D}_{n,\nu'+1,\mu'}(\bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{l}}'_{\nu'-\alpha}, \boldsymbol{0}; \bar{\boldsymbol{m}}'_\alpha, -\bar{\boldsymbol{m}}_{\mu'-\alpha}) \\
& \times \mathscr{D}_{n,\nu,\mu}(\bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{l}}'_{\nu'-\alpha}; \bar{\boldsymbol{l}}_{\nu-\nu'+\alpha}, \bar{\boldsymbol{m}}_{\mu'-\alpha}) \qquad (12)
\end{aligned}
$$

$$
\mu_3 = \min(n-2\nu'+\nu,\ n-\nu) \qquad \mu_4 = \min(n-2\nu'+\nu,\ n-\nu-1)
$$

$$
\mu_5 = \min(n-2\nu'+\nu-1,\ n-\nu).
$$

Analogously, a formula for V_n can be obtained but equations (10)-(12) suffice for calculating E_n and V_n.

The sequence of computations is as follows. By using the starting value $\mathscr{D}_{0,0,0}=1$ in (12) one finds $E_0=\varepsilon_A-B/2$. Equation (10) determines the components

$$
V_1\mathscr{D}_{1,0,0}=0 \qquad V_1\mathscr{D}_{1,1,0}(\boldsymbol{m}) = V_1\mathscr{D}_{1,0,1}(\boldsymbol{m}) = -\sqrt{S\omega}\,\delta_{\boldsymbol{m},\boldsymbol{0}},
$$

and, after insertion into (11), it is found that $V_1^2 = S\omega(2\bar{n}+1)$. Proceeding in the same way one more pair of elements of fraction (7) can be calculated:

$$
E_1 = \varepsilon_A + \frac{\omega}{2\bar{n}+1} \qquad V_2^2 = 2(2\bar{n}+1)S\omega + \frac{4\bar{n}(\bar{n}+1)}{(2\bar{n}+1)^2}\,\omega^2 + \frac{B^2}{24}.
$$

Further analytical calculations are cumbersome and to move forward a computer has to be used.

At $T=0$, only the terms with $\nu=\nu'=\alpha=0$ give a contribution to (11) and (12). In this connection only the components with $\nu=0$ have to be considered in recurrence relation (10). Note that $\mathscr{D}_{n+1,0,\mu}$ is only expressed through $\mathscr{D}_{n,0,\mu}$ and $\mathscr{D}_{n-1,0,\mu}$. In this case, equations (10)-(12) are reduced to the formulae obtained earlier (Sherman 1985),

on the basis of which the absorption spectra of a crystal at $T = 0$ has been computed (Sherman 1986). The employment of the algorithm developed allows us to obtain the equations for the correlator at finite temperatures which are similar and only slightly more involved than these formulae. This similarity of basic formulae gives a possibility of actually using the same calculation procedure at $T \neq 0$ that has been utilised at $T = 0$. This circumstance is a consequence of a similarity of the Lanczos recurrence relations to equations (3) and (3′) pointed out above. A calculation of the absorption spectra for finite temperatures will be carried out in the forthcoming paper.

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