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Solution of the local polaron model with a boson continuum

Michele Cini† and Massimiliano Cuozzo‡

INFM, Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica, 1-00133 Roma, Italy

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Abstract. We study the zero-temperature Green function for the local polaron model that describes the interaction of an electron in an empty band with a boson continuum; the coupling takes place at one site in the lattice. To this end, we propose a new exact approach which consists in two steps: first, the problem is reduced to the solution of an infinite linear algebraic system of recursion equations by the method of excitation amplitudes; then, a systematic expansion of the solution is generated by Feenberg's formalism. Previously, the problem had been solved exactly in the narrow-band limit; otherwise, the solution was achieved for one or a few boson modes. Here we consider a boson continuum and obtain an infinite expansion of the self-energy in terms of the dressed Green function. In this case, the recursive, continued-fraction technique is equivalent to self-consistent perturbation theory. The results are illustrated by selected numerical examples, and show that the satellites are much more sensitive to the boson dispersion than the main line.

1. Introduction

The local polaron model describes a single particle (e.g. an electron or hole) which evolves in an empty band and interacts with a boson field only when a particular 'electronic' state (e.g. a site in the lattice) is populated. The Hamiltonian of this model is $H = H_F + H_B + H_I$, where

$$H_F = \varepsilon_a c_a^\dagger c_a + \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k [V_{ka} c_k^\dagger c_a + \text{HC}] \tag{1}$$

is a Fano model Hamiltonian, $c_a^\dagger$ is the creation operator of the local state, $c_k^\dagger$ creates a band state, ε_a and ε_k are the energy levels of the local state and of the band states;

$$H_B = \sum_q \omega_q b_q^\dagger b_q \tag{2}$$

describes the free-boson field, and the field–electron interaction is of the local type:

$$H_I = c_a^\dagger c_a \sum_q g_q (b_q^\dagger + b_q). \tag{3}$$

For $V_{ka} = 0$, when the band reduces to a core-like level, this can be solved exactly as shown by Langreth [1]. A similar model with dispersionless bosons was first introduced by Hewson and Newns [2] in the context of a theory of image force effects in chemisorption, and the bosons were surface plasmons. The present model was introduced by one of us [3]

† BITNET: CINI@ROMA2.INFN.IT.
‡ BITNET: CUOZZO@ROMA2.INFN.IT.

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in a theory of photoemission spectra from valence states. The spectrum is related to the density of states which can be obtained from the local Green's function

$$G(\omega) \equiv \langle a| \frac{1}{\omega - H + \mathrm{i}\delta} |a\rangle \tag{4}$$

where $|a\rangle = c_a^+|0\rangle$. The model (1)–(3) allows us to study the competition between screening (which takes place in a time of the order of the inverse boson frequencies) and band diffusion, whose time-scales are determined by the inverse band width, and by the analytic structure (e.g. Van Hove singularities) of the band profile. The exact solution was found by one of us [3] for any shape of the electronic level, subject to the condition that all of the bosons have the same frequency ω_0. The recursion method of excitation amplitudes, which was introduced to solve this problem, has been applied in a variety of contexts [4], and particularly to non-linear optics [5], when the relevant bosons are photons; its main advantage is that it is non-perturbative and electron–boson interactions are automatically treated to all orders. Also, it includes all of the electronic degrees of freedom from the start, since it gives $G(\omega)$ directly in terms of the propagator G_0 of H_F. For a class of problems, it is much more rewarding than the standard techniques. The simple, closed exact solution of [3] was in fact reproduced by the standard perturbation methods [6], but is much more difficult to derive in that way. However, the application of the excitation amplitude approach was limited to problems involving a few boson modes because otherwise the solution of the recurrence equations becomes too demanding.

Yet, the case of a boson continuum is physically very interesting, and it is clear that it can lead to qualitatively different phenomena. We just mention that in the continuum case the bosons have a group velocity, and therefore there is a new time-scale in the problem. In the present paper, we wish to propose a method for overcoming that limitation, and dealing with a boson continuum—that is, with a boson mode having dispersion in frequency.

2. Excitation amplitudes

Let us introduce the excitation amplitudes, defined by

$$\Psi(q_1, q_2, \ldots, q_N, \omega) \equiv \langle a| b_{q_1} b_{q_2} \cdots b_{q_N} \frac{1}{\omega - H + \mathrm{i}\delta} |a\rangle. \tag{5}$$

By the method of excitation amplitudes one can reduce the problem exactly to an infinite set of linear recurrence equations. We refer the reader to reference [3] for the derivation. The interacting propagator, which coincides with the zeroth amplitude, is given by

$$G(\omega) = \Psi(\omega) = G_0(\omega)\left[1 + \sum_q g_q \Psi(q, \omega)\right]. \tag{6a}$$

Here,

$$G_0(\omega) \equiv \langle a| \frac{1}{\omega - H_F + \mathrm{i}\delta} |a\rangle$$

is the non-interacting local Green function which we consider known. The general recurrence relation is

$$\Psi(q_1, q_2, \ldots, q_n, \omega) = G_0(\omega - \omega_{q_1} - \omega_{q_2} - \cdots - \omega_{q_n}) \times \left[g_{q_1} \Psi(q_2, \ldots, q_n, \omega) + g_{q_2} \Psi(q_1, q_3, \ldots, q_n, \omega) + \cdots \right.$$

$$+ g_{q_n}\Psi(q_1, q_2, \ldots, q_{n-1}, \omega) + \sum_{q'} g_{q'}\Psi(q_1, q_2, \ldots, q_n, q', \omega)\Big]. \tag{6b}$$

A clear advantage of this approach is that of expressing G in terms of G_0, which is already fully dressed by the hopping interactions V.

If $\omega_{\boldsymbol{q}} \equiv \omega_0$ is independent of $\boldsymbol{q}$, equation (6) is solved by introducing the quantities

$$\Phi_k(\omega) = \sum_{q_1 \cdots q_k} g_{q_1} g_{q_2} \cdots g_{q_k} \Psi(q_1, q_2, \ldots, q_k, \omega)$$

and setting

$$g_0^2 = \sum_{\boldsymbol{q}} g_{\boldsymbol{q}}^2.$$

In terms of the Φ_k the system becomes tridiagonal and thus the solution is a continued fraction [3]:

$$G(\omega) = \cfrac{G_0(\omega)}{1 - \cfrac{g_0^2 G_0(\omega) G_0(\omega - \omega_0)}{1 - \cfrac{2g_0^2 G_0(\omega - \omega_0) G_0(\omega - 2\omega_0)}{1 - \cfrac{3g_0^2 G_0(\omega - 2\omega_0) G_0(\omega - 3\omega_0)}{1 - \cfrac{4g_0^2 G_0(\omega - 3\omega_0) G_0(\omega - 4\omega_0)}{1 - \cdots}}}}}. \tag{7}$$

The same method and solution apply if there is just one mode of frequency ω_0 and coupling g_0. In the presence of $N = 2$ or $N = 3$ boson modes, the set (6*b*) can be resolved along similar lines, in terms of matrix continued fractions [4]. However, the amount of computation involved grows very quickly with the number of modes. We wish to show below that some simplicity is regained in the $N \to \infty$ limit, which is the case of a continuous boson dispersion law. To this end, we find it expedient to rephrase the set (6*b*) in a different form. Let us start with a numerable set of modes, and define $\Psi_{l_1, l_2, \ldots, l_n}(\omega)$ as the amplitude which has l_i boson modes with energy ω_i in its argument; $\Psi \equiv 0$ if any of the l_i are negative. Using these new definitions the system becomes

$$\begin{aligned} G(\omega) = \Psi_{0,0,\ldots,0}(\omega) &= G_0(\omega)[1 + g_{q_1}\Psi_{1,0,\ldots,0}(\omega) + g_{q_2}\Psi_{0,1,\ldots,0}(\omega) + \cdots \\ &\quad + g_{q_n}\Psi_{0,\ldots,0,1}(\omega)] \cdots \\ \Psi_{l_1, l_2, \ldots, l_n}(\omega) &= G(\omega - l_1\omega_{q_1} - l_2\omega_{q_2} - \cdots - l_n\omega_{q_n})[g_{q_1}\Psi_{l_1+1, l_2, \ldots, l_n}(\omega) \\ &\quad + g_{q_2}\Psi_{l_1, l_2+1, \ldots, l_n}(\omega) + \cdots + g_{q_n}\Psi_{l_1, l_2, \ldots, l_n+1}(\omega) + l_1 g_{q_1}\Psi_{l_1-1, l_2, \ldots, l_n}(\omega) \\ &\quad + l_2 g_{q_2}\Psi_{l_1, l_2-1, \ldots, l_n}(\omega) + \cdots + l_n g_{q_n}\Psi_{l_1, l_2, \ldots, l_n-1}(\omega)] \cdots . \end{aligned} \tag{8}$$

This rephrasing explicitly shows the permutation symmetry of the amplitudes with respect to their bosonic indices, and, for example, $\Psi(q_1, q_2, \omega)$ and $\Psi(q_2, q_1, \omega)$ are seen to be the same thing, namely $\Psi_{1,1,0,\ldots,0}(\omega)$.

3. Feenberg expansion

3.1. Self-energy

A systematic expansion for the solution of linear algebraic problems was proposed by Feenberg [7, 8] and is summarized in appendix 1. A more complete account of Feenberg's method and its applications to atomic physics was given by Swain [9]. If $\mathbf{A}$ is an $M \times M$ matrix, let $A = \det(\mathbf{A})$ and let A_i be the determinant obtained from A by taking away

the ith row and column; similarly denote by A_{ij} that obtained by taking away the ith and jth rows and columns, and so on. By definition, $A_{123\cdots M} = 1$. The ith component of the solution of a system $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$ is

$$x_i = \frac{b_i}{D_i} - \sum_j{}^* \frac{a_{ij}b_j}{D_{ij}} + \sum_{jk}{}^* \frac{a_{ij}a_{jk}b_k}{D_{ijk}} - \sum_{jkl}{}^* \frac{a_{ij}a_{jk}a_{kl}b_l}{D_{ijkl}} - \cdots \tag{9}$$

where the asterisk on the summation means that the summation indices must be different from each other and from any other indices appearing in the summand,

$$D_i \equiv \frac{A}{A_i} \qquad D_{ij} \equiv \frac{A}{A_{ij}}$$

and so on. Each contribution to a $\sum^*$ is called an *irreducible process* (see appendix 1). In (8), only the first component of $\boldsymbol{b}$ is non-vanishing, and by solving for $x_0 \equiv G(\omega)$ we obtain

$$G(\omega) = \frac{G_0(\omega)}{D_0}. \tag{10}$$

In Feenberg's method one is not forced to write down the matrix $\mathbf{A}$ explicitly; all that we need is to know the non-vanishing a_{ij} connecting a given entry to all of the others. To clarify this point let us consider the amplitude $\Psi_{2,0,\ldots,0}(\omega)$. This is only linked to $\Psi_{3,0,\ldots,0}(\omega)$, to $\Psi_{1,0,\ldots,0}(\omega)$ and to $\Psi_{2,\ldots,1,\ldots,0}(\omega)$ (considering all of the possible positions of 1). For example, it is not linked to $\Psi_{0,\ldots,2,\ldots,0}(\omega)$ or to $\Psi_{0,\ldots,1,\ldots,2,\ldots,0}(\omega)$. In general, a given state can only be linked to those with one boson more or one boson less. Thus it is better to work referring only to the population numbers $\{l_i\}$ rather than to a particular base, and a slight change of notation is useful. Let us think of the excitation amplitude $\{l_i\}$ as the 'state' $|j\rangle$ in the following way:

$$\Psi_{l_1,l_2,\ldots,l_n}(\omega) \equiv |l_1, l_2, \ldots, l_n\rangle \equiv |\{l_j\}\rangle \equiv |j\rangle.$$

Let us write $\Psi_{0,0,\ldots,0}(\omega) \equiv |0\rangle$. Thus a_{ij} is the matrix element connecting the 'state' $|i\rangle$ and the 'state' $|j\rangle$—that is, the matrix element which links the amplitude with population number $\{l_i\}$ to the amplitude with population number $\{l_j\}$.

The D-quantities can be expanded in a similar fashion to x_i. Let us write out the first terms of D_0:

$$D_0 = 1 - \sum_j{}^* \frac{a_{0j}a_{j0}}{D_j^0} - \sum_{j,k,l}{}^* \frac{a_{0j}a_{jk}a_{kl}a_{l0}}{D_{jkl}^0} - \sum_{j,k,l,m,n}{}^* \frac{a_{0j}a_{jk}a_{kl}a_{lm}a_{mn}a_{n0}}{D_{jklmn}^0} - \cdots. \tag{11}$$

The arguments of the sums are products of matrix elements which have the same initial and final index '0' (in this sense we call them 'loops') and there are only products with an even number of matrix elements. Clearly, $a_{0j} = G_0(\omega)$ for all of the possible states $|j\rangle$ linked to $|0\rangle$. Thus,

$$D_0 = 1 - G_0(\omega)\left[\sum_j{}^* \frac{a_{j0}}{D_j^0} - \sum_{j,k,l}{}^* \frac{a_{jk}a_{kl}a_{l0}}{D_{jkl}^0} - \sum_{j,k,l,m,n}{}^* \frac{a_{jk}a_{kl}a_{lm}a_{mn}a_{n0}}{D_{jklmn}^0} - \cdots\right]. \tag{12}$$

Introducing

$$\Sigma(\omega) = \sum_j{}^* \frac{a_{j0}}{D_j^0} - \sum_{j,k,l}{}^* \frac{a_{jk}a_{kl}a_{l0}}{D_{jkl}^0} - \sum_{j,k,l,m,n}{}^* \frac{a_{jk}a_{kl}a_{lm}a_{mn}a_{n0}}{D_{jklmn}^0} - \cdots \tag{13}$$

we may write $D_0 = 1 - G_0(\omega)\Sigma(\omega)$ and using (12) we get Dyson's equation:

$$G(\omega) = \frac{G_0(\omega)}{1 - G_0(\omega)\Sigma(\omega)}.$$

Thus, Σ is the proper self-energy.

3.2. Rules for the loop expansion

Explicitly, equation (13) reads

$$\Sigma(\omega) = \sum_{q_j}^{*} g_{q_j}^2 \frac{G_0(\omega-\omega_{q_j})}{D^0_{\omega_{qj}}} + \sum_{q_j,q_k}^{*} g_{q_j}^2 g_{q_k}^2 \frac{G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qk}}} + \cdots \tag{14}$$

and can be continued by applying Feenberg's rules. The expansion is the sum of the contributions of loops that begin and end with the $|0\rangle$ state, and represent irreducible processes. During their 'life' the loops may visit only an odd number of intermediate states, due to the presence of an odd number of matrix elements in the definition of Σ. The rules for the contribution of each loop to the self-energy are as follows.

(1) For each intermediate state, include a propagator

$$G_0\left(\omega - \sum_j l_j\omega_j\right)$$

where l_j is the occupation of the boson j in the intermediate state.

(2) Include a factor g_q^2 for every switched-on boson mode with energy ω_q.

(3) Divide the contribution of every loop by a Feenberg D where the high index is '0' and the low indices depend on the states visited by the loop.

(4) A numerical factor $f_{q_j,q_k,q_l,\ldots}$ must be included; this arises according to the above discussion from the l-factors in (8) which are different from unity when there are several equal bosons switched on. We can dispense with a general expression for these f since they will disappear in the continuum limit (see below).

(5) Sum over all of the indices of the bosons of the intermediate states.

In order to analyse the expansion, we need a few definitions. A loop can be represented graphically as a series of dots, one for each boson mode which is turned on or off in the irreducible process. A part of a loop where all nodes represent bosons which are turned on (off) is an 'ascending' ('descending') part. Thus, we can split the set of all loops into two distinct classes, as follows. 'Arch loops' consist of one ascending part, followed by a descending part. We call all of the others 'zigzag loops'.

For example, the contribution Σ_5 due to the terms which visit five intermediate states comes from the graphs of figure 1, where 1(a), 1(b) and 1(c) are arch contributions, and 1(d) is a zigzag one. The mathematical contributions are

$$1(a)\qquad G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_j}-\omega_{q_k}-\omega_{q_l}) \times G_0(\omega-\omega_{q_k}-\omega_{q_l})G_0(\omega-\omega_{q_l})$$

$$1(b)\qquad G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_j}-\omega_{q_k}-\omega_{q_l}) \times G_0(\omega-\omega_{q_k}-\omega_{q_l})G_0(\omega-\omega_{q_k})$$

$$1(c)\qquad G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_j}-\omega_{q_k}-\omega_{q_l}) \times G_0(\omega-\omega_{q_j}-\omega_{q_l})G_0(\omega-\omega_{q_l})$$

$$1(d)\qquad G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_k})G_0(\omega-\omega_{q_k}-\omega_{q_l})G_0(\omega-\omega_{q_l}).$$

The D-denominators read

$$1(a)\qquad D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{ql}}$$

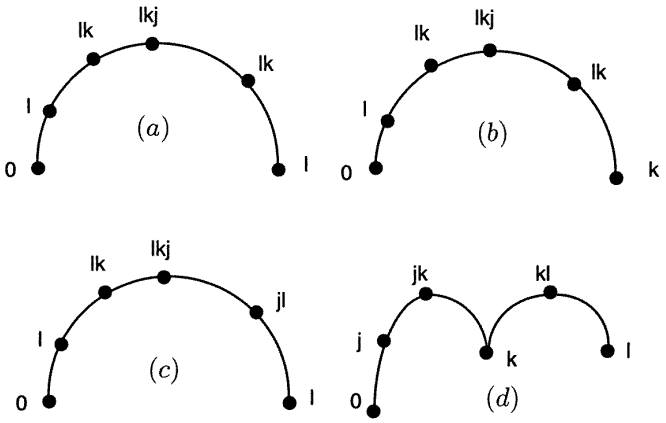

Figure 1. Irreducible processes which contribute to Σ_5. Note that q_k, q_l and q_j must all be different.

$1(b)$ $\quad D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{qk}}$

$1(c)$ $\quad D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qj}+\omega_{ql},\omega_{ql}}$

$1(d)$ $\quad D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qk},\omega_{qk}+\omega_{ql},\omega_{ql}}$.

Finally, we get

$$\begin{aligned}\Sigma_5(\omega) = \sum_{q_j,q_k,q_l}{}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 f_{q_j,q_k,q_l} G_0(\omega-\omega_{q_j}) G_0(\omega-\omega_{q_j}-\omega_{q_k}) G_0(\omega-\omega_{q_j}-\omega_{q_k}-\omega_{q_l}) \\ \times \left[\frac{G_0(\omega-\omega_{q_k}-\omega_{q_l}) G_0(\omega-\omega_{q_l})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{ql}}} + \frac{G_0(\omega-\omega_{q_k}-\omega_{q_l}) G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{qk}}} \right. \\ \left. + \frac{G_0(\omega-\omega_{q_j}-\omega_{q_l}) G_0(\omega-\omega_{q_l})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qj}+\omega_{ql},\omega_{ql}}} \right] + \sum_{q_j,q_k,q_l}{}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 f_{q_j,q_k,q_l} \\ \times \frac{G_0(\omega-\omega_{q_j}) G_0(\omega-\omega_{q_j}-\omega_{q_k}) G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qk},\omega_{qk}+\omega_{ql},\omega_{ql}}} \\ \times G_0(\omega-\omega_{q_k}-\omega_{q_l}) G_0(\omega-\omega_{q_l}). \qquad (15)\end{aligned}$$

The self-energy expression including the loops which visit up to five intermediate states is a bit involved, but is readily obtained along these lines. It reads

$$\begin{aligned}\Sigma(\omega) = \sum_{q_j}{}^{*} g_{q_j}^2 \frac{G_0(\omega-\omega_{q_j})}{D_{\omega_{qj}}} + \sum_{q_j,q_k}{}^{*} g_{q_j}^2 g_{q_k}^2 \frac{G_0(\omega-\omega_{q_j}) G_0(\omega-\omega_{q_j}-\omega_{q_k}) G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qk}}} \\ + \sum_{q_j,q_k,q_l}{}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 f_{q_j,q_k,q_l} G_0(\omega-\omega_{q_j}) G_0(\omega-\omega_{q_j}-\omega_{q_k}) \\ \times G_0(\omega-\omega_{q_j}-\omega_{q_k}-\omega_{q_l}) \\ \times \left[\frac{G_0(\omega-\omega_{q_k}-\omega_{q_l}) G_0(\omega-\omega_{q_l})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{ql}}} + \frac{G_0(\omega-\omega_{q_k}-\omega_{q_l}) G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qk}+\omega_{ql},\omega_{qk}}} \right. \\ \left. + \frac{G_0(\omega-\omega_{q_j}-\omega_{q_l}) G_0(\omega-\omega_{q_l})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qj}+\omega_{qk}+\omega_{ql},\omega_{qj}+\omega_{ql},\omega_{ql}}} \right] + \sum_{q_j,q_k,q_l}{}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 f_{q_j,q_k,q_l}\end{aligned}$$

$$\times \frac{G_0(\omega-\omega_{q_j})G_0(\omega-\omega_{q_j}-\omega_{q_k})G_0(\omega-\omega_{q_k})}{D^0_{\omega_{qj},\omega_{qj}+\omega_{qk},\omega_{qk},\omega_{qk}+\omega_{ql},\omega_{ql}}}$$
$$\times G_0(\omega-\omega_{q_k}-\omega_{q_l})G_0(\omega-\omega_{q_l})+\cdots. \tag{16}$$

The above rules hold for any discrete set of ω_j. Supplemented by the corresponding expansions of the denominators they yield a systematic expansion of the self-energy in terms of G_0, which is the Fano–Anderson propagator in the absence of any coupling to the bosons. This method is complicated by the presence of the f-factors and provides an efficient algorithm only if the potential energy due to the bosons is small compared to the kinetic energy, and therefore a few terms suffice. In the next section we show that considerable progress can be achieved in the continuum limit $N \to \infty$.

3.3. Simplified rules for the continuum limit

All the factors $f_{q_1,q_2,\ldots,q_N}$ can be replaced by unity for $N \to \infty$. This simplification can easily be proved by a combinatorial argument, showing that the amplitude of repeatedly exciting the same boson mode gives a contribution to the total amplitude which is $O(1/N)$. On the other hand, consider the last term of equation (6*b*), namely,

$$G_0(\omega-\omega_{q_1}-\omega_{q_2}-\cdots-\omega_{q_n})\sum_{q'} g_{q'}\Psi(q_1,q_2,\ldots,q_n,q',\omega)$$

which introduces the new variable q' into the equation for

$$\Psi(q_1,q_2,\ldots,q_n,\omega).$$

It is clear that q' appears only as an integration variable; the set $\{q'=q_1\}U\{q'=q_2\}\cdots U\{q'=q_n\}$ has a vanishing measure in the continuum limit, and contributes nothing. Thus, as far as the calculation of G is concerned, we may consider that each mode is excited at most once.

A further, major simplification can be obtained by a close examination of the expansion. Feenberg's method allows us to develop the local Green function as a series of terms. The denominator of each term is a *Feenberg D* which may be expanded in the same way, although the processes (or graphs) occurring in the denominators do not generally start from $|0\rangle$. When each *Feenberg D* is expanded, the whole series is finally written in terms of continued fractions. We can hope to simplify matters only if there is a simple relationship between the 'floors'. We said above that it is possible to classify the loops as *arches* or *zigzags*. All of the terms may be further classified as *dominant* or *dominated*. We describe as dominant the graphs that during their evolution never switch off a boson belonging the initial state; the others are dominated. Two dominant graphs having different initial states but visiting the same number of intermediate states give simply related mathematical contributions; indeed, they can be obtained from each other by a shift due to the different energies of the bosons of the rising states. Let us explain this property by an example. The following two dominant loops arise from different initial states and visit one intermediate state:

(i) $|0\rangle \to |\omega_q\rangle \to |0\rangle \Rightarrow G_0(\omega)G_0(\omega-\omega_q)$

(ii) $|\omega_1,\omega_2,\ldots,\omega_N\rangle \to |\omega_1,\omega_2,\ldots,\omega_N,\omega_q\rangle \to |\omega_1,\omega_2,\ldots,\omega_N\rangle$
$\Rightarrow G_0(\omega-\omega_1-\omega_2-\cdots-\omega_N)G_0(\omega-\omega_1-\omega_2-\cdots-\omega_N-\omega_q).$

We can see that (i) and (ii) differ by a shift.

On the other hand, dominated graphs depend strongly on the initial states and hence their mathematical contributions are not simply related. Consider the following dominated loop visiting one intermediate state:

$$|\omega_1, \omega_2, \ldots, \omega_N\rangle \to |\omega_2, \omega_3, \ldots, \omega_N\rangle \to |\omega_1, \omega_2, \ldots, \omega_N\rangle$$
$$\Rightarrow G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N) G_0(\omega - \omega_2 - \omega_3 - \cdots - \omega_N).$$

It is clear that it is not simply related to any loop rising from the $|0\rangle$ state, and the dominated loops are much more difficult to deal with than the dominant ones.

Fortunately, only the dominant graphs remain in the continuum limit. To understand that we recall the self-energy rules. We have to include a $g_{\boldsymbol{q}}^2$-factor for each boson which is switched on in the irreducible process. Since we want to work with a finite total coupling, that is $\sum_q g_q^2 < \infty$, this fact implies that $g_{\boldsymbol{q}}^2$ becomes infinitesimal in the continuum limit, $g_{\boldsymbol{q}}^2 \to g(\boldsymbol{q})^2\ \mathrm{d}\boldsymbol{q}$. We get a finite contribution only if $\boldsymbol{q}$ is summed over. The last of the self-energy rules prescribes that one has to sum over all of the intermediate states of graphs. This sum involves integration over all of the modes that are turned on in intermediate states, but do not belong to the initial state. This is best seen by an example. Consider a dominant and a dominated loop that both visit one intermediate state. The dominant loop

$$|\omega_1, \omega_2, \cdots, \omega_n\rangle \to |\omega_1, \omega_2, \cdots, \omega_n, \omega_q\rangle \to |\omega_1, \omega_2, \cdots, \omega_n\rangle$$

yields the finite contribution

$$\sum_q g_q^2 G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N) G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N - \omega_q)$$
$$\underset{N\to\infty}{\longrightarrow} \int \mathrm{d}q\ g^2(q) G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N)$$
$$\times\ G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N - \omega_q)$$

while the dominated loop

$$|\omega_1, \omega_2, \omega_3, \cdots, \omega_n\rangle \to |\omega_2, \omega_3, \cdots, \omega_n\rangle \to |\omega_1, \omega_2, \omega_3, \cdots, \omega_n\rangle$$

yields

$$g_{q_1}^2 G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N) G_0(\omega - \omega_2 - \cdots - \omega_N)$$
$$\underset{N\to\infty}{\longrightarrow} \mathrm{d}q_1\ g^2(q_1) G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N)$$
$$\times\ G_0(\omega - \omega_1 - \omega_2 - \cdots - \omega_N - \omega_q)$$

and vanishes for $N \to \infty$. This happens with all dominated loops and so in the continuum limit their contributions become infinitesimal. Thus, in the continuum limit,

$$D^0_{\omega_j} = 1 - \sum_p g_p^2 \frac{G_0(\omega - \omega_j) G_0(\omega - \omega_j - \omega_p)}{D^{0,\omega_j}_{\omega_j + \omega_p}} - \cdots. \tag{17}$$

This D is composed of the same loops as D_0 with the difference that the initial states are shifted by ω_j. Therefore, $D^0_{\omega_j} = D_0(\omega - \omega_j)$. In general, every D with only one low index is equal to D_0 shifted of the energy represented by that index. Using a known property of the Feenberg D, we obtain

$$D^0_{\omega_j, \omega_j + \omega_k, \omega_k} = D^0_{\omega_j} D^{0,\omega_j}_{\omega_j + \omega_k} D^{0,\omega_j, \omega_j + \omega_k}_{\omega_k} \to D_0(\omega - \omega_j) D_0(\omega - \omega_j - \omega_k) D_0(\omega - \omega_k) \tag{18}$$

and Σ becomes

$$\Sigma(\omega) = \sum_{q_j}^{*} g_{q_j}^2 \frac{G_0(\omega - \omega_{q_j})}{D_0(\omega - \omega_{q_j})} + \sum_{q_j q_k}^{*} g_{q_j}^2 g_{q_k}^2 \frac{G_0(\omega - \omega_{q_j}) G_0(\omega - \omega_{q_j} - \omega_{q_k}) G_0(\omega - \omega_{q_k})}{D_0(\omega - \omega_{q_j}) D_0(\omega - \omega_{q_j} - \omega_{q_k}) D_0(\omega - \omega_{q_k})} + \cdots . \tag{19}$$

Finally, using

$$\frac{G_0(\omega)}{D_0(\omega)} = G(\omega)$$

we find

$$\Sigma(\omega) = \sum_{q_j}^{*} g_{q_j}^2 G(\omega - \omega_{q_j}) + \sum_{q_j q_k}^{*} g_{q_j}^2 g_{q_k}^2 G(\omega - \omega_{q_j}) G(\omega - \omega_{q_j} - \omega_{q_k}) G(\omega - \omega_{q_k}) + \cdots . \tag{20}$$

The effect of the D-denominators is just to dress the Green function.

In the continuum limit the rules for building the self-energy reduce to the following simplified set.

(1) For each intermediate state, include a dressed propagator

$$G\left(\omega - \sum_j l_j \omega_j\right)$$

where l_j is the occupation of the boson j in the intermediate state; l_j is allowed to be 0 or 1.

(2) Include a factor g_q^2 for every switched-on boson mode with energy ω_q.

(3) Sum over all of the indices of the bosons of the intermediate states not belonging to the initial one.

For example, including all processes that visit up to five intermediate states, we get

$$\begin{aligned}\Sigma(\omega) = {} & \sum_{q_j}^{*} g_{q_j}^2 G(\omega - \omega_{q_j}) + \sum_{q_j, q_k}^{*} g_{q_j}^2 g_{q_k}^2 G(\omega - \omega_{q_j}) G(\omega - \omega_{q_j} - \omega_{q_k}) G(\omega - \omega_{q_k}) \\ & + \sum_{q_j, q_k, q_l}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 G(\omega - \omega_{q_j}) G(\omega - \omega_{q_j} - \omega_{q_k}) G(\omega - \omega_{q_j} - \omega_{q_k} - \omega_{q_l}) \\ & \times [G(\omega - \omega_{q_l} - \omega_{q_k}) G(\omega - \omega_{q_l}) + G(\omega - \omega_{q_k} - \omega_{q_l}) G(\omega - \omega_{q_k}) \\ & + G(\omega - \omega_{q_j} - \omega_{q_l}) G(\omega - \omega_{q_l})] + \sum_{q_j, q_k, q_l}^{*} g_{q_j}^2 g_{q_k}^2 g_{q_l}^2 G(\omega - \omega_{q_j}) \\ & \times G(\omega - \omega_{q_j} - \omega_{q_k}) G(\omega - \omega_{q_k}) G(\omega - \omega_{q_k} - \omega_{q_l}) G(\omega - \omega_{q_l})\end{aligned} \tag{21}$$

The expansion can be carried out in principle to any desired order and used for a self-consistent solution together with Dyson's equation. It is clear that it is much simpler and more powerful than that of the previous section: we got rid of the f-factors and are expressing Σ in terms of the fully dressed G, rather than G_0.

Equation (21) can also be obtained by more standard diagrammatic methods. The first term corresponds to the second-order skeleton diagram; the second is the single overlapping fourth-order diagram and the rest corresponds to the three types of overlapping skeleton diagram which occur in order six. Thus, if the bosons form one continuum the present recursion method turns out to be equivalent to self-consistent perturbation theory [10],

although it has clear advantages if sharp boson modes are also present. We have checked by direct analytical calculation that the results (21) reproduce the first five denominators of equation (7) in the appropriate limit (that is, when the continuum is shrunk to a single frequency ω_0); in that case, however, the continued-fraction expression is much more convenient. Moreover, recursion methods tend to be particularly suitable for numerical implementation in complex situations where the problem must be handled approximately.

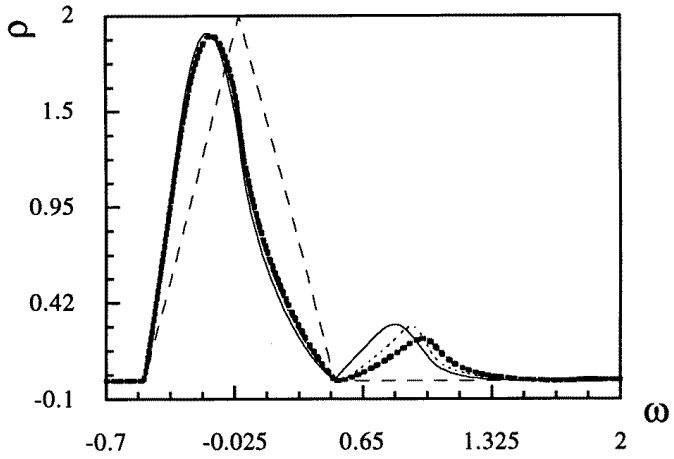

Figure 2. The effects of the boson dispersion for $\omega_p = 2a$ and $b = 0.1$. Dashed curve: the non-interacting density of states ρ^0 for the triangular band. The other curves yield the interacting ρ. Solid curve: the dispersionless limit of equation (3); light-dotted curve: $\Delta\omega = \omega_p/8$; heavy-dotted curve: $\Delta\omega = \omega_p/4$; the energies are in units of the band width $2a$.

4. Numerical results

We performed many numerical calculations in order to get preliminary physical insight, and allow for further tests of the above analysis. In particular, we have used the calculated spectra to check the first moments arising from our theory against exact moments [11]; also, all of our codes have been routinely checked in the narrow-band limit by comparison with Langreth's solution [1]. For illustration, we consider the triangular-shaped electronic band $\rho^{(0)}(\omega) = (-1/\pi)\mathrm{Im}\, G_0(\omega)$ arising from

$$G_0(\omega) = a^{-1}\tan^{-1}\left(\frac{2a}{p}\right) - \frac{p}{4a^2}\ln\left(\frac{p^2+4a^2}{p^2}\right) \tag{22}$$

where a is the half-width and $p = 0^+ - \mathrm{i}\omega$. As an example, we studied the interaction with a boson continuum $\omega \in (\omega_p, \omega_p + \Delta\omega)$ arising from a linear dispersion law

$$\omega(q) = \omega_p + \Delta\omega\,\frac{q}{q_{\max}} \tag{23}$$

which could mimic e.g. a surface plasmon field, with cut-off wave vector $q_{\max}$. In our test calculations, the electron–boson coupling is taken in the form

$$g_q^2 = b\frac{\omega_p^2}{q_{\max}} \tag{24}$$

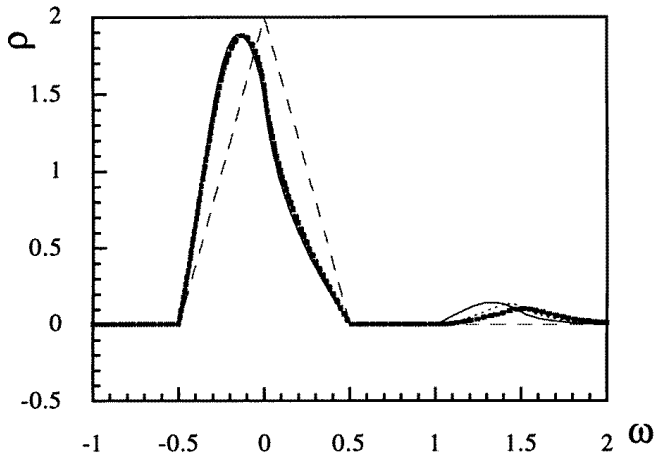

Figure 3. The effects of the boson dispersion for $\omega_p = 3a$ and $b = 0.06$. Dashed curve: the non-interacting density of states ρ^0 for the triangular band. The other curves yield the interacting ρ. Solid curve: the dispersionless limit of equation (3); light-dotted curve: $\Delta\omega = \omega_p/8$; heavy-dotted curve: $\Delta\omega = \omega_p/4$; the energies are in units of the band width $2a$.

where b is a constant parameter, and energies are measured in units of the band width $2a$. Figure 2 shows the results for the non-interacting $\rho^{(0)}(\omega)$ (dashed curve) and for the interacting $\rho(\omega)$ for $\omega_p = 1, b = 0.1$, and three different values for the dispersion width $\Delta\omega$. In all cases the interaction produces a renormalization and narrowing of the main peak, and the rise of satellites. The modification of the main line from the triangular shape is caused by the potential due to the bosons that dynamically screen the electron when it sits at site a: the renormalized site is more attractive for the electron, and this causes a narrowing. The line shape of the main peak weakly depends on $\Delta\omega$; the satellite shape is much more sensitive to the width of the boson continuum. In the dispersionless limit of equation (3) ($\Delta\omega \to 0$) the first satellite looks very much like a reduced copy of the main peak; with increasing boson dispersion in energy, it gets increasingly broadened, since there is uncertainty about the energy of the boson wave packet involved. This trend is confirmed by the data of figure 3, that refer to a somewhat smaller b and a larger ω_p. Comparing the two cases we notice that the influence of $\Delta\omega$ on the shape of the satellite is somewhat more marked in figure 2. This may be easily interpreted. In figure 3 the boson modes are fast compared with the electronic degrees of freedom, while in figure 2, where $\omega_0 = 2a$, there is more competition between screening and band motion, and the fact that some modes are faster than others has a marked influence on the dynamics.

5. Conclusions

The outcome of the present method is a viable algorithm for computing exact solutions to problems involving an electronic continuum interacting with a boson one. The possibility of dealing with boson dispersion in frequency removes an important shortcoming of the method of excitation amplitudes and widens its scope in the various fields to which it has been applied to date. Various applications to electron spectroscopies and non-linear optics may be anticipated. The method of excitation amplitudes has already been applied successfully

to finite temperatures [4, 12, 13], and a similar extension of the present treatment is clearly feasible: one has to apply Feenberg's method to the solution of the finite-temperature recurrence relations.

The fact that only fully dressed propagators occur in our expressions ensures a much faster convergence than is possible otherwise. The explicit expression (21) for the self-energy truncated to five intermediate states should already be adequate for many applications, although we can continue the expansion when this is needed.

The above test calculations show that the effect of boson dispersion broadens and lowers the satellites, leaving the principal peak almost unaltered. The effects of dispersion are particularly important when the onset of the continuum is at low energies.

Appendix 1. The Feenberg method

Selecting an arbitrary integer $i \in (1, M)$, $\det(\mathbf{A})$ is given by the Laplace expansion

$$A = \sum_j (-1)^{i+j} a_{ij} A^{ij} \tag{A1}$$

where A^{ij} is the determinant obtained by removing the ith row and the jth column from A. With the definitions surrounding equation (9) in the text, it is not difficult to prove the less well known, but equivalent Feenberg expansion

$$A = a_{ii}A_i - \sum_j{}^* a_{ij}a_{ji}A_{ij} + \sum_{ij}{}^* a_{ij}a_{jk}a_{ki}A_{ijk} - \sum_{ijkl}{}^* a_{ij}a_{jk}a_{kl}a_{li}A_{ijkl} + \cdots. \tag{A2}$$

Like Laplace's, this is also a recursion formula, and the smaller determinants can be expanded in a similar way: for instance,

$$\begin{aligned} A_{uv} = a_{ii}A_{iuv} &- \sum_j{}^* a_{ij}a_{ji}A_{ijuv} + \sum_j{}^*\sum_k{}^* a_{ij}a_{jk}a_{ki}A_{ijkuv} \\ &- \sum_l{}^*\sum_k{}^*\sum_j{}^* a_{ij}a_{jk}a_{kl}a_{li}A_{ijkluv} + \cdots. \end{aligned} \tag{A3}$$

Comparing (A1) and (A2), one finds

$$A^{ij} = -(-1)^{i+j}\left[a_{ji}A_{ij} - \sum_k{}^* a_{jk}a_{ki}A_{ijk} + \sum_l{}^*\sum_k{}^* a_{jk}a_{kl}a_{li}A_{ijkl} - \cdots\right]. \tag{A4}$$

Thus we can insert the above results into the solution of any well-posed linear system $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$, which is given by Cramer's formula

$$x_i = \sum_j^N (-1)^{i+j} b_j \frac{A^{ji}}{A}. \tag{A5}$$

The algorithm can be cast in a convenient continued-fraction form, by defining the Feenberg D-ratios:

$$D_i = \frac{A}{A_i} \qquad D_{ij} = \frac{A}{A_{ij}} \qquad D^i_j = \frac{A_i}{A_{ij}} \qquad D^i_{jk} = \frac{A_i}{A_{ijk}} \qquad D^{il}_{jk} = \frac{A_{il}}{A_{ijkl}}$$

and the like, whereby (A5) becomes equation (9). The Feenberg D-ratios can be expanded. From (A2) one obtains

$$D_i = \frac{A}{A_i} = a_{ii} - \sum_j{}^* \frac{a_{ij}a_{ji}A_{ij}}{A_i} + \sum_j{}^*\sum_k{}^* a_{ij}a_{jk}a_{ki}\frac{A_{ijk}}{A_i}$$

$$-\sum_{l}^{*}\sum_{k}^{*}\sum_{j}^{*} a_{ij}a_{jk}a_{kl}a_{li}\frac{A_{ijkl}}{A_i}+\cdots$$
$$=a_{ii}-\sum_{j}^{*}\frac{a_{ij}a_{ji}}{D_j^i}+\sum_{j}^{*}\sum_{k}^{*}\frac{a_{ij}a_{jk}a_{ki}}{D_{jk}^i}-\sum_{l}^{*}\sum_{k}^{*}\sum_{j}^{*}\frac{a_{ij}a_{jk}a_{kl}a_{li}}{D_{jkl}^i}+\cdots.$$

D-denominators with several low indices can be expressed in terms of those with one; for instance (equation (18) is another example of that)

$$D_{ij}=\frac{A}{A_{ij}}=\frac{A}{A_i}\frac{A_i}{A_{ij}}=D_iD_j^i=D_jD_i^j.$$

High indices just reduce the sizes of the determinants, and in view of (A3) we can write

$$D_i^{uv}=a_{ii}-\sum_{j}^{*}\frac{a_{ij}a_{ji}}{D_j^{uvi}}+\sum_{j}^{*}\sum_{k}^{*}\frac{a_{ij}a_{jk}a_{ki}}{D_{jk}^{uvi}}-\sum_{l}^{*}\sum_{k}^{*}\sum_{j}^{*}\frac{a_{ij}a_{jk}a_{kl}a_{li}}{D_{jkl}^{uvi}}+\cdots. \tag{A6}$$

Each term in these restricted summations $\sum^*$ can be thought of as an 'irreducible process' taking us from i to several intermediate 'states' $j,k,\ldots$, and back to i. The 'states' must be different from each other and from any other index appearing in the summand. Thus, the rules for writing down the contribution from each irreducible process to a given D can be read off from equation (A6).

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[10] See e.g.
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