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Improved calculation of the electron self-energy due to electron–phonon coupling in solids

A Fortini

Laboratoire de Physique du Solide, ESPCI 10, rue Vauquelin, F-75231, Paris Cedex 05, France

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Abstract. An improved method for solving time-dependent problems in quantum mechanics, in the customary cases of constant or harmonic perturbation, is applied to the calculation of the self-energy of electrons interacting with phonons in solids. The mixing of unperturbed Bloch states, resulting from the actual coupling, is self-consistently taken into account, and the related quantum probability amplitudes are determined through direct integration over the quasiparticle spectrum. Laplace transform and elementary mathematics are used, thereby enhancing the physical transparency, and bringing out approximations in every stage. Explicit illustrative results are worked out in the simple case of slowly varying self-energy parameters. The method is critically compared with the standard Green function approach, and further encourages more detailed applications.

1. Introduction

The calculation of self-energies is the key element in a number of interacting particle many-body problems, particularly in condensed matter. As a typical example, the electron self-energy due to electron–phonon coupling in solids has been of considerable importance, because of its major role in the theoretical interpretation of superconductivity, enhanced in recent years by the advent of high-temperature superconductivity. Determinant features of this interaction were initially pointed out by Frölich in a pioneering work [1], followed by Bardeen and Pines [2]. These early treatments were of a rather static nature, and the dynamical aspects of the coupling were more explicitly introduced later, in particular by Migdal [3], Gorkov [4] and Eliashberg [5]. Today, most existing works in that field, and also in other many-body problems, rely on Green function techniques.

However, the physics underlying Green function methods and inherent unavoidable approximations are somewhat concealed by formal mathematical procedures implemented therein. The purpose of this paper is to propose an alternative method to address situations of the type mentioned above, in which each stage in the progress from the Schrödinger equation to the inquired answers, can be well monitored. This will be based mainly on the use of the Laplace transform, in conjunction with an improved method to solve the time-dependent Schrödinger equation, in the customary cases of constant or harmonic perturbations [6], ensuring norm conservation at any time and any order of the coupling strength, and including at once the Dyson equation of self-energy.

The Laplace transform offers several advantages well suited to physical applications. For example, it permits us to deal with evolution processes starting properly from $t = 0$, and to extract conveniently long-term behaviours, while convergence requirements are very wide (the integrand must not increase faster than the exponential). Appropriate functions

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are naturally introduced without the need of analytic continuation, or the insertion of small imaginary parts to ensure mathematical convergence. The consideration of evolution in negative times [7] is avoided, as well as the introduction of the Matsubara periodic function in the calculation of statistical averages [8].

The major results of the method will be briefly recalled in section 2, with some suitable adaptation. They will be applied in section 3 to the electron–phonon interaction in metals, with some emphasis on the Frölich coupling. The main step will be the calculation of the evolution operator including the self-energy, on the unperturbed state basis, taking into account in a self-consistent way the mixing of states due to the coupling, and the related spreading of the Fermi distribution. Some simplifying assumptions will be adopted so as to enlighten methodological aspects, for example the salient features in the description of the interactions in terms of quasiparticles. Section 4 will be devoted to a summary and a brief discussion of the results, compared with the standard Green function approach.

2. The determinantal solution of the evolution operator

Let H_0 denote an unperturbed Hamiltonian, with eigenstates $b, c, \ldots$ and related eigenvalues $E_b, E_c, \ldots$. Energies will be expressed in frequency units throughout. First we assume a constant perturbation V, applied from $t = 0$. The evolution of the system is then described by the customary operator $U(t)$, satisfying the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}U(t)}{\mathrm{d}t} = [H_0 + VY(t)]U(t) \tag{1}$$

where $Y(t)$ is the Heaviside step function. We shall work with the Laplace transform of $U(t)$

$$U(\nu) = \int_0^\infty \mathrm{e}^{-\nu t}U(t)\,\mathrm{d}t$$

which satisfies the transformed equation,

$$\nu U(\nu) = U_0 - \mathrm{i}(H_0 + V)U(\nu) \tag{2}$$

with $U_0 = U(t = 0)$. Introducing the operator $d = \nu I + \mathrm{i}H_0$ (with I the identity operator) which is diagonal on the basis of the H_0 eigenstates, and the temporary notation $K = \mathrm{i}V$, the above equation can be rewritten more briefly,

$$(d + K)U(\nu) = U_0. \tag{3}$$

Regarding equation (3) as a linear system in the discretized Hilbert space, before passing to the thermodynamic limit, the matrix elements $U_b^c = \langle c|U|b\rangle$ between the starting state b and any c, $[U_b^c(t = 0) = \delta_b^c]$ are written in terms of the related determinant D and minors D_b^c of the matrix $I + d^{-1}K$,

$$U_b^c = D_b^c/d_b D. \tag{4}$$

As shown in [6] with the help of elementary properties of determinants, the natural solution which can be derived upon expansion of determinants in increasing powers of the kernel K, exhibits unphysical closed sequences of transitions which can be removed through division by the diagonal minor D_b^b relative to the starting state b,

$$U_b^c = D_b^c(D_b^b)^{-1}/d_b D(D_b^b)^{-1}. \tag{5}$$

The determinant quotients can then be given a more explicit operational expression, on defining the matrix $S_b = I + d^{-1}KQ_b$, where Q_b denotes the projector on the Hilbert space complementary to the state b (see appendix A)

$$U_b^b = \frac{1}{d_b(1 + \langle b|S_b^{-1}d^{-1}K|b\rangle)} \qquad U_b^c = -\frac{\langle c|S_b^{-1}d^{-1}K|b\rangle}{d_b(1+\rangle b|S_b^{-1}d^{-1}K|b\rangle)} \qquad (c \neq b). \tag{6}$$

As in the starting determinantal forms (4) or (5), these expressions are exact results. In particular, the unitarity of the solution is preserved at any time and with any order of the kernel K, providing the highest order kept in the upper and lower series, upon expansion of the S_b^{-1}'s are in accordance. These expansions which yield vortex corrections beyond the lowest order in K, are close to perturbation series, except for the exclusion of the initial b state from intermediate summations, as imposed by the Q_b's. Because of the same exclusion of the b states, only proper self-energy parts arise in the denominators of equations (6), in the form required by the Dyson theorem, i.e. after summing over all diagrams which can be split into several parts by cutting internal lines [7].

Apart from a factor i, the Laplace transform $U_b^b(\nu)$ is analogous to the Green function Fourier transform, the important properties of which are easily recovered. The poles of $U_b^b(\nu)$ which give rise to a quasistationary (damped) function of time, will provide the quasiparticle spectrum, while its real part will provide the related spectral density (see appendix B).

It may occur that the fractional forms (6) are not sufficient. The method can then be pushed one step further [6], leading for example to improved forms of the self-energy. Expressions of type (6) will thus be written in terms of determinant ratios, up to a desired form of the solution. Only in the final form, will the thermodynamic limit be re-established in the quasicontinuous parts of the spectrum.

Finally, the preceding results can be extended to the case of harmonic perturbation, in which $V(t)$ (still assumed to be applied at $t = 0$) is taken in the form

$$V(t) = g\exp(-\mathrm{i}\omega t) + g^+\exp(\mathrm{i}\omega t). \tag{7}$$

Equation (2) becomes

$$\nu U(\nu) = U_0 - \mathrm{i}[H_0U(\nu) + gU(\nu + \mathrm{i}\omega) + g^+U(\nu - \mathrm{i}\omega)] \tag{8}$$

which represents a set of recursion equations linking $U[\nu + \mathrm{i}(n-1)\omega]$, $U(\nu + \mathrm{i}n\omega)$ and $U[\nu+\mathrm{i}(n+1)\omega]$, where n is an integer. It is convenient to introduce the following notations for the matrix elements of d and U

$$d_{cn} = \langle c|d(\nu + \mathrm{i}n\omega)|c\rangle = \nu + \mathrm{i}(E_c + n\omega) \qquad U_b^{c(n)} = \langle c|U(\nu + \mathrm{i}n\omega)|b\rangle.$$

Fourier indices n can be included in the Hilbert space, besides normal quantum numbers $b, c, \ldots$ as investigated by Shirley [9]. This allows us to regard the $U_b^{c(n)}$'s as the cn components of the $U|b\rangle$ vector [6], and to rewrite the set of equations (8) as follows

$$d_{cn}U_b^{c(n)} + \mathrm{i}[g_k^cU_b^{k(n+1)} + g_k^{+c}U_b^{k(n-1)}] = \delta_b^c \tag{9}$$

with n assigned some fixed reference value in a given state. Now, the solutions (6) can easily be generalized by introducing the following matrix elements of the kernel in equation (9),

$$K_{c_1n_1}^{c_2n_2} = \mathrm{i}(g_{c_1}^{c_2}\delta_{n_1}^{n_2-1} + g_{c_1}^{+c_2}\delta_{n_1}^{n_2+1}).$$

For any starting value of n, we have

$$U_b^{b(n)} = \frac{1}{d_{bn}(1 + \langle bn|S_{bn}^{-1}d^{-1}K|bn\rangle)} \qquad U_b^{c(n')} = -\frac{\langle cn'|S_{bn}^{-1}d^{-1}K|bn\rangle}{d_{bn}(1 + \langle bn|S_{bn}^{-1}d^{-1}K|bn\rangle)} \tag{10}$$

with $S_{bn} = I + d^{-1}K\,Q_{bn}$, $c \neq b$ and (or) $n' \neq n$.

Hereafter, we shall be mainly interested in the departure from the unperturbed behaviour in equations (6) and (10), giving rise to off-diagonal elements and to the K contribution in the denominators (self-energy).

2.1. Thermodynamic average

We now turn to the calculation of the thermodynamic average of observables O

$$\langle O\rangle = Z^{-1}\,\mathrm{Tr}(\mathrm{e}^{-\beta H}O)$$

with $Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H}$ and $\beta = 1/k_BT$. As harmonic perturbation only gives rise to translations by ω in the Laplace space, it will be sufficient to consider the case of constant perturbation.

Let us gain some insight into the self-consistent determination of the long-term steady state of the whole system. The initial many-body eigenstates $|B\rangle$ of energy E_B, assumed to be close to the most probable ones from both a quantum and statistical point of view, are submitted to the evolution $U(t)$ defined by the Schrödinger equation, and consisting of internal transitions between basis states. The initial definition of the $|B\rangle$'s is then self-consistently refined so as to retrieve the same starting $|B\rangle$'s at any time. On the other hand, provided H_0 denotes the total unperturbed Hamiltonian including both interacting subsystems, after the time-independent potential V has been applied, the solution of the Schrödinger equation can also be formally written as $U(t) = \mathrm{e}^{-\mathrm{i}Ht}[H = H_0 + V]$. Then in a sufficiently accurate theoretical description one should necessarily find, at least approximately, that diagonal elements are recovered, i.e.

$$\mathrm{e}^{-\mathrm{i}Ht}|B\rangle = \mathrm{e}^{-\mathrm{i}E_Bt}|B\rangle.$$

The basic assumption of the quasiparticle concept, in the Fermi liquid theory, states that this is possible providing the quasiparticle lifetime is long enough. It follows that, on substituting β for the imaginary time $\mathrm{i}t$,

$$\mathrm{e}^{-\beta H}|B\rangle = \mathrm{e}^{-\beta E_B}|B\rangle.$$

Hence, the expression of the statistical average

$$\langle O\rangle = Z^{-1}\sum_B \langle B|O|B\rangle \mathrm{e}^{-\beta E_B}. \tag{11}$$

This can be written more explicitly if many-body interactions are described by means of independent quasiparticles. Then, in the occupation number representation, the E_B's are eigenvalues of some energy operator E in the form

$$E = \sum_k E_k c_k^+ c_k$$

and, as is well known, the statistical operator can be expressed in terms of individual statistics [10]. For fermions,

$$Z^{-1}\mathrm{e}^{-\beta E} = \prod_k [(1-f_k)c_kc_k^+ + f_kc_k^+c_k] \tag{12}$$

where $f_k \equiv f(E_k)$ is the Fermi function of individual energies E_k. In the case of bosons in states q of energy ω_q, we have, similarly,

$$Z^{-1}\mathrm{e}^{-\beta E} = \prod_q (1-\mathrm{e}^{-\beta\omega_q})\mathrm{e}^{-\beta\omega_q a_q^+ a_q}. \tag{13}$$

As physically expected, the quantum statistics of independent particles can be used for quasiparticles.

3. Electron self-energy in coupling with phonons

In order to realize at best the efficiency of the determinantal method, we now proceed to apply the general solutions (10) to a specific problem of major interest, such as the electron–phonon coupling which has been extensively studied until now [11–17]. In particular we aim to see how the method may help in calculating the related electron self-energy. Since the interest is mainly focused on the efficiency of the method, irrelevant details will be ignored. Thus, it will be sufficient to restrict ourselves to one electronic band, without specifying band and spin indices, and one-phonon branch in a lattice of N cells, with one atom (of mass M) per cell. The coupling potential between an electron in the basis of Bloch states $\boldsymbol{k}$ of energy $\varepsilon_{\boldsymbol{k}}$, and the phonon of wavevector $\boldsymbol{q}$, frequency $\omega_{\boldsymbol{q}}$, and polarization $\sigma_{\boldsymbol{q}}$, will be taken in the usual form

$$V_{\boldsymbol{k}} = \sum_{\boldsymbol{q}} (g_{\boldsymbol{k}}^{\boldsymbol{k}+\boldsymbol{q}} \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}} t} a_{\boldsymbol{q}} c_{\boldsymbol{k}+\boldsymbol{q}}^{+} c_{\boldsymbol{k}} + g_{\boldsymbol{k}}^{\boldsymbol{k}-\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\omega_{\boldsymbol{q}} t} a_{\boldsymbol{q}}^{+} c_{\boldsymbol{k}-\boldsymbol{q}}^{+} C_{\boldsymbol{k}}) \tag{14}$$

with

$$g_{\boldsymbol{k}}^{\boldsymbol{k}\pm\boldsymbol{q}} = -N^{\frac{1}{2}} \alpha_{\boldsymbol{q}} \sigma_{\boldsymbol{q}} \langle \boldsymbol{k} \pm \boldsymbol{q} | \nabla_{\boldsymbol{r}} v(\boldsymbol{r}) | \boldsymbol{k} \rangle \qquad \alpha_{\boldsymbol{q}} = (\hbar / 2M\omega_{\boldsymbol{q}})^{\frac{1}{2}}.$$

$c_{\boldsymbol{k}}, c_{\boldsymbol{k}}^{+}$ and $a_{\boldsymbol{q}}, a_{\boldsymbol{q}}^{+}$ denote the customary annihilation and creation operators of electrons and phonons, respectively. $v(\boldsymbol{r} - \boldsymbol{R}_n)$ is the interaction potential between the electron at $\boldsymbol{r}$ and the ion at the lattice site $\boldsymbol{R}_n$.

We first note that because of the mixing between Bloch states owing to the interaction, the step-like shape of the Fermi function is spread about the Fermi level, thus allowing for transitions in both directions between $\boldsymbol{k}$ and $\boldsymbol{k}'$, even at $T = 0$ K. Thus we have to start with an N-body wavefunction incorporating this important physical feature and to proceed self-consistently. In the occupation number representation, collective Bloch states are of the type

$$|b\rangle = |1_{\boldsymbol{k}_1}, 0_{\boldsymbol{k}_2}, 1_{\boldsymbol{k}_3}, \ldots 1_{\boldsymbol{k}_j}, \ldots 0_{\boldsymbol{k}_l}, \ldots\rangle \tag{15}$$

where 0 and 1 represent unoccupied and occupied states, respectively. The simplest proper wavefunction of the dressed electrons, allowing for intermediate occupations of any $\boldsymbol{k}$, will be obtained by taking the most general combination

$$|\psi_B\rangle = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c_{\boldsymbol{k}}^{+}) |0\rangle. \tag{16}$$

$|0\rangle$ is the vacuum state, $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ the probability amplitudes for the $\boldsymbol{k}$ state to be either empty or occupied, respectively. The number of particles is left undetermined, in accordance with a grand canonical distribution which we shall adopt. Actually, electrons involved in the interaction with phonons are concentrated in a thin shell of the $\boldsymbol{k}$-space near the Fermi surface, and represent a rather small fraction of the total number. All other electrons are 'frozen' by the exclusion principle, and behave like a reservoir imposing their chemical potential to the interacting ones. It follows that the energy needed to add up a carrier at the Fermi level in the interacting system is just zero, so that the carrier energies must be referred to the Fermi level, which, as usual, will be taken for the energy origin. In fact, the basic state defined in equation (16) is thought to a dynamical steady state sustained by the interactions, in so far as the quasiparticle damping is not too strong. The occupation numbers $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ must satisfy the normalization condition

$$|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1 \tag{17}$$

which ensures, in turn, the normalization of $|\psi_B\rangle$. They can be taken with the same phase, without loss of generality, and are to be determined self-consistently. When the

contribution of particular components, $\boldsymbol{k}, \boldsymbol{k}', \ldots$ is under consideration, the definition (16) will be rewritten for convenience, in the following appropriate form

$$|\psi_B\rangle = (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^+_{\boldsymbol{k}})(u_{\boldsymbol{k}'} + v_{\boldsymbol{k}'} c^+_{\boldsymbol{k}'})|\psi_{0\boldsymbol{k},0\boldsymbol{k}'}\rangle.$$

In $\psi_{0\boldsymbol{k},0\boldsymbol{k}'}$ $\boldsymbol{k}$ and $\boldsymbol{k}'$ are certainly empty, i.e.

$$|\psi_{0\boldsymbol{k},0\boldsymbol{k}'}\rangle = \prod_{\boldsymbol{k}'' \neq \boldsymbol{k},\boldsymbol{k}'} (u_{\boldsymbol{k}''} + v_{\boldsymbol{k}''} c^+_{\boldsymbol{k}''})|0\rangle.$$

The evolution rate of the state ψ_B resulting from the electron–phonon coupling can now be worked out, using equations (10). For simplicity, we shall restrict ourselves to the lowest order of the coupling matrix $g^{\boldsymbol{k}\pm\boldsymbol{q}}_{\boldsymbol{k}}$, involving one-phonon processes only, and to low enough temperature where phonon absorption can be ignored. Since the n indices refer to the *variation* of the phonon number, one can take $n = 0$ in the basic state, specified by $B0$. The general solution (10) then becomes, to second order of the kernel K,

$$\begin{aligned} U^{B(0)}_B &= \frac{1}{d_{B0} - \langle\psi_{B0}|K\,Q_{B0}d^{-1}K|\psi_{B0}\rangle} \\ U^{C(n)}_B &= -\frac{\langle\psi_{Cn}|K|\psi_{B0}\rangle}{d_{Cn}[d_{B0} - \langle\psi_{B0}|K\,Q_{B0}d^{-1}K|\psi_{B0}\rangle]}. \end{aligned} \tag{18}$$

First we have

$$d_{B0} = \langle\psi_{B0}|(\nu + \mathrm{i}H_0)|\psi_{B0}\rangle = \nu + \mathrm{i}\sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}}. \tag{19}$$

Then, substituting $K = \mathrm{i}\sum_{\boldsymbol{k},\boldsymbol{k}'} g^{\boldsymbol{k}'}_{\boldsymbol{k}} a^+_{\boldsymbol{k}-\boldsymbol{k}'} c^+_{\boldsymbol{k}'} c_{\boldsymbol{k}}$, restricted to the emission of a phonon in the state of momentum $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$, we have to calculate

$$d^{-1}K|\psi_{B0}\rangle = \mathrm{i}\sum_{\boldsymbol{k},\boldsymbol{k}'} d^{-1} g^{\boldsymbol{k}'}_{\boldsymbol{k}} a^+_{\boldsymbol{k}-\boldsymbol{k}'} c^+_{\boldsymbol{k}'} c_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^+_{\boldsymbol{k}})(u_{\boldsymbol{k}'} + v_{\boldsymbol{k}'} c^+_{\boldsymbol{k}'})|\psi_{0\boldsymbol{k},0\boldsymbol{k}'}, 0_{\boldsymbol{q}}\rangle.$$

$0_{\boldsymbol{q}}$ means that $n = 0$ in the mode $\boldsymbol{q}$. Obviously, the action of $c^+_{\boldsymbol{k}'} c_{\boldsymbol{k}}$ on collective electron states of the type (15) in ψ_{B0}, can only proceed according to the scheme

$$(\ldots 0_{\boldsymbol{k}'}, \ldots 1_{\boldsymbol{k}}, \ldots) \to (\ldots 1_{\boldsymbol{k}'}, \ldots 0_{\boldsymbol{k}}, \ldots)$$

with the probability amplitude $u_{\boldsymbol{k}'} v_{\boldsymbol{k}}$. The resultant eigenvalues of d^{-1} are all distinct from each other but they can be averaged without significant error, since the overall energy distribution is sharply peaked on its mean value $\varepsilon_B = \sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}}$ (equation (19)). In the initial state, d^{-1} is thus averaged into $(\nu + \mathrm{i}\varepsilon_B)^{-1}$, and since in the above $\boldsymbol{k} \to \boldsymbol{k}'$ transition the energy is necessarily increased by $\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}}$, the averaged value of d^{-1} becomes $[\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{k}-\boldsymbol{k}'})]^{-1}$ in the final state. A detailed proof is given in appendix C. The situation being relatively similar for the $\boldsymbol{k}' \to \boldsymbol{k}$ transitions, one obtains

$$d^{-1}K|\psi_{B0}\rangle = \mathrm{i}\sum_{\boldsymbol{k}'\boldsymbol{k}} \frac{u_{\boldsymbol{k}'} v_{\boldsymbol{k}} g^{\boldsymbol{k}'}_{\boldsymbol{k}}}{\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{k}-\boldsymbol{k}'})} |\psi_{0\boldsymbol{k},1\boldsymbol{k}'}, 1_{\boldsymbol{k}-\boldsymbol{k}'}\rangle. \tag{20}$$

Owing to the presence of the emitted phonon, the undressed intermediate states are orthogonal to ψ_{B0} as required. It is now possible to write out the self-energy to second order

$$\begin{aligned} \mathrm{i}\Sigma_{B0} &= d_{B0}\langle\psi_{B0}|(I + d^{-1}K\,Q_{B0})^{-1}d^{-1}K|\psi_{B0}\rangle = -\langle\psi_{B0}|K\,Q_{B0}d^{-1}K|\psi_{B0}\rangle + \cdots \\ &= \sum_{\boldsymbol{k}',\boldsymbol{k}} |g^{\boldsymbol{k}'}_{\boldsymbol{k}}|^2 \frac{|u_{\boldsymbol{k}'}|^2 |v_{\boldsymbol{k}}|^2}{\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{k}-\boldsymbol{k}'})}. \end{aligned} \tag{21}$$

3.1. Single-particle self-energy

Heretofore the results refer to the overall system, and we now proceed to seek how they could be derived equivalently in a one-particle scheme, in the spirit of a mean-field approximation. In the case of independent particles, the poles of the Laplace transform $U(\nu)$ reduce to a sum over individual energies. Therefore, an equivalent one-body description can only be derived from a recast of the energy arising in the many-body denominators into a sum of identical $\boldsymbol{k}$ contributions. Of course, the procedure is only approximate because, conversely, the convolution of the resulting one-body Laplace transforms does not necessarily restore rigorously the initial many-body form.

The required form of the denominators in equations (18) will be obtained by substituting $|u_{\boldsymbol{k}'}|^2 = 1 - |\nu_{\boldsymbol{k}'}|^2$, and collecting terms in $|\nu_{\boldsymbol{k}}|^2, |\nu_{\boldsymbol{k}'}|^2, \ldots$ in expression (21) of the self-energy, which gives

$$d_{B0} + \mathrm{i}\Sigma_{B0} = \nu + \mathrm{i}\sum_{\boldsymbol{k}} |\nu_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} |\nu_k|^2 \sum_{\boldsymbol{k}'} |g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2 \times \left[\frac{1}{\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{k}-\boldsymbol{k}'})} - |\nu_{\boldsymbol{k}'}|^2 \frac{\nu + \mathrm{i}(\varepsilon_B + \omega_{\boldsymbol{k}-\boldsymbol{k}'})}{[\nu + \mathrm{i}(\varepsilon_B + \omega_{\boldsymbol{k}-\boldsymbol{k}'})]^2 + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}}^2} \right]. \tag{22}$$

On account of the symmetry relationship of the phonon energies, $\omega_{\boldsymbol{k}-\boldsymbol{k}'} = \omega_{\boldsymbol{k}'-\boldsymbol{k}}$, the symmetric terms in $|\nu_{\boldsymbol{k}}|^2 |\nu_{\boldsymbol{k}'}|^2$ have been combined with each other. The first term in the rectangular bracket represents a simple correction to the unperturbed electron energy, and in the second one we recognize the Frölich coupling, which may give rise to an attractive interaction [1].

Separating out a single $\boldsymbol{k}$ contribution now reduces to a translation of ν by an amount equal to $(-\mathrm{i})$ time the total energy of all other particles, in states $\boldsymbol{k}' \neq \boldsymbol{k}$. In the denominators of the self-energy itself, $\mathrm{i}\Sigma_{B0}$, the total electron energy only involves its unperturbed part ε_B, which we split conveniently as $\varepsilon_B = \varepsilon_{B\boldsymbol{k}} + |\nu_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}}$. It follows that the same translation can accordingly be restricted to $\varepsilon_{B\boldsymbol{k}}$ therein. In fact, this customary approximation also lies in the natural limits of the treatment (corrections are omitted in corrective terms). As aforementioned, this could be improved by pushing the method one step further, in which the perturbation corrections would appear, in turn, in the self-energy denominators.

For notational simplicity, the unperturbed energy of the $\boldsymbol{k}$ state, $|\nu_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}}$, which will simply give rise to a factor $\exp(-\mathrm{i}|\nu_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}} t)$, in the original time-dependent functions, will also be temporarily included in the translation, and only written out when needed. Taking apart the occupation factor $|\nu_{\boldsymbol{k}}|^2$ (see below), the resulting single-particle self-energy $\Sigma_{\boldsymbol{k}}(\nu)$, such that $\Sigma_{B0} = \sum_{\boldsymbol{k}} \Sigma_{\boldsymbol{k}}(\nu)$, will then be given by

$$\Sigma_{\boldsymbol{k}}(\nu) = \Xi_{\boldsymbol{k}}(\nu) - \mathrm{i}\Gamma_{\boldsymbol{k}}(\nu) = -\mathrm{i}\sum_{\boldsymbol{k}'} |g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2 \left[\frac{1}{\nu + \mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})} - |\nu_{\boldsymbol{k}'}|^2 \frac{\nu + \mathrm{i}\omega_{\boldsymbol{q}}}{(\nu + \mathrm{i}\omega_{\boldsymbol{q}})^2 + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}}^2} \right]. \tag{23}$$

Strictly speaking, knowledge of the self-energy is sufficient to derive most physical quantities of interest, as the energy spectrum and the density of states of quasiparticles. However, it might be useful to introduce an *effective* single-particle interaction potential in the framework of the same formalism, and to appreciate the related approximations. Such a potential must lead to the same expression (23) of the self-energy, in a parallel one-particle treatment, still based on the general solution (10) for $U(\nu)$.

Let us consider, for definiteness, the $\boldsymbol{k} \to \boldsymbol{k}'$ transitions pertaining to phonon emission. We therefore factorize out the related one-particle energy denominator $\nu + \mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})$, in equation (23). The quasiparticle approximation, valid for times smaller than the quasiparticle

lifetime, allows us to take $t \sim 0$, i.e. $\nu \to \infty$, in the remaining factor. Thus we obtain the physically expected result

$$\Sigma_{\boldsymbol{k}}(\nu) = -\mathrm{i}\sum_{\boldsymbol{k}'} \frac{|g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2 |u_{\boldsymbol{k}'}|^2}{\nu + \mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})} \tag{24}$$

which clearly imposes the following effective potential

$$\mathcal{V}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} g_{\boldsymbol{k}}^{\boldsymbol{k}'} u_{\boldsymbol{k}'} a_{\boldsymbol{q}}^{+} c_{\boldsymbol{k}'}^{+} c_{\boldsymbol{k}}. \tag{25}$$

$\Sigma_{\boldsymbol{k}}(\nu)$ is just retrieved using $\mathcal{V}_{\boldsymbol{k}}$ in the single-particle general form

$$\Sigma_{\boldsymbol{k}}(\nu) = -\mathrm{i}\langle \boldsymbol{k}|\mathcal{V}_{\boldsymbol{k}} Q_{\boldsymbol{k}} d^{-1} \mathcal{V}_{\boldsymbol{k}}|\boldsymbol{k}\rangle$$

(the n indices are omitted), and the single-particle solutions (including the translation by $|\nu_{\boldsymbol{k}}|^2 \varepsilon_{\boldsymbol{k}}$) can be written, accordingly, as follows

$$U_{\boldsymbol{k}}^{\boldsymbol{k}}(\nu) = \frac{1}{\nu + \mathrm{i}|\nu_{\boldsymbol{k}}|^2 \Sigma_{\boldsymbol{k}}(\nu)} \qquad U_{\boldsymbol{k}}^{\boldsymbol{k}'}(\nu) = \frac{\mathrm{i} g_{\boldsymbol{k}}^{\boldsymbol{k}'} u_{\boldsymbol{k}'} \nu_{\boldsymbol{k}}}{[\nu + \mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})][\nu + \mathrm{i}|\nu_{\boldsymbol{k}}|^2 \Sigma_{\boldsymbol{k}}(\nu)]}. \tag{26}$$

Expressions (26) describe a typical sequence of events, occurring continuously in the dynamical evolution of the $\boldsymbol{k}$ components of the quasiparticle states, assumed to be initially occupied (to the fractional amount $|\nu_{\boldsymbol{k}}|^2$). The real part of $\mathrm{i}\Sigma_{\boldsymbol{k}}(\nu)$ in the denominators gives rise to the decay of the initial occupancy, described by the diagonal elements $U_{\boldsymbol{k}}^{\boldsymbol{k}}(\nu)$, in a few lifetimes. In the meantime, the denominator $\nu + \mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})$ in the off-diagonal elements $U_{\boldsymbol{k}}^{\boldsymbol{k}'}(\nu)$ will give rise to a steady-state in $\exp[-\mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})t]$, restoring the unperturbed states (see equations (29) and (30) below).

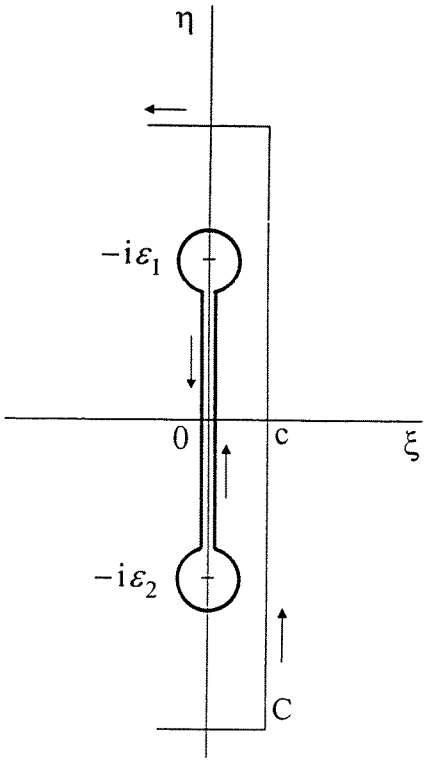

Figure 1. Contour in the complex plane of the Laplace variable $\nu(\xi, \eta)$, used in the calculation of the evolution operator. The cut is generated by the quasicontinuous set of poles along the η-axis, in the presence of coupling.

Before proceeding further, we have to make some additional remarks on expressions (26) and to give a more explicit form to the self-energy. Owing to the discretized summation over $\boldsymbol{k}'(=\boldsymbol{k}-\boldsymbol{q})$ in equations (23)–(24), the poles of the $U(\nu)$ components are roots of an equation of very high order. It can be shown [6] that they are, in addition, the product by $(-\mathrm{i})$ of the eigenvalues of a Hermitian operator, say H_0+V, and, therefore, purely imaginary quantities. Thus, collisions give rise to a quasicontinuous spectrum extending in the vicinity of the unperturbed roots $-\mathrm{i}\varepsilon_{\boldsymbol{k}}$, along the imaginary axis, in the complex plane of the Laplace variable $\nu(\xi,\eta)$. Their extension, schematically pictured by the segment $(-\mathrm{i}\varepsilon_2,-\mathrm{i}\varepsilon_1)$ (figure 1), depends on both the range of the collision potential and the $\omega_{\boldsymbol{q}}$ spectrum. In the quasicontinuum limit, this pole array tends towards a cut, outside which there is no pole in the complex plane. The integration along the cut requires the prior summation by $\boldsymbol{k}'$ (or $\boldsymbol{q}$) which is, therefore, to be evaluated for $\nu\to\pm 0+\mathrm{i}\eta$, so reducing to a Cauchy type of integration. From equation (23) we find

$$\Xi_{\boldsymbol{k}}(\eta)-\mathrm{i}\Gamma_{\boldsymbol{k}}(\eta)=\lim_{\xi\to\pm 0}\int_0^\infty |g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2 s(\omega_{\boldsymbol{q}})\left[-\frac{1}{\eta+\varepsilon_{\boldsymbol{k}'\boldsymbol{k}}+\omega_{\boldsymbol{q}}-\mathrm{i}\xi}\right.$$
$$\left.+\frac{1}{2}|\nu_{\boldsymbol{k}'}|^2\left(\frac{1}{\eta+\varepsilon_{\boldsymbol{k}'\boldsymbol{k}}+\omega_{\boldsymbol{q}}-\mathrm{i}\xi}+\frac{1}{\eta+\varepsilon_{\boldsymbol{k}\boldsymbol{k}'}+\omega_{\boldsymbol{q}}-\mathrm{i}\xi}\right)\right]\mathrm{d}\omega_{\boldsymbol{q}}.$$

$s(\omega_{\boldsymbol{q}})$ denotes the phonon density of states. Hence, in terms of the effective potential above defined (equations (24)–(25)),

$$\begin{aligned}\Xi_{\boldsymbol{k}}(\eta)&=-\int_0^\infty\frac{|g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2|u_{\boldsymbol{k}'}|^2 s(\omega_{\boldsymbol{q}})}{\eta+\varepsilon_{\boldsymbol{k}'\boldsymbol{k}}+\omega_{\boldsymbol{q}}}\,\mathrm{d}\omega_{\boldsymbol{q}}\\ \Gamma_{\boldsymbol{k}}(\eta)&=\frac{\pi}{2}\int_0^\infty|g_{\boldsymbol{k}}^{\boldsymbol{k}'}|^2|u_{\boldsymbol{k}'}|^2 s(\omega_{\boldsymbol{q}})\delta(\eta+\omega_{\boldsymbol{q}}+\varepsilon_{\boldsymbol{k}'\boldsymbol{k}})\,\mathrm{d}\omega_{\boldsymbol{q}}.\end{aligned}\tag{27}$$

The definition of $\Gamma_{\boldsymbol{k}}(\eta)$ is slightly changed into $\mathrm{sgn}(\xi)\Gamma_{\boldsymbol{k}}(\eta)$ so as to single out the change of sign with ξ. The integral in the first equation is to be taken in principal part. Equations (27) define the self-energy components as functions of the quasiparticle energy variable $-\eta$.

The original of the first equation (26) can now be written as follows

$$U_{\boldsymbol{k}}^{\boldsymbol{k}}(t)=\frac{\mathrm{e}^{-\mathrm{i}|\nu_{\boldsymbol{k}}|^2\varepsilon_{\boldsymbol{k}}t}}{2\pi\mathrm{i}}\int_{\mathrm{cut}}\frac{\mathrm{e}^{\mathrm{i}\eta\varepsilon_{\boldsymbol{k}}t}\mathrm{i}\,\mathrm{d}\eta}{\mathrm{i}[\eta+|\nu_{\boldsymbol{k}}|^2\Xi_{\boldsymbol{k}}(\eta)]+\mathrm{sgn}(\xi)|\nu_{\boldsymbol{k}}|^2\Gamma_{\boldsymbol{k}}(\eta)}.\tag{28}$$

The imaginary part of the poles in the integrand yields the quasiparticle spectrum. At the Fermi level, $\varepsilon_{\boldsymbol{k}}=\varepsilon_{\boldsymbol{k}F}=0$, we have $\eta_F=0$, and the damping function $\Gamma_{\boldsymbol{k}}(\eta)$ generally starts from zero because of phase space limitations, which validates the Fermi liquid scheme [7].

Further calculations require detailed knowledge of the electron and phonon spectra. A simple result is obtained if the self-energy components are slowly varying functions, averaged into constants, $\bar{\Xi}_{\boldsymbol{k}}$, $\bar{\Gamma}_{\boldsymbol{k}}$, in the relevant integration range. Only the right-hand edge of the cut gives a nonzero result

$$U_{\boldsymbol{k}}^{\boldsymbol{k}}(t)\cong\frac{\mathrm{e}^{-\mathrm{i}|\nu_{\boldsymbol{k}}|^2\varepsilon_{\boldsymbol{k}}t}}{2\pi\mathrm{i}}\int_{-\infty}^{+\infty}\frac{\mathrm{e}^{\mathrm{i}\eta t}\mathrm{i}\,\mathrm{d}\eta}{\mathrm{i}[\eta+|\nu_{\boldsymbol{k}}|^2\bar{\Xi}_{\boldsymbol{k}}]+|\nu_{\boldsymbol{k}}|^2\bar{\Gamma}_{\boldsymbol{k}}}=\exp[-\mathrm{i}|\nu_{\boldsymbol{k}}|^2(\varepsilon_{\boldsymbol{k}}+\bar{\Xi}_{\boldsymbol{k}}-\mathrm{i}\bar{\Gamma}_{\boldsymbol{k}})t].\tag{29}$$

A similar expression for the off-diagonal elements (26) can be directly derived from the preceding one, with the help of elementary rules,

$$U_{\boldsymbol{k}}^{\boldsymbol{k}'}(t)=\mathrm{i}g_{\boldsymbol{k}}^{\boldsymbol{k}'}u_{\boldsymbol{k}'}\nu_{\boldsymbol{k}}\mathrm{e}^{-\mathrm{i}|\nu_{\boldsymbol{k}}|^2\varepsilon_{\boldsymbol{k}}t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}}+\omega_{\boldsymbol{q}})t}\int_0^t\mathrm{e}^{\mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}}+\omega_{\boldsymbol{q}})t'}\mathrm{e}^{\mathrm{i}|\nu_{\boldsymbol{k}}|^2\varepsilon_{\boldsymbol{k}}t'}U_{\boldsymbol{k}}^{\boldsymbol{k}}(t')\,\mathrm{d}t'$$

$$= g_{\boldsymbol{k}}^{\boldsymbol{k}'} u_{\boldsymbol{k}'} v_{\boldsymbol{k}} \frac{\exp[-\mathrm{i}|v_{\boldsymbol{k}}|^2(\varepsilon_{\boldsymbol{k}} + \bar{\Xi}_{\boldsymbol{k}} - \mathrm{i}\bar{\Gamma}_{\boldsymbol{k}})t] - \exp[-\mathrm{i}(|v_{\boldsymbol{k}}|^2\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}})t]}{\mathrm{i}(\varepsilon_{\boldsymbol{k}'\boldsymbol{k}} + \omega_{\boldsymbol{q}}) - |v_{\boldsymbol{k}}|^2(\mathrm{i}\bar{\Xi}_{\boldsymbol{k}} + \bar{\Gamma}_{\boldsymbol{k}})}. \tag{30}$$

We note that the relevant quantities relative to quasiparticle states are weighted by the bare particle quantum occupation, $|v_{\boldsymbol{k}}|^2$. This is of course a natural consequence of the forced reduction to a one-particle problem, and the fractional initial occupation of the $\boldsymbol{k}$ state which is simply passed on to the quasiparticle state throughout the formalism. It follows that this weighting factor must be dropped (i.e. $|v_{\boldsymbol{k}}|^2\nu$ substituted for ν) to find the proper quasiparticle spectrum and the damping function from the poles of $U_{\boldsymbol{k}}^{\boldsymbol{k}}(\nu)$ (equations (26)), as was done in equations (23)–(24).

The results (29)–(30) exhibit well the essential features of the above-mentioned time dependence, and especially the vanishing of quasiparticle states in a few lifetimes, $\tau_{\boldsymbol{k}} = \bar{\Gamma}_{\boldsymbol{k}}^{-1}$.

3.2. Density of states and probability amplitudes $u_{\boldsymbol{k}}$, $v_{\boldsymbol{k}}$.

Analogously to Green function methods, the density of states $\rho_k(\eta)$ at given $\boldsymbol{k}$ and $-\eta$, is deduced from the real part of the diagonal elements $U_{\boldsymbol{k}}^{\boldsymbol{k}}(\nu)$, in the limit $\xi \to +0$. A detailed proof is given in appendix B. More precisely one obtains $\rho_{\boldsymbol{k}}(\eta)/|v_{\boldsymbol{k}}|^2$, for the above-mentioned reasons, thereby eliminating the weighting factor $|v_{\boldsymbol{k}}|^2$. From equations (23) and (26), we thus have

$$\rho_{\boldsymbol{k}}(\eta) = \frac{1}{\pi}\mathrm{Re}\,\frac{1}{\mathrm{i}[\eta + \varepsilon_{\boldsymbol{k}} + \Xi_{\boldsymbol{k}}(\eta)] + \Gamma_{\boldsymbol{k}}(\eta)} = \frac{1}{\pi}\frac{\Gamma_{\boldsymbol{k}}(\eta)}{[\eta + \varepsilon_{\boldsymbol{k}} + \Xi_{\boldsymbol{k}}(\eta)]^2 + \Gamma_{\boldsymbol{k}}^2(\eta)}. \tag{31}$$

The unperturbed energy ε_k is reinserted, except, for simplicity, in the self-energy which is only poorly dependent on it owing to the integration by $\omega_{\boldsymbol{q}}$.

$\rho_{\boldsymbol{k}}(\eta)$ should satisfy the general sum rule

$$\int_{-\infty}^{+\infty} \rho_{\boldsymbol{k}}(\eta)\,\mathrm{d}(-\eta) = 1 \tag{32}$$

which simply expresses that the initial norm of the $\boldsymbol{k}$ state is redistributed over the whole spectrum by the interaction. In the present formalism, this is satisfied as a consequence of the norm conservation in the solution $U(t)$. Even though the latter remains at any time, the quasiparticle approximation imposes limitation to small times. It is shown in appendix D that the sum rule (32) for $\rho_{\boldsymbol{k}}(\eta)$ as given by (31), can be derived, in particular at $t = 0$, from the unitarity of $U(t)$ expressed in the Laplace space.

The *total* density of states is deduced from $\rho_{\boldsymbol{k}}(\eta)$ through integration over $\boldsymbol{k}$, using the bare particle density of states, $\rho^{(0)}(\varepsilon_{\boldsymbol{k}})$,

$$\rho(\eta) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\Gamma_{\boldsymbol{k}}(\eta)\rho^{(0)}(\varepsilon_{\boldsymbol{k}})\,\mathrm{d}\varepsilon_{\boldsymbol{k}}}{[\eta + \varepsilon_{\boldsymbol{k}} + \Xi_{\boldsymbol{k}}(\eta)]^2 + \Gamma_{\boldsymbol{k}}^2(\eta)}. \tag{33}$$

As expected, the broadening of the bare particle levels is determined by the coupling strength, $\Gamma_k \propto |g_{\boldsymbol{k}}^{\boldsymbol{k}-q}|^2$.

We finally turn to the calculation of the probability amplitudes, $|u_{\boldsymbol{k}}|^2, |v_{\boldsymbol{k}}|^2$. As the latter describe the change of bare particle states dues to the interaction, they are naturally defined at $T = 0K$, where all states below the Fermi level are occupied,

$$|v_{\boldsymbol{k}}|^2 = \int_{-\infty}^{0} \rho_{\boldsymbol{k}}(\eta)\,\mathrm{d}(-\eta). \tag{34}$$

In the above simplifying assumptions, this gives

$$|\nu_{\boldsymbol{k}}|^2 = \frac{1}{\pi}\int_{-\infty}^{0} \frac{\bar{\Gamma}_{\boldsymbol{k}}\,\mathrm{d}(-\eta)}{(\eta+\varepsilon_{\boldsymbol{k}}+\bar{\Xi}_{\boldsymbol{k}})^2+\bar{\Gamma}_{\boldsymbol{k}}^2} = \frac{1}{2}-\frac{1}{\pi}\mathrm{arctg}\frac{\varepsilon_{\boldsymbol{k}}+\bar{\Xi}_{\boldsymbol{k}}}{\bar{\Gamma}_{\boldsymbol{k}}}. \tag{35}$$

$|\nu_{\boldsymbol{k}}|^2$ tends towards 1 if $\varepsilon_{\boldsymbol{k}} \to -\infty$, and towards 0 if $\varepsilon_{\boldsymbol{k}} \to +\infty$, so recovering the smearing of the Fermi function of bare particles over a range $\Gamma_{\boldsymbol{k}}$, of the order of the interaction strength.

At finite temperature the statistical average must be included in the initial state, which at once represents the steady state in our self-consistent treatment. The momentum $\boldsymbol{k}$ is still regarded as a good quantum number in passing from bare particles to quasiparticles, and the quasiparticle creation and annihilation operators are close to those of bare particles, apart from a frequency shift and a small dispersion due to damping [18], as accounted for in the density of states $\rho_{\boldsymbol{k}}(\eta)$. Since quasiparticles behave like independent fermions (equation (12)), a simple way to include the thermodynamical average in the occupation probability of the $\boldsymbol{k}$ state will consist in inserting the Fermi statistics, via the density of states, in equation (34)

$$|\nu_{\boldsymbol{k}}(T)|^2 = \int_{-\infty}^{+\infty} \rho_{\boldsymbol{k}}(\eta)\, f(-\eta)\,\mathrm{d}(-\eta). \tag{36}$$

We have a similar complementary expression for $|u_{\boldsymbol{k}}(T)|^2$.

4. Summary and conclusions

In summary, we have proposed a new means of solving the dynamics of interacting electron systems, especially the calculation of self-energy, seemingly simpler than the widely spread Green function methods. The components of the many-body interacting states on the unperturbed states are determined in a self-consistent way through the resolution of the Laplace transformed equation of the evolution operator, within the framework of a so-called determinantal method, previously published. Owing to the conservation of the norm in the solution, the proper self-energy parts, as given by the Dyson equation, arise directly therein, in a quite natural way, along with the quasiparticle spectrum. The related density of states is shown to derive from the diagonal elements of the evolution operator, and the probability amplitudes entering the definition of the dressed states, including statistics, are directly calculated through integration over the quasiparticle spectrum, in the Laplace space.

The overall behaviour is well pictured by the evolution, in real time, of typical individual processes, in a direct treatment, involving elementary mathematics based on the linear system theory and the Laplace transform, which renders it relatively easy to read the physical content. Also, inherent approximations are well brought out, such as limitations imposed by the quasiparticle damping, the reduction to a one-body problem, or in the introduction of the statistics. The need to proceed self-consistently with fractional occupations due to the coupling itself is emphasized. As a consequence, all relevant quasiparticles quantities then arise with the same occupation weight. In an early paper by Frölich [1], these occupations were properly taken into account from the beginning, and determined by an extremum method. This is not always clear in Green function techniques, where particles (holes) travelling in positive (negative) time are *artificially* added to the system. Statistical factors are then introduced in the averaging procedure [19, 20], while the quantum occupations in the ground state are retrieved from the discontinuities of the Green function, in a quite formal way [18].

For the sake of simplicity, the problem was illustrated by the electron–phonon coupling in a metal, at lowest order, ignoring screening, Coulombic correlations, and extra damping effects. Explicit results were obtained in equations (29–30) and (35), within our simplified assumption of constant self-energy components. This could be appreciably improved by taking into account the η dependence of the self-energy, at least in the form of suitable expansions, which should then yield the mass renormalization owing to the interactions, such as in Eliashberg's theory [5, 20, 21]. Also the higher-order terms arising in the expansion of the S_{bn}^{-1}'s (equations (10)) (vertex corrections) could be taken into account. In the case of electron–phonon coupling, they were shown by Migdal [3] to be only of order of the adiabatic parameter, $(m/M)^{\frac{1}{2}}$, but the occurrence of strong interactions requiring such corrections was recently pointed out [21, 22]. Finally, the reliability of the method provides us with opportunity to further more detailed studies in which these refinements could be included.

Appendix A. Operational form of the determinantal solution

Given the starting state b, introduce the convenient notation $|U\rangle = U(t)|b\rangle$, with $|U_0\rangle \equiv |b\rangle$. Equation (3) is then rewritten in the following form

$$|U\rangle = (I + d^{-1}K)^{-1}d^{-1}|b\rangle.$$

As d is diagonal, we have $d^{-1}|b\rangle = d_b^{-1}|b\rangle$, with d_b scalar. Further, P_b and Q_b denoting the projectors on the b state and its complementary space, respectively, one can substitute $(I + d^{-1}KQ_b)|b\rangle$ for $|b\rangle$ in the r.h.s. without change. Then, reversing the operators in the r.h.s., we obtain

$$(I + d^{-1}KQ_b)^{-1}(I + d^{-1}K)|U\rangle = d_b^{-1}|b\rangle.$$

Obviously the determinant of the matrix $I + d^{-1}KQ_b$ is the diagonal minor D_b^b of the matrix $I + d^{-1}K$, hence recovering the solution in the form (5). The above equation is then rewritten more compactly, using the splitting $d^{-1}K \equiv d^{-1}KQ_b + d^{-1}KP_b$,

$$(I + S_b^{-1}d^{-1}KP_b)|U\rangle = d_b^{-1}|b\rangle$$

with $S_b = I + d^{-1}KQ_b$. As the matrix $I + S_b^{-1}d^{-1}KP_b$ has only non-zero elements in the principal diagonal and the column b, solving this system leads straightforwardly to equations (6).

Appendix B. Quasiparticle density of states

Let Δ denote the determinant of the matrix $d + K$. Expanding Δ with respect to the b row gives

$$\Delta = d_b\Delta_b^b + K_\ell^b\Delta_b^\ell, \tag{B.1}$$

($\ell \neq b$). Bearing in mind that $d_k = \nu + \mathrm{i}\varepsilon_k$, we have

$$\Delta_b^b = \frac{\partial\Delta}{\partial(\mathrm{i}\varepsilon_b)}. \tag{B.2}$$

Alternatively, Δ can also be written in terms of its imaginary roots $-\mathrm{i}E_j$, assuming the multiplicity m_j,

$$\Delta = \prod_j(\nu + \mathrm{i}E_j)^{m_j}. \tag{B.3}$$

The E_j's denote the energy of states derived from the unperturbed ones, b, by the interaction K. Hence, combining (B.2) and (B.3), one obtains the following expression of the diagonal elements of the evolution operator

$$U_b^b(\nu) = \frac{\Delta_b^b(\nu)}{\Delta(\nu)} = \frac{\partial \ln \Delta}{\partial(\mathrm{i}\varepsilon_b)} = \sum_j \frac{m_j}{\nu + \mathrm{i}E_j} \frac{\partial E_j}{\partial \varepsilon_b}. \tag{B.4}$$

The limiting value of this expression for $\xi \to +0$ is then

$$\lim_{\xi \to +0} \sum_j \frac{m_j}{\xi + \mathrm{i}(\eta + E_j)} \frac{\partial E_j}{\partial \varepsilon_b} = \sum_j m_j \frac{\partial E_j}{\partial \varepsilon_b} \left[-\frac{\mathrm{i}}{\eta + E_j} + \pi \delta(\eta + E_j) \right]$$

the real part of which can be shown to define a density of states

$$\rho_b(\eta) = \frac{1}{\pi} \mathrm{Re}[\lim_{\xi \to +0} U_b^b(\nu)] = \sum_j m_j \frac{\partial E_j}{\partial \varepsilon_b} \delta(\eta + E_j). \tag{B.5}$$

Indeed, if we multiply each side of equation (B.5) by one b quantum of energy, say $\delta\varepsilon_b$, the resulting expression of $\rho_b(\eta)\delta\varepsilon_b$ can be seen to represent the summation of the individual $m_j\delta(\eta+E_j)$'s, each one of them being integrated over the shift $\delta E_j = (\partial E_j/\partial\varepsilon_b)\delta\varepsilon_b$ induced by $\delta\varepsilon_b$. It follows that $\rho_b(\eta)\delta\varepsilon_b$ is just the number of quasiparticle states generated by the initial b state, so defining $\rho_b(\eta)$ as the quasiparticle *density of states at a given b state*.

Appendix C. Energy denominators in the $k \to k'$ transitions

We calculate the change of the d^{-1} mean eigenvalue upon the electron transition $\boldsymbol{k} \to \boldsymbol{k}'$, with respect to its initial value, $(\nu + \mathrm{i}\varepsilon_B)^{-1}$. Ignoring the phonon states, we have

$$d^{-1} c_{k'}^+ c_k |\psi_B\rangle = (c_{k'}^+ c_k d^{-1} + [d^{-1}, c_{k'}^+ c_k])|\psi_B\rangle. \tag{C.1}$$

Let us separate out the $\boldsymbol{k}$ and $\boldsymbol{k}'$ states in the unperturbed energy

$$d^{-1} = \frac{1}{\nu + \mathrm{i}H_{0k'k} + \mathrm{i}E_{k'k}}$$

with $H_{0k'k} = \sum_{k'' \neq k',k} \varepsilon_{k''} c_{k''}^+ c_{k''}$ and $E_{k'k} = \varepsilon_{k'} c_{k'}^+ c_{k'} + \varepsilon_k c_k^+ c_k$. Obviously, $E_{k'k}$ and $c_{k'}^+ c_k$ commute with $H_{0k'k}$ and the magnitude of the $E_{k'k}$ eigenvalues are very small compared with those of $H_{0k'k}$ which involve a summation over states. Thus, we can write the following first-order expression without significant error,

$$d^{-1} = \frac{1}{\nu + \mathrm{i}H_{0k'k}} - \left(\frac{1}{\nu + \mathrm{i}H_{0k'k}} \right)^2 \mathrm{i}E_{k'k}.$$

Hence,

$$[d^{-1}, c_{k'}^+ c_k] = -\left(\frac{1}{\nu + \mathrm{i}H_{0k'k}} \right)^2 \mathrm{i}[E_{k'k}, c_{k'}^+ c_k] = -\left(\frac{1}{\nu + \mathrm{i}H_{0k'k}} \right)^2 \mathrm{i}\varepsilon_{k'k} c_{k'}^+ c_k.$$

$(\varepsilon_{k'k} = \varepsilon_{k'} - \varepsilon_k)$. Equation (C.1) becomes

$$d^{-1} c_{k'}^+ c_k |\psi_B\rangle = \left[\frac{1}{\nu + \mathrm{i}\varepsilon_B} - \left(\frac{1}{\nu + \mathrm{i}\varepsilon_{Bk'k}} \right)^2 \mathrm{i}\varepsilon_{k'k} \right] c_{k'}^+ c_k |\psi_B\rangle$$

with $\varepsilon_{Bk'k}$ eigenvalue of $H_{0k'k}$. As $|\varepsilon_{k'k}| \ll |\varepsilon_B|$, $|\varepsilon_{Bk'k}|$, and $|\varepsilon_{Bk'k}| \cong |\varepsilon_B|$, we can also write,

$$d^{-1} c_{k'}^+ c_k |\psi_B\rangle = \frac{\mathrm{i}}{\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{k'k})} c_{k'}^+ c_k |\psi_B\rangle = \frac{\mathrm{i}}{\nu + \mathrm{i}(\varepsilon_B + \varepsilon_{k'k})} u_{k'} v_k |\psi_{1k'0k}\rangle.$$

Appendix D. Norm of the evolution operator in the Laplace space

The norm of the evolution operator can be directly calculated in the Laplace space, by means of convolution integration. Consider the diagonal component $U_k^k(\nu)$, equation (26). The norm at $t = 0$, is thus given by

$$|U_k^k(t=0)|^2 = \lim_{\nu\to\infty} \frac{\nu}{2\pi \mathrm{i}} \int_C \frac{\mathrm{d}\nu'}{[\nu - \nu' + \mathrm{i}|\nu_k|^2\Sigma_k(\nu-\nu')][\nu' - \mathrm{i}|\nu_k|^2\Sigma_k^*(\nu')]}.$$

The result is insensitive to $|\nu_k|^2$ which can be dropped. The integrand now exhibits a second cut translated by ν from the first one (figure D1), but according to the convolution theorem which requires $c < \xi$, this cut is out of the contour C. Therefore, the integration is only to be taken along the cut lying on the η'-axis, where, from equation (23) (with the slight redefinition of $\Gamma_k(\eta)$ in equation (27)),

$$\Sigma_k(\nu') \to_{\xi'\to\pm 0} \Xi_k(\eta') = \mathrm{i}\,\mathrm{sgn}(\xi')\Gamma_k(\eta').$$

Hence, by reinserting $|\nu_k|^2\varepsilon_k$ and eliminating $|\nu_k|^2$, we obtain

$$\begin{aligned}|U_k^k(t=0)|^2 &= \frac{1}{2\pi\mathrm{i}}\int_{\mathrm{cut}} \frac{\mathrm{d}\nu'}{\nu' - \mathrm{i}\varepsilon_k - \mathrm{i}\Sigma_k^*(\nu')} \\ &= \frac{1}{2\pi\mathrm{i}}\left[\int_{-\infty}^{+\infty} \frac{\mathrm{d}\eta'}{\eta' - \varepsilon_k - \Xi_k(\eta') - \mathrm{i}\Gamma_k(\eta')}\right. \\ &\quad \left. + \int_{+\infty}^{-\infty} \frac{\mathrm{d}\eta'}{\eta' - \varepsilon_k - \Xi_k(\eta') + \mathrm{i}\Gamma_k(\eta')}\right]\end{aligned}$$

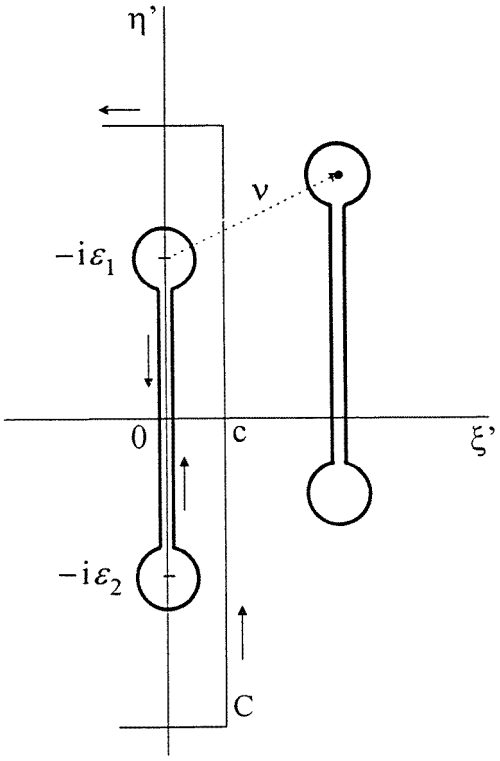

Figure D1. Contour used in the complex plane of the Laplace variable $\nu'(\xi', \eta')$ for the calculation of the norm of the quasiparticle states, with the help of the convolution theorem. The cut translated by ν, with $\xi > 0$, is located outside the contour.

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\Gamma_{\boldsymbol{k}}(\eta')\,\mathrm{d}\eta'}{[\eta' - \varepsilon_{\boldsymbol{k}} - \Xi_{\boldsymbol{k}}(\eta')]^2 + \Gamma_{\boldsymbol{k}}^2(\eta')}.$$

The integration is the same as in equation (32), and the result is necessarily 1, because of norm conservation. This can be readily verified in the simple model with constant self-energy components.

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