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# Scattering, Dissipation, and Transport in Mesoscopic Systems

FERNANDO SOLS

*Beckman Institute and Department of Physics,*
*University of Illinois at Urbana Champaign, 405 N. Matthews Ave., Urbana, Illinois 61801*
*and *Departamento de Fisica de la Materia Condensada, C-XII,*
*Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

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A theoretical study of dissipative scattering in mesoscopic systems is presented. Within the single electron and localized phonon approximations, exact expressions for the transmission and reflection probabilities between the various leads and channels are derived in terms of dressed two-particle Green's functions. These general results are obtained through two different procedures: one approach is based on a direct study of the microscopic stationary scattering amplitudes while in a second method the reduced density matrix of a scattered wave packet is analyzed. In both approaches the phonon bath degrees of freedom are traced out in such a way that an effective description of the electron dissipative dynamics emerges. The scattering probabilities are shown to satisfy symmetry relations which exactly account for the presence of a dissipative thermal bath. A lattice formulation of the calculational method is also presented, and an explicit proof of unitarity is obtained by invoking the continuity equation. By introducing time-ordering in the Keldysh contour, a diagrammatic perturbation theory in the electron–phonon interaction is developed. Unitarity is shown to be automatically preserved to all orders in perturbation theory. The use of diagrams is illustrated by applying them to some simple cases involving one- and two-phonon processes. Finally, a discussion is presented on the computation of the current from the inelastic scattering probabilities. The existence of an ambiguity in the assignment of quantum statistical factors to the outgoing scattering channels is pointed out. It is argued that a more consistent picture is obtained if no statistical restrictions are explicitly introduced in the electron final states. The novel formulation which is presented here provides a theoretical framework for quantitative studies of the interplay between quantum interference and dissipation in the transport properties of very small structures. 

## 1. INTRODUCTION

The recent development of cryogenic and lithographic techniques has generated a strong interest in a novel regime of electron transport where the wave nature of the electron plays a fundamental role. The commonly accepted view is that the electron phase is randomized by inelastic processes, which at low temperatures can be very rare. If the inelastic mean free path is larger than the mean free path due to elastic scattering by impurities, a wealth of new phenomena emerge that cannot be described within the framework of semiclassical transport theory, where quantum effects only enter through the band structure and the cross section of (usually)

* Permanent address.



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uncorrelated scattering events. The physical systems where the electron phase coherence is preserved at a scale much larger than the atomic dimensions are often referred to as mesoscopic systems [1]. Among the new phenomena originated by electron quantum interference are weak localization [2], the Aharonov–Bohm (A-B) effect [3], universal conductance fluctuations [4], resonant tunneling [5, 6], and electron waveguide behavior [7]. The prospect of applying some of these new effects to the design of electronic devices based on novel principles has strongly contributed to the current interest in the physics of mesoscopic systems [8]. This is particularly true in the case of resonant tunneling [6], A-B effect [9], and electron waveguide transport [10, 11], where some specific proposals have been made. Common to all these phenomena is the preservation of phase coherence at a length scale where quantum interference develops. Dephasing, or randomization of the phase, is caused by the interaction with an environment with many internal degrees of freedom whose dynamics becomes correlated with the motion of the electron. Stern *et al.* [12] have recently studied in some depth the concept of phase randomization by a dissipative environment, and their analysis has later been refined by Loss and Mullen [13]. These authors emphasize that, in order for effective dephasing to occur, the electron motion along different paths (that would interfere in the absence of dissipation) must become correlated with the evolution of the bath into corresponding orthogonal states. The loss of phase coherence is generally accompanied by a transfer of energy between the carriers and the bath, although this is not strictly necessary. If the dissipative environment supports low energy excitations (like, e.g., acoustic phonons or electron–hole pairs), the dephasing length $l_\phi$ may be smaller than the inelastic length $l_{in}$, since the former is associated with the transfer of a quantum of energy that can be arbitrarily small, while the second is rather the length the carrier travels before it loses an amount of energy comparable to its kinetic energy [14]. The concept of mean free path is useful for transport in extended systems such as quantum wires or quantum wells. However, the situation in a typical quasi-one-dimensional nanostructure with feature size below the dephasing length is better described by a scattering picture where probabilities are the relevant quantities that measure the importance of the various physical processes. In this paper we shall use dephasing and inelastic scattering as exchangeable terms and they both will refer to processes where the final and initial bath states are orthogonal. The electron–electron interaction can also cause dephasing [15], but we shall not consider it here.

Since the early work by Landauer [16], it has been common to assume that dissipation occurs only in reservoirs which are physically separated from the region where elastic scattering (and all associated quantum interference phenomena) takes place. This view is certainly adequate in the limit where inelastic scattering is extremely rare and has the additional advantage of providing a powerful computational tool, since the sample transport properties can be obtained from the scattering of independent electrons. More recently, Büttiker [17–19] has included dissipation in the sample region by introducing extra reservoirs with no net current flow. The electrons leaving the reservoir are assumed to have no phase-coherence with the

electrons entering it. Dissipation is then described in terms of a generalized Landauer problem, where a variety of voltage leads are attached to the sample [19]. This approach has also been followed by D'Amato and Pastawski [19a], who have studied the conductance of a disordered linear chain, and by Hershfield [19b], who has developed a numerical algorithm to include the effect of dephasing leads. The phenomenological description of dissipation in terms of additional reservoirs has been shown by Datta [20] to be equivalent to a model of point-like phonon scatterers. This equivalence has been used by Pastawski [20a] to develop a unified description of classical and quantum transport. In these works, localized phonons are effectively treated in the self-consistent Born (or ladder) approximation.

Dissipation is easily described in its extreme form, when a series of physical processes that would occur coherently in the absence of dissipation can be treated as completely uncorrelated. An example of this can be found in resonant tunneling, which, in the regime of strong intra-well dissipation, can be viewed as a two-step process in which the electron first tunnels into the resonant site and later leaves it without phase memory of its arrival. This is the regime of sequential tunneling, which is opposite to the coherent tunneling that takes place in the absence of dissipation [18]. Tejedor *et al.* [21] have shown that a magnetic field parallel to the interface can be used to distinguish between coherent and sequential tunneling and to move continuously between the two regimes within a given structure by controlling the degree of localization within the resonant well. It is clearly desirable to improve our understanding of dissipation by studying models in which some type of realistic electron–phonon interaction is explicitly considered. Recently, several works have appeared in which phonon coupling to the quasi-bound state of a resonant tunneling structure has been included [22–25]. The simplifying approximation of a wide-band has been introduced in all these works. Hyldgaard and Jauho [26] have extended these studies to resonant tunneling in superlattices.

The purpose of this paper is to develop a systematic approach to the study of dissipation in mesoscopic systems. The ultimate goal is to provide a quantitative description of the electron–phonon interaction in ultrasmall structures. This ambitious task is, however, quite arduous and one must resort to a variety of approximations, particularly in the early stages. We have introduced two main simplifications in our analysis. First, we employ a single-electron picture and, second, we assume that dissipation takes place in a finite region of space. These two approximations have been used in most of the recent work on dissipation in quantum transport where some type of electron–phonon interaction has been explicitly included [22–27]. Although the first approximation prevents us from studying the role of the Pauli exclusion principle and Coulomb correlation in dissipation, we expect it to keep many essential features of the interplay between quantum interference and dissipation. Apart from the obvious simplifications that arise from considering a single-particle picture, there are other good reasons for introducing such an approximation. Most importantly, the single-electron picture has been widely used in the study of transport in semiconductors [28] and there is a great variety of situations (such as transport by nondegenerate plasmas in semiconductors) where it can be considered legitimate. A detailed account of the merits of the single-

particle approach has recently been given by Rammer [29], who has developed a single electron theory of quantum transport within a density matrix formulation. While he has presented a real time description of the electron dynamics, we have focused on the study of stationary scattering, where physics can be formulated in energy space. We expect our stationary scattering approach to be advantageous in the description of steady-state transport. Furthermore, as we shall see, an energy formulation often permits a better understanding of the physical meaning of expressions or diagrams that would remain obscure in their time-dependent counterparts.

The second simplification that we have introduced is the assumption that the electron interacts with phonons only in a finite region of space. This approximation allows us to adopt a simple scattering picture in which the channels for asymptotic propagation are known exactly. The scattering channels are the various transverse modes in the different leads connected to the nanostructure under study. A more realistic model in terms of extended phonons (which in turn can be scattered by the structure) would be considerably more complicated and must be studied separately. In addition, it should be pointed out that a model of localized phonons is quite adequate in some situations where, due to the specifics of the structure, phonon modes develop that have most of their amplitude in the scattering region. These are cases in which the lattice vibrations are sensitive to the geometry, also because of their wave nature. In this sense, we can assert that the geometry affects the electron motion both by changing its wave function and by modifying the phonons that tend to destroy the coherence. Whether this modification of the phonon modes enhances or inhibits dephasing remains to be seen and certainly constitutes a question of great interest.

The resulting scattering problem that we shall study is schematically depicted in Fig. 1 and can be formulated as follows: an electron comes from lead $a$ in transverse mode $m$ with energy $E_i$ and can be transmitted with a certain probability into mode $n$ of lead $b$ with energy $E_f$ after having interacted with the boundaries, impurities, and phonons in the central region (the "sample"). We are essentially following the Landauer approach in which the resistance of a sample is viewed as a direct consequence of its scattering properties [16]. However, we include the possibility of inelastic processes within (or in the vicinity of) the sample. As in the standard Landauer picture, we assume that the electron reservoirs introduce additional randomization of the relative phase between the electron waves that enter and leave the reservoir.

In Section 2, we derive general expressions for the inelastic transmission and reflection probabilities in terms of two-particle Green's functions. The reason why two-particle Green's functions (with four field operators) appear in a single-particle problem is that we calculate probabilities instead of probability amplitudes (which would be given by one-electron Green functions). In connection with this rather important point, we also discuss the relation between the irreducibility of the two-particle Green function and the occurrence of inelastic scattering in which the phonon bath changes state. An interesting feature of our scattering analysis is that the fundamental property of microscopic reversibility gives rise to a detailed

balance equation that guarantees the suppression of net currents in the absence of a driving force. The situation is similar to that encountered in Boltzmann equation studies. However, we deal here with scattering probabilities (associated to a one-event process) instead of scattering rates (which give the frequency of uncorrelated scattering events). An interesting by-product of the found symmetry relation is the compatibility between microscopic reversibility and irreversible thermalization.

Our starting point is the relation between the Green's functions and the elements of the discrete $S$-matrix (transmission and reflection coefficients) that was derived by Fisher and Lee [30] for one-dimensional scattering and was later generalized by Stone, Szafer, and Baranger [31, 32] to arbitrary multilead structures. Formally, the phonon bath is introduced by simply adding new labels to the equations. The Hilbert space is thus enlarged to include both the states of the particle and the states of the phonon system. The total system formed by the electron plus the phonons is a Hamiltonian system where energy is conserved. From the point of view of scattering, the phonon indices appear on a formally identical footing to that of the electron lead and channel quantum numbers. Leggett [33] has recently pointed out the formal similarity between phonon states and electron transverse modes. Of course, this similarity disappears when an explicit account of the quantum statistics is taken in the process of ensemble averaging. Since we are only interested in the electron dynamics, we trace out the phonon degrees of freedom by taking a thermal average for the initial states and an equal weight sum over all possible final states. This is the approach to dissipation in quantum mechanics that has been emphasized by Leggett and collaborators [34, 35] following the seminal work of Feynman and Vernon.

The work of Section 2 is complemented by three appendices. In Appendix A, we present an alternative derivation of the relation between Green's functions and scattering amplitudes that is based on a real time analysis of a scattered wave packet. Appendix B deals with a lattice formulation that may be required in other contexts. The equations for inelastic resonant tunneling [22] are rederived exactly. Finally, in Appendix C we show that unitarity can be inferred from the general expressions for the inelastic scattering probabilities by invoking the continuity equation satisfied by the electron current and density operators.

In Section 3, we present an alternative derivation of the equations for the inelastic transmission and reflection probabilities based on an analysis of the reduced density matrix (that which results from taking the trace over the phonon coordinates in the total density matrix). The reason for presenting an alternative derivation is threefold. First, it provides us with an independent check of the equations derived in Section 2. Second, it gives additional insight into the physics described by those equations. The scattering probabilities are obtained by analyzing the real time evolution of a wave packet that is scattered by the sample. The stationary scattering properties are obtained by considering the limiting case of a monochromatic wave packet. In particular, an interesting solution is given to the apparent paradox that the reduced density matrix depends only on one time argument (see Eqs. (33) and (36)) while a calculation of the scattering probabilities seems to require full knowledge of the dependence of the two-particle Green func-

tion on its three significant time variables (see Eq. (14)). The solution lies in the correlation which exists between time and space dependence in the asymptotic regions, where the electron propagates freely. Finally, an analysis of the inelastic scattering problem in terms of the reduced density matrix creates a bridge with the literature on dissipation in quantum mechanics [35], where the density matrix approach has been widely used.

Equations (14) and (16) for the inelastic scattering probabilities derived in Sections 2 and 3 are formally exact. However, an exact evaluation of the Green's functions involved that fully includes the effect of boundaries, impurities, and phonons is not possible in general. One has to resort to various types of approximations. One possibility is to treat the phonons exactly and include the elastic scattering approximately, but this is only possible in tight-binding formulations where the phonons couple to one electron site [22, 28]. It is more common to assume that the electron motion in the presence of boundaries and impurities is known exactly and include the effects of phonons approximately. In this work we follow the second approach because there is a wide variety of situations where the elastic one-electron problem can be solved exactly by analytical or numerical methods. We wish to develop a diagrammatic perturbation theory in the electron–phonon coupling that allows us to include the effect of phonons in a systematic fashion and eventually to introduce correlative approximations by summing a given class of diagrams. This program is carried out in Section 4. A diagrammatic representation is derived by applying Wick's theorem to a time-ordered version of the Green's functions introduced in Sections 2 and 3. A nice feature of our perturbative analysis is that unitarity is automatically preserved to all orders in perturbation theory. This is possible because we develop a perturbation theory for scattering probabilities—rather than amplitudes, whose sum must be unity regardless of the value of the electron–phonon coupling constant.

In Section 5, we illustrate the use of the diagram rules derived in Section 4 by applying them to some simple cases. We calculate all one-phonon diagrams and explicitly check unitarity in one particular case. We also study a group of two-phonon diagrams which include real emission and absorption processes. The particular case where the same phonon is first emitted and then absorbed (or vice versa) yields an additional elastic chanel that has been known to be important in other contexts.

Finally, in Section 6, we present a discussion on the computation of the net current in a given lead as a function of the chemical potential of the various leads in terms of previously computed inelastic transmission probabilities. This is an attempt to generalize the Landauer–Büttiker equations [19, 37] to the case where inelastic scattering occurs in the sample. We employ counting arguments which are similar to those used by Büttiker [19, 37] in his initial derivation of the conductance of multilead structures in the independent electron approximation (which is correct in the absence of dissipation). This may seem the logical first step towards a multilead conductance formula which accounts for realistic dissipation. After all, the counting argument used in Ref. [37] for the elastic regime proved to be essentially correct, as confirmed by the later work of Ref. [32] and by the numerous

successful applications of the results there obtained. However, the generalization of the multilead conductance formula to the dissipative case is considerably more problematic, particularly in what regards the inclusion (or not inclusion) of the Fermi statistics in the final states. In Section 6, we present two different *ansätze* for the computation of the current in the leads, one in which the Pauli exclusion principle is introduced in the outgoing channels and another one in which it is not. Both ansätze have been used previously in the literature in one form or another. In the particular case where there are only two leads, the magnetic field is zero, and dissipation is absent, both current ansätze are equivalent but this is not true in the general case. We argue that, although the option without explicit inclusion of Fermi statistics in the final states is probably closer to the correct solution, neither of the two ansätze is entirely free of contradictions. This often neglected ambiguity in the computation of the current strongly suggests that the generalization of the Landauer–Büttiker equations to the presence of dissipation (and thus of dynamic electron–electron interactions) requires more careful theoretical work than one would expect from the success of simple counting arguments in the independent electron picture. In this regard we note that the generalization of the linear response analysis of Refs. [31, 32] is not straightforward, since in those works the assumption of independent electrons (which is not valid in the presence of electron–phonon coupling) is introduced at the outset. A more appropriate starting point may be provided by an exact expression for the conductance coefficients in terms of many-body scattering states that has been recently derived by the author within the framework of a gauge-invariant formulation of linear transport [37a]. Recently, Feng [38] has studied an exactly solvable model in which a generalization of the Landauer formula for at least the two-terminal case seems to be possible. However, Feng's choice of an electron–phonon interaction in which the phonons couple separately to each of the unperturbed scattering eigenstates completely precludes the dephasing effect of dissipation, since the phase coherence contained within each scattering state—which is the essence of quantum interference—is preserved intact. Thus the validity and generality of his results must be taken with caution until theoretical work dealing with more realistic electron phonon couplings is available. A promising approach is that taken by Anda and Flores [39] who have employed the Keldysh method to compute the transport properties of resonant tunneling heterostructures, following the early work by Combescot et al. [39a] on inelastic tunneling. However, at least in its present form, the Keldysh formalism does not readily lead to a scattering picture of the electron transport problem that can be applied in the most general situation (without specific assumptions about the phonon interaction and the couplings between leads and sample). In summary, the work presented in Section 6 about the computation of the current is of a more tentative nature than that of the other sections. We point out, however, the existence of an ambiguity in the choice of current formula that has often remained unnoticed in the literature. We hope that this discussion will stimulate further theoretical work on the correct method of computing the current.

In this work we have borrowed some concepts from the literature on dissipation

in quantum mechanics, which has considerably grown in the last ten years due to the interest on macroscopic quantum phenomena. Most of the work in this field has dealt with the effect of an environment with many degrees of freedom (the "bath") on the dynamics of a single degree of freedom (the "particle"). Dissipation is a manifestation of the lack of knowledge or control on the detailed behavior of the bath. It is well described mathematically by the reduced density matrix, which is obtained by tracing out the bath coordinates from the total density matrix. The equivalent procedure in a stationary scattering approach consists in summing over all possible final bath states while thermally averaging over the initial ones. Most of the work on dissipation in quantum mechanics has been based on path-integral formulations. Here we show that similar ideas can be implemented in the framework of Schrödinger mechanics and that they can in particular be applied to the study of dissipative scattering. The formal connection between dissipation in mesoscopic systems and macroscopic quantum phenomena is not accidental but rather quite deep, since mesoscopic systems provide a natural scenario for the study of the crossover from the quantum-mechanical world of atoms and molecules to the semiclassical world of macroscopic bodies. The transition between quantum and classical behavior is fundamentally driven by dissipation, which is a phenomenological way of referring to the effect on a few interesting dynamic variables of a large number of uncontrolled degrees of freedom.

## 2. Inelastic Scattering Probabilities in Terms of Two-Particle Green Functions

### A. *General Relations*

Our starting point is a relation between the electron Green's function and the $S$-matrix elements of a general multilead structure (like the one in Fig. 1) which was obtained by Stone and Szafer [31] in the context of a linear response derivation of the Landauer–Büttiker formula. They found

$$G_{nm}^{0(+)}(x_a, x_a') = \frac{-i}{\hbar v_{ma}} \left\{ \delta_{nm} \exp[ik_{ma}(x_a' - x_a)] + \left(\frac{k_{ma}}{k_{na}}\right)^{1/2} r_{nm,aa} \exp(ik_{na}x_a + ik_{ma}x_a') \right\} \tag{1a}$$

$$G_{nm}^{0(+)}(x_b, x_a) = \frac{-i}{\hbar v_{ma}} t_{nm,ba} \left(\frac{k_{ma}}{k_{nb}}\right)^{1/2} \exp(ik_{nb}x_b + ik_{ma}x_a), \tag{1b}$$

where $t_{nm,ba}$ is the probability amplitude that an incident electron in transverse mode $m$ of lead $a$ is transmitted into mode $n$ of lead $b$, $r_{nm,aa}$ is the reflection coefficient to go from mode $m$ to mode $n$ within lead $a$, and $k_{ma}$ and $v_{ma}$ are the electron wavevector and velocity in mode $m$ of lead $n$ at energy $E$ (note that the

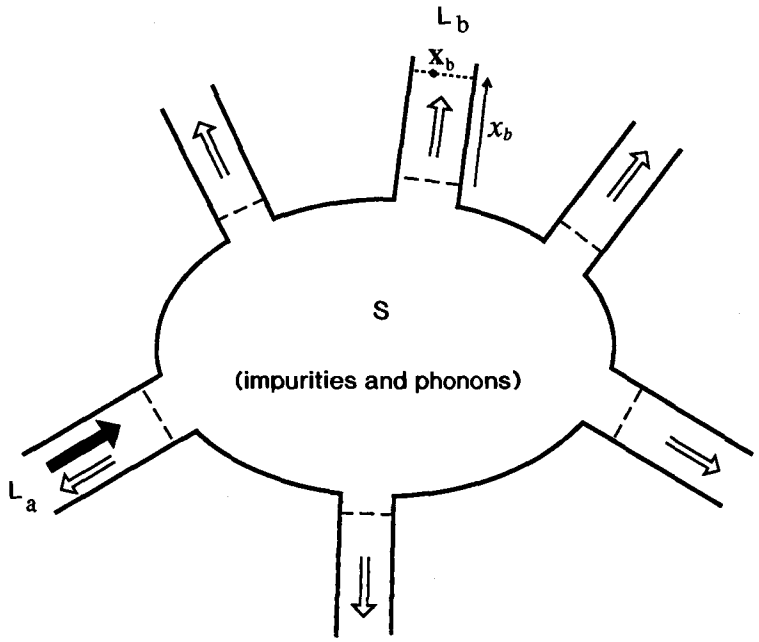


FIG. 1. Schematic representation of a generic multilead structure. The arrows indicate the propagation of a scattered electron. $S$ is the sample region which include impurities phonons, and boundaries. The asymptotic regions $L_a$, $L_b$, ... are formed by semi-infinite leads where the electron propagates freely.

index convention differs from that of Ref. [31]). The retarded ($G_0^{(+)}$) and advanced ($G_0^{(-)}$) Green's functions are defined as

$$G_{nm}^{0(\pm)}(x_b, x_a; E) = \langle x_b, \chi_n | \, G_0^{(\pm)}(E) \, | x_a, \chi_m \rangle,$$
$$G_0^{(\pm)}(E) \equiv (E - H_0 \pm i\eta)^{-1}, \tag{2}$$

where $\chi_m(y_a)$ is the wave function for the transverse mode $m$ in lead $a$, and $\mathbf{x}_a = (x_a, y_a)$ is a point in lead $a$ (see Fig. 1). Here, and in the rest of this paper, the limit $\eta \to 0^+$ is implicitly assumed. In Eq. (1a), $x'_a \geqslant x_a$ must be taken, where, by convention, $x_a$ grows in the outward direction;

$$H_0 = -\frac{\hbar^2 \nabla^2}{2M} + U(\mathbf{x}) \tag{3}$$

is the one-electron Hamiltonian that includes the effect of boundaries and impurities.

Equation (1) generalizes a relation previously obtained by Fisher and Lee [30] for one-dimensional scattering. In Appendix A, we provide an alternative derivation of the relations (1) that is based on a wave packet approach to the scattering problem. Apart from its own interest, one important reason for presenting this alternative derivation is that it allows us to appreciate in a simpler context (namely,

in the absence of phonon scattering) some technical points that will be essential in the density matrix analysis of Section 3.

We argue at this point that dissipation can be included by introducing in (1) extra-indices associated to the states of the phonons bath $|\alpha\rangle$, $|\beta\rangle$, etc. The scattering states of our complete physical systems now require the additional specification of the bath state. Thus, for instance, $t_{nm,ba,\beta\alpha}$ is the probability amplitude that an electron coming from lead $a$ in transverse mode $m$ finding the bath in initial state $|\alpha\rangle$, is transmitted into channel $n$ of lead $b$ leaving the bath in state $|\beta\rangle$, at a given total energy $E = E_i + \varepsilon_\alpha = E_f + \varepsilon_\beta$, where $E_i$ and $E_f$ are the initial and final electron energies (energy has to be conserved in the Hamiltonian system formed by the electron plus the phonon bath).

We focus for the moment on the transmission probability and rewrite (1b) with new bath indices,

$$t_{nm,ba,\beta\alpha} = i\hbar(v_{nb\beta} v_{ma\alpha})^{1/2} \times \exp(-ik_{Enb\beta} x_b - ik_{Ema\alpha} x_a) \langle x_b, \chi_n; \beta | \, G^{(+)}(E) \, | x_a, \chi_m; \alpha \rangle, \tag{4}$$

where

$$G^{(+)}(E) = (E - H + i\eta)^{-1} = \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \, e^{iEt/\hbar} \theta(t) \, e^{-iHt/\hbar} \, e^{-\eta|t|} \tag{5}$$

is the retarded Greenian for the total system, $\theta(t)$ is the step function and, in the total Hamiltonian

$$H = H_0 + H_B + V, \tag{6}$$

$H_B$ describes the isolated phonon bath while $V$ is the electron–phonon interaction. We introduce for convenience a field-theoretical description of the electron in which

$$|x_a, \chi_m; \alpha\rangle \equiv \psi_m^+(x_a) \, |0, \alpha\rangle, \tag{7}$$

where $|0\rangle$ is the vacuum of electrons and the field operator $\psi_m^+(x_a)$ creates an electron in the transverse mode $m$ of lead $a$ with longitudinal coordinate $x_a$. As a result, the transmission probability can be written

$$\begin{aligned} T_{nm,ba,\beta a}(E) &\equiv |t_{nm,ba,\beta a}(E)|^2 \\ &= v_{Enb\beta} v_{Ema\alpha} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, e^{iE(t-s)/\hbar} \theta(s) \\ &\quad \times \theta(t) e^{-i\varepsilon_\beta(t_0 - s_0 + t)/\hbar} e^{i\varepsilon_\alpha(t_0 - s_0 + s)/\hbar} \langle 0, \alpha | \, \psi_m(x_a, s_0 - s) \psi_n^+(x_b, s_0) \, |0, \beta\rangle \\ &\quad \times \langle 0, \beta | \, \psi_n(x_b, t_0 + t) \, \psi_m^+(x_a, t_0) \, |0, \alpha\rangle, \end{aligned} \tag{8}$$

where the Heisenberg field operators have been introduced:

$$\psi_m(x_a, t) = e^{iHt/\hbar} \psi_m(x_a) \, e^{-iHt/\hbar}. \tag{9}$$

In deriving (8) we have used the fact that $H \, |0, \alpha\rangle = \varepsilon_\alpha \, |0, \alpha\rangle$. Due to time trans-

lational invariance (8) is independent of the variables $s_0$ and $t_0$, which have been introduced for convenience.

We are interested in quantities that describe the reduced dynamics of the electron, i.e., the dynamics that results from tracing out the bath coordinates. In particular, we would like to know the inelastic transmission probability $T_{nm,ba}(E_f, E_i)$ defined in such a way that the probability that an incident electron in mode $m$ of lead $a$ with energy $E_i$ is transmitted into mode $n$ of lead $b$ with energy between $E_f$ and $E_f + dE_f$ is $T_{nm,ba}(E_f, E_i)\, dE_f$. Such a probability distribution must be given by the relation

$$T_{nm,ba}(E_f, E_i) = \sum_{\alpha} P_\alpha \sum_{\beta} T_{nm,ba,\beta\alpha}(E_i + \varepsilon_\alpha)\, \delta(E_f - E_i + \varepsilon_\beta - \varepsilon_\alpha), \tag{10}$$

where

$$P_\alpha \equiv e^{-\beta\varepsilon_\alpha}/Z_B \tag{11}$$

is the thermal equilibrium distribution function for the isolated bath (note that $\alpha$ is a bath state and not a phonon mode) and the delta function guarantees the conservation of the total energy $E = E_i + \varepsilon_\alpha = E_f + \varepsilon_\beta$. In (10), it is assumed that the phonons are initially in thermal equilibrium and a sum is performed over all possible final bath states $|\beta\rangle$. The phenomenological description that results from tracing our the phonon coordinates contains the essence of dissipation.

We wish to emphasize that, although we usually refer to a phonon bath, Eq. (10) (and all those subsequently derived therefrom) is of a more general nature. As long as $H_B$ and $V$ are not specified, our expressions apply to any type of inelastic scattering where the dissipative degrees of freedom are assumed to be initially in thermal equilibrium.

Now we introduce the expression (8) into Eq. (10) and take advantage of its independence on the variables $t_0$ and $s_0$ (and in particular on their difference) and write the delta function as

$$\delta(E_f - E_i + \varepsilon_\beta - \varepsilon_\alpha) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d(t_0 - s_0)\, e^{i(E_f - E_i + \varepsilon_\beta - \varepsilon_\alpha)(t_0 - s_0)/\hbar}. \tag{12}$$

The terms in the phase which are proportional to $(\varepsilon_\beta - \varepsilon_\alpha)$ (note also the presence of the total energy $E$) cancel out and (10) becomes

$$\begin{aligned} T_{nm,ba}(E_f, E_i) = \frac{v_f v_i}{2\pi\hbar} \sum_{\alpha} P_\alpha \sum_{\beta} \iiint_{-\infty}^{\infty} & ds\, dt\, d(t_0 - s_0) \\ & \times e^{i[(E_f - E_i)(t_0 - s_0) + E_f t - E_i s]/\hbar} \theta(t)\, \theta(s) \langle 0, \alpha |\, \psi_m(x_a, s_0 - s) \\ & \times \psi_n^+(x_b, s_0)\, |0, \beta\rangle \langle 0, \beta |\, \psi_n(x_b, t_0 + t)\, \psi_m^+(x_a, t_0)\, |0, \alpha\rangle. \end{aligned} \tag{13}$$

By completeness, the sum over final bath states $|\beta\rangle$ yields the identity and can be removed. In going from (8) to (13), the velocities $v_{Emn\alpha} = v_{Eima}$ and $v_{Enb\beta} = v_{Efnb}$ have been replaced by $v_i$ and $v_f$, respectively, since these are quantities that depend

only on the initial and final electron states ($v_i$ is a function of $a$, $m$, and $E_i$). We rename $s_0 - t_0 \equiv \tau$ and make $t_0 = 0$ without loss of generality. The final result is

$$T_{nm,ba}(E_f, E_i) = \frac{v_f v_i}{2\pi\hbar} \iiint_{-\infty}^{\infty} d\tau\, ds\, dt\, e^{i[(E_i - E_f)\tau + E_f t - E_i s]/\hbar} \theta(t)\, \theta(s)$$
$$\times \langle \psi_m(x_a, \tau - s)\, \psi_n^+(x_b, \tau)\, \psi_n(x_b, t)\, \psi_m^+(x_a, 0) \rangle, \qquad (14)$$

where the expectation value of an operator $A$ is taken as the equilibrium thermal average over the phonon states in the absence of the electron:

$$\langle A \rangle = \sum_{\alpha} P_\alpha \langle 0, \alpha |\, A\, | 0, \alpha \rangle. \qquad (15)$$

Equation (14) is one of the central results of this work. It closely resembles the expression obtained by Wingreen *et al.* [22] in their analysis of the role of phonons in resonant tunneling. Actually, in Appendix B, where a lattice formulation of this study is presented, we show that with some suitable modifications our previous derivation can be used to exactly reproduce the result of Ref. [22]. We have thus generalized the equation for $T(E_f, E_i)$ derived by Wingreen *et al.* [22] to an arbitrary mesoscopic structure with many leads and many transverse channels on each lead and in which phonons are distributed in an extended finite region. In the next section, we give an alternative derivation of (14) based on a density matrix approach.

Finally, we note that a similar analysis for the reflection probability yields

$$R_{nm,aa}(E_f, E_i) = T_{nm,aa}(E_f, E_i) + \delta_{nm}\, \delta(E_f - E_i)[1 + 2\hbar v_i\, \mathrm{Im}\, G_{nn}^{(+)}(x_a, x_a; E_i)], \qquad (16)$$

where the first term on the right is to be taken as shorthand notation for an expression that is formally equivalent to (14) with $b = a$ and $x_b = x_a$. The second term on the r.h.s. of (16) is a correction to the full propagation contained in the first term. It removes the effect of direct propagation from $|\chi_m, x_a\rangle$ to $|\chi_m, x_a\rangle$ without reflection on the sample, much as in (1a). The dressed one-particle Green's function

$$G_{nm}^{(+)}(x_b, x_a; E) = \int_{-\infty}^{\infty} \frac{dt}{\hbar} e^{iEt/\hbar} [-i\theta(t) \langle \psi_n(x_b, t)\, \psi_m^+(x_a, 0) \rangle] \qquad (17)$$

(of which here we consider the case $b = a$ and $n = m$) stems from the interference between full and direct propagation (corresponding to the l.h.s. and first term of r.h.s. of (1a), respectively) that results from computing a probability.

The unitarity condition that all scattering probabilities must add up to one is not obviously satisfied by Eqs. (14) and (16). One may think that, in order to show that unitarity is preserved in the dissipative scattering, one has to go back to the basic relation (10) and its reflection counterpart and argue that the $S$-matrix of the total system electron plus bath is unitary. However, we show in Appendix C that unitarity can be explicitly derived from the general Eqs. (14) and (16) by invoking the continuity equation satisfied by the electron current and density operators.

B. *Elastic Scattering and Reducibility*

There is an essential relation between the irreducibility of the two-particle Green's function in Eq. (14) and the occurrence of inelastic scattering, by which we mean the existence of outgoing scattering channels in which the bath changes state, $|\beta\rangle \neq |\alpha\rangle$. To see this, we note that if one introduces the approximation

$$\begin{aligned}&\langle \psi_m(x_a, \tau - s)\, \psi_n^+(x_b, \tau)\, \psi_n(x_b, t)\, \psi_m^+(x_a, 0)\rangle \\ &\quad \approx \langle \psi_m(x_a, \tau - s)\, \psi_n^+(x_b, \tau)\rangle \langle \psi_n(x_b, t)\, \psi_m^+(x_a, 0)\rangle, \end{aligned} \tag{18}$$

the dependence on $\tau$ is lost because of time translational invariance and the integration over $\tau$ yields $2\pi\hbar\, \delta(E_f - E_i)$, which corresponds to elastic scattering. However, the expression resulting from introducing (18) in (14) is different from that which would be obtained in the total absence of phonons. The reason is that the approximation (18) amounts to neglecting inelastic scattering while including the dressing by phonons of the elastic peak. In an extended solid, the same effect is known as polaron shift or mass renormalization. If we define $T^0$ as the transmission probability that results from introducing the approximation (18), we easily find that

$$T^0_{nm,ba}(E_f, E_i) = T^0_{nm,ba}(E_i)\, \delta(E_f - E_i), \tag{19}$$

where

$$T^0_{nm,ba}(E) = \hbar^2 v_{Enb} v_{Ema} \, |G^{(+)}_{nm}(x_b, x_a; E)|^2 \tag{20}$$

and $G^{(+)}_{nm}(x_b, x_a; E)$ is the dressed single particle Green's function that was already defined in (17). Analogously,

$$R^0_{nm,aa}(E) = \hbar^2 v_{Ena} v_{Ema} \, |G^{(+)}_{nm}(x_a, x_a; E)|^2 + \delta_{nm}[1 + 2\hbar v_{Ena} G^{(+)}_{nn}(x_a, x_a; E)]. \tag{21}$$

If, in addition, we define $\delta G^{(+)}$ as the difference between the dressed and bare one-particle propagators,

$$\delta G^{(+)} \equiv G^{(+)} - G_0^{(+)}.$$

Equations (20) and (21) can be rewritten as

$$T^0_{nm,ba}(E) = |t_{nm,ba}(E) + i\hbar (v_{Enb} v_{Ema})^{1/2}\, e^{-i(k_{Enb} x_b + k_{Ema} x_a)}\, \delta G^{(+)}_{nm}(x_b, x_a; E)|^2 \tag{22a}$$

$$R^0_{nm,aa}(E) = |r_{nm,aa}(E) + i\hbar (v_{Ena} v_{Ema})^{1/2}\, e^{-i(k_{Ena} x_a + k_{Ema} x_a)}\, \delta G^{(+)}_{nm}(x_a, x_a; E)|^2, \tag{22b}$$

where $t_{nm,ba}$ and $r_{nm,aa}$ are the $S$-matrix elements in the total absence of phonons. While the obtention of (22a) is straightforward, the derivation of (22b) requires slightly more algebra. It is interesting to compare (22) with Eq. (1). Clearly, the second term within the absolute value signs corresponds to a modification of the effective elastic scattering amplitude due to the presence of phonons.

It is clear from the definitions (17), (20), and (21), and by inspection of Eq. (13) that $T^0$ and $R^0$ only contain contributions from processes where the initial and final

bath states are identical, i.e., where $|\beta\rangle = |\alpha\rangle$. Therefore, it is the fact that some final bath states may be different from the initial one, i.e., that some *real* modification can be introduced in the phonon bath, that renders the two-particle Green's function of Eq. (14) irreducible to the product of two single particle Green's functions. Thus we see that the dressed single particle Green's function only contains information on the elastic scattering processes, in which no trace is left in the phonon bath, while a complete (and in general irreducible) two-particle Green's function is required to fully describe dissipative scattering.

We have just seen the decoupled propagators only contain contributions from elastic scattering. However, not all the elastic processes are contained in $T^0$ and $R^0$. To see this, we note that, because of the definition (15), $T^0$ can be written

$$T^0_{nm,ba}(E) = \hbar^2 v_{Enb} v_{Ema} \left| \sum_\alpha P_\alpha G^{(+)}_{\alpha\alpha,nm}(x_b, x_a; E) \right|^2, \tag{23}$$

where

$$G^{(+)}_{\alpha\alpha,nm}(x_a, x_b; E) \equiv \int_{-\infty}^{\infty} \frac{dt}{\hbar} e^{iEt/\hbar} [-i\theta(t) \langle 0, \alpha | \psi_n(x_b, t) \psi^+_m(x_a, 0) | 0, \alpha \rangle]. \tag{24}$$

On the other hand, the total elastic contribution $T^{\text{el}}$ is obtained from (13) by restricting the sum over final states $|\beta\rangle$ to the case $|\beta\rangle = |\alpha\rangle$. Thus one can write

$$T^{\text{el}}_{nm,ba}(E) = \hbar^2 v_{Enb} v_{Ema} \sum_\alpha P_\alpha |G^{(+)}_{\alpha\alpha,nm}(x_b, x_a; E)|^2. \tag{25}$$

From comparison of (23) and (25) it is clear that, in general, $T^{\text{el}} \neq T^0$. The type of elastic processes that are contained in $T^{\text{el}}$ but not in $T^0$ are those in which the same phonon is first emitted and then reabsorbed, or vice versa, or combinations thereof. In principle, it is also possible to obtain the same effect if the two phonons are different but have the same energy. However, these processes would not be included in the definition (25), since they correspond to the case $\varepsilon_\beta = \varepsilon_\alpha$, but $|\beta\rangle \neq |\alpha\rangle$. The possibility of resonant elastic scattering is also encountered in other contexts, like, e.g., in the theory of Raman scattering [40]. The importance of the various types of elastic contributions (which may or may not correspond to distinct physical processes) has to be studied case by case in the different physical applications of this formalism.

We will return briefly to the above discussion in Section 4, where a diagrammatic perturbation theory is presented, and in Section 5, where some two-phonon diagrams are calculated.

### C. *Symmetry Properties*

Due to the fundamental time-reversal invariance of the total Hamiltonian (6), one can derive from general principles the microscopic symmetry relation

$$t_{nm,ba,\beta\alpha}(E) = t_{mn,ab,\alpha\beta}(E). \tag{26}$$

If this symmetry property is introduced in the basic equation (10), one obtains

$$T_{nm,ba}(E, E') = e^{\beta(E'-E)} T_{mn,ab}(E', E), \tag{27}$$

which is a detailed balance equation that guarantees the suppression of current in the absence of driving forces (see, however, the discussion in Section 6). For the derivation of (27), crucial use as been made of energy conservation and of the fact that the bath is initially in an equilibrium (Boltzmann) distribution.

An interesting corollary of the symmetry relation (27) is the compatibility between irreversible thermalization and microscopic reversibility. In effect, we can think of a sufficiently large phonon bath such that any electron that enters the bath will leave it in a thermal energy distribution, regardless of its initial energy. In the absence of other electrons the inelastic transmission probability would be of the type

$$T_{nm,ba}(E_f, E_i) = Ce^{-\beta E_f} \tag{28}$$

(where $C$ is a constant), i.e., a Boltzmann distribution independent of the electron initial quantum numbers and of the final channel indices (equipartition of energy). No matter how "irreversible" the scattering probability (28) looks at first sight, it satisfies the symmetry relation (27) and is therefore entirely compatible with the reversibility of the microscopic laws.

## 3. Density Matrix Approach

Here we rederive the results of Section 2 following a density matrix approach that has been widely used in the literature on dissipation in quantum mechanics [34–36], usually in the context of time dependent formulations. We show here that this approach can also be applied to the study of stationary dissipative scattering. To establish a connection between real time dynamics and scattering properties in energy space, it is convenient to consider the evolution of an incident wave packet, as is done in Appendix A for the case of phonon-free scattering. The technical points on the validity of the conceptual framework apply identically here and will not be discussed again.

### A. *The Propagator*

If $\bar{\rho}(t_0)$ is the density matrix of the total system (electron plus phonons) at a time $t_0$, then at another time $t$

$$\bar{\rho}(t) = e^{-iH(t-t_0)/\hbar} \bar{\rho}(t_0)\, e^{iH(t-t_0)/\hbar}, \tag{29}$$

where $H$ is the total Hamiltonian given in (6). It is common to assume decoupled initial conditions for the particle-bath system,

$$\bar{\rho}(t_0) = \rho_P \cdot \rho_B, \tag{30}$$

where $\rho_P$ is the density matrix for the electron (which usually is taken in a pure state, $\rho_P = |\psi\rangle\langle\psi|$) and $\rho_B = e^{-\beta H_B}/Z_B$ describes the bath in thermal equilibrium. In the particular problem which we are considering, the assumption of decoupled initial conditions is entirely appropriate, since at $t = t_0$ the incident electron wave packet is complete localized in one of the asymptotic leads and no interaction with the phonons in the same region has yet occurred. The subsequent evolution of the density matrix is given by (29). Since we are not explicitly interested in the phonon dynamics, we focus on the reduced density matrix that results from tracing out the phonon coordinates,

$$\rho(t) \equiv Tr_B \bar{\rho}(t), \tag{31}$$

which in principle describes completely the electron dynamics. Note that this step is similar in spirit to that given in Eq. (10), where an equal weight sum is done on the final phonon states (equivalent to the $Tr_B$ of (31)) and initial thermal equilibrium is assumed for the bath (equivalent of (30)). At $t = t_0$, of course, $\rho(t_0) = \rho_P$. The reduced density matrices at different times are related by a propagator $J$,

$$\rho(t) = J(t, t_0)\, \rho(t_0) \tag{32}$$

or, in a coordinate representation,

$$\rho(\mathbf{x}, \mathbf{x}'; t) = \iint d\tilde{\mathbf{x}}\, d\tilde{\mathbf{x}}'\, J(\mathbf{x}, \mathbf{x}', t; \tilde{\mathbf{x}}, \tilde{\mathbf{x}}', t_0)\, \rho(\tilde{\mathbf{x}}, \tilde{\mathbf{x}}'; t_0), \tag{33}$$

where $\rho(\mathbf{x}, \mathbf{x}'; t) \equiv \langle \mathbf{x}|\, \rho(t)\, |\mathbf{x}'\rangle$. Below we derive an expression for the propagator $J$ in terms of a two-particle Green's function.

Equations (29) and (31) can be combined into

$$\begin{aligned}\rho(\mathbf{x}, \mathbf{x}'; t) &= \sum_{\beta} \langle \mathbf{x}, \beta|\, e^{-iH(t-t_0)/\hbar} \frac{e^{-\beta H_B}}{Z_B} \rho_P\, e^{iH(t-t_0)/\hbar}\, |\mathbf{x}', \beta\rangle \\ &= \iint d\tilde{\mathbf{x}}\, d\tilde{\mathbf{x}}' \sum_{\beta} \sum_{\alpha} \frac{e^{-\beta E_\alpha}}{Z_B} \langle \mathbf{x}, \beta|\, e^{-iH(t-t_0)/\hbar}\, |\tilde{\mathbf{x}}, \alpha\rangle \\ &\quad \times \langle \tilde{\mathbf{x}}', \alpha|\, e^{iH(t-t_0)/\hbar}\, |\mathbf{x}', \beta\rangle\, \rho(\tilde{\mathbf{x}}, \tilde{\mathbf{x}}'; t_0),\end{aligned} \tag{34}$$

where completeness has been introduced in the second equality. As in Section 2, we introduce second quantization for the electron:

$$|\mathbf{x}, \alpha\rangle = \psi^+(\mathbf{x})\, |0, \alpha\rangle. \tag{35}$$

If a Heisenberg picture is adopted (see Eq. (9)) one can write ($t_0 = 0$)

$$J(\mathbf{x}, \mathbf{x}', t; \tilde{\mathbf{x}}, \tilde{\mathbf{x}}', 0) = \theta(t) \langle \psi(\tilde{\mathbf{x}}', 0)\, \psi^+(\mathbf{x}', t)\, \psi(\mathbf{x}, t)\, \psi^+(\tilde{\mathbf{x}}, 0) \rangle, \tag{36}$$

where the step function $\theta(t)$ has been introduced to emphasize retarded propagation and, more important, to remind that the evolution of the *reduced* density matrix is not time symmetric. In fact, the result (36) does depend on the particular

choice of initial conditions (30). This should have been expected, since the reduced electron motion depends implicity on the bath dynamics, and information on it has been lost in the tracing process (different total density matrices can yield the same reduced density matrix). Therefore, for a relation like (33) to be meaningful, and explicit prescription has to be given to obtain the initial total density matrix from the reduced one. This is what we mean by sensitivity to the choice of initial conditions. However, for reasons commented before (namely, the adequacy of (30)), this dependence does not affect the generality of our scattering analysis. Rammer [29] has performed a diagrammatic analysis of the propagator $J(\mathbf{x}, \mathbf{x}', t; \tilde{\mathbf{x}}, \tilde{\mathbf{x}}, 0)$. However, unlike we do here, he does not use second quantization for the single electron.

A quick comparison of Eqs. (14) and (36) seems to suggest a paradox: a computation of the transmission probability requires full knowledge of the dependence of the two-particle Green's function on its three meaningul time variables, while the propagator $J(t)$ only requires knowledge of the dependence of an equivalent (except for the trivial transformation (41)) Green's function on one time variable. One may naively conclude that, given that less information is contained in the expression for $J(\mathbf{x}, \mathbf{x}; t; \tilde{\mathbf{x}}, \mathbf{x}', 0)$ than is required in the calculation of $T_{nm,ba}(E_f, E_i)$, the general belief that the reduced density matrix contains all the information on the particle dynamics is wrong, since, in particular, it cannot be used to compute inelastic scattering probabilities (which require three time variables). However, a more careful consideration suggests that there must be a flaw in the previous argument, since, with complete knowledge of $J(t)$ one should be able to follow the evolution of an incident wave packet and, by analyzing it at a much later time, one could infer the scattering probabilities. But, if that is effectively so, how can one recover the required information on three time variables from an expression like (36) that only contains one? The solution to this apparent contradiction lies in the realization that, while $T_{nm,ba}(E_f, E_i)$ requires detailed knowledge of the temporal dependence of the Green's function, very little information is needed on its spatial dependence (only its value at two points $x_b$ and $x_a$ in modes $\chi_n$ and $\chi_m$). On the other hand, full knowledge of $J(\mathbf{x}, \mathbf{x}', t; \tilde{\mathbf{x}}, \tilde{\mathbf{x}}', 0)$ (and thus of $\rho(\mathbf{x}, \mathbf{x}'; t)$) requires complete information on the *spatial* dependence of the Green's function and very little on its *temporal* dependence. If the two approaches are complete, there must be a trade of information between temporal and spatial properties. The conversion between time and space dependence can be made in the asymptotic leads, where the electron propagates freely and a well-defined correlation between time evolution and spatial behavior exists. Below we implement this idea and show that one can effectively use Eqs. (33) and (36) to derive Eqs. (14) and (16).

B. *Scattering Probabilities*

Let us consider an initial wave packet

$$\Psi^{-}_{E_i ma}(\mathbf{x}, t_0) = \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E_i}{\Delta\varepsilon}\right) \xi^{-}_{\varepsilon ma}(\mathbf{x})\, e^{-i\varepsilon t_0/\hbar} \tag{37}$$

that at $t_0 \sim -T$ is approaching the sample from lead $a$ in mode $m$, with an energy distribution that is strongly peaked around $E_i$ with a small width $\Delta\varepsilon$ and which at the same time is sufficiently localized in space for the amplitude in the sample region to be negligible (see Appendix A for an explanation of the notation in Eq. (37) and for a detailed account of the assumptions involved). With decoupled initial conditions, the reduced density matrix at $t_0 \sim -T$ is that of a pure state,

$$\rho^{-}_{E_i ma}(t_0) = |\Psi^{-}_{E_i ma}(t_0)\rangle\langle\Psi^{-}_{E_i ma}(t_0)|. \tag{38}$$

The evolution of the density matrix at a later time is given by (32). We wish to extract information on the scattering probabilities by analyzing $\rho^{-}_{E_i ma}(t)$ at a much later time $t \sim T$, when the wave function has evolved into several (or a continuum of) outgoing wave packets that lie entirely in the asymptotic leads. For that purpose, we first note that, in general, if a density matrix, $\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j|$, is written in terms of eigenstates of an operator $A$, $A|i\rangle = a_i|i\rangle$, then the probability that an observable $A$ takes the eigenvalue $a_i$ is simply $P(a_i) = \rho_{ii} = \langle i|\rho|i\rangle$. By extending this argument to the continuum of energy eigenstates in the asymptotic leads, $\xi^{\pm}_{Enb}(\mathbf{x})$, we write

$$T_{nm,ba}(E_f, E_i) = \langle \xi^{+}_{E_f nb}| J(t, t_0)\, \rho^{-}_{E_i ma}(t_0) |\xi^{+}_{E_f nb}\rangle, \tag{39}$$

where $\Delta\varepsilon \to 0$, $t \sim T$, and $t_0 \sim -T$ (see once more Appendix A for details on the notation). The normalization $\langle \xi^{+}_{Ena}| \xi^{+}_{E'na}\rangle = \delta(E - E')$ (see Eq. (A5)) gives Eq. (39) the right units of energy probability distribution. From (36)–(38), Eq. (39) can be more explicitly written

$$\begin{aligned} T_{nm,ba}(E_f, E_i) = {} & \iint_{L_b} d\mathbf{x}\, d\mathbf{x}' \iint_{L_a} d\tilde{\mathbf{x}}\, d\tilde{\mathbf{x}}' \iint d\varepsilon\, d\varepsilon' \\ & \times \frac{1}{\Delta\varepsilon} \Phi^*\left(\frac{\varepsilon - E_i}{\Delta\varepsilon}\right) \Phi\left(\frac{\varepsilon' - E_i}{\Delta\varepsilon}\right) e^{i(\varepsilon - \varepsilon')t_0/\hbar} \\ & \times [\xi^{+}_{E_f nb}(\mathbf{x}')\, \xi^{-}_{\varepsilon ma}(\tilde{\mathbf{x}})]^*\, \xi^{+}_{E_f nb}(\mathbf{x})\, \xi^{-}_{\varepsilon' ma}(\tilde{\mathbf{x}}') \\ & \times \theta(t - t_0)\langle \psi(\tilde{\mathbf{x}}, t_0)\, \psi^{+}(\mathbf{x}, t)\, \psi(\mathbf{x}', t)\, \psi^{+}(\tilde{\mathbf{x}}', t_0)\rangle. \end{aligned} \tag{40}$$

Here we recall that the incoming (outgoing) wave packet is entirely localized in the semi-infinite lead $L_a(L_b)$ and the domain of the space integral in (40) can be replaced by $L_a \cup L'_a(L_b \cup L'_b)$, as derived in Appendix A. If now we introduce the transformation

$$\psi^{+}_m(x_a) = \int dy_a\, \chi_m(y_a)\, \psi^{+}(\mathbf{x}_a). \tag{41}$$

which can be easily derived from the definitions (7) and (35), Eq. (40) becomes

$$T_{nm,ba}(E_f, E_i) = \iiiint_{-\infty}^{\infty} dx_a\, dx_b\, dx'_b\, dx'_a \iint d\varepsilon\, d\varepsilon' \times \frac{1}{\Delta\varepsilon} \Phi^*\left(\frac{\varepsilon - E_i}{\Delta\varepsilon}\right) \Phi\left(\frac{\varepsilon' - E_i}{\Delta\varepsilon}\right) e^{i(\varepsilon - \varepsilon')t_0/\hbar} \times \frac{e^{ik_{Efnb}(x_b - x'_b)}\, e^{i(k_{Ema}x_a - k_{\varepsilon' nm}x'_a)}}{(2\pi\hbar)^2 v_{Efnb}(v_{\varepsilon ma} v_{\varepsilon' ma})^{1/2}} \times \theta(t - t_0)\langle \psi_m(x_a, t_0)\, \psi_n^+(x_b, t)\, \psi_n(x'_b, t)\, \psi_m^+(x'_a, t_0)\rangle. \quad (42)$$

In order to proceed further, we analyze a more general Green's function

$$G_{mnnm}(x_a, x_b, x'_b, x'_a; t_a, t_b, t'_b, t'_a) \equiv \theta(t_b - t_a)\, \theta(t'_b - t'_a)\langle \psi_m(x_a, t_a)\, \psi_n^+(x_b, t_b)\, \psi_n(x'_b, t'_b)\, \psi_m^+(x'_a, t'_a)\rangle \quad (43a)$$

of which the expression (42) contains a particular case ($t'_a = t_a = t_0$ and $t'_b = t_b = t$). Let us introduce the Fourier transform of (43a):

$$G_{mnnm}(x_a, x_b, x'_b, x'_a; t_a, t_b, t'_b, t'_a) \equiv \iiiint \frac{d\varepsilon_a\, d\varepsilon_b\, d\varepsilon'_b\, d\varepsilon'_a}{(2\pi)^4} \times e^{i(\varepsilon_b t_b - \varepsilon_a t_a + \varepsilon'_a t'_a - \varepsilon'_b t'_b)/\hbar} G_{mnnm}(x_a, x_b, x'_b, x'_a; \varepsilon_a, \varepsilon_b, \varepsilon'_b, \varepsilon'_a). \quad (43b)$$

Since both the incoming and the outgoing wave packets are entirely localized in the asymptotic regions, it is possible to find two reference points $\bar{\mathbf{x}}_a \in L_a$ and $\bar{\mathbf{x}}_b \in L_b$ such that $\bar{x}_a < x_a, x'_a$ and $\bar{x}_b < x_b, x'_b$ for all the values of $x_a, x'_a, x_b$, and $x'_b$ that effectively contribute to the integrals in (42). In these conditions, one can write

$$G_{mnnm}(x_a, x_b, x'_b, x'_a; \varepsilon_a, \varepsilon_b, \varepsilon'_b, \varepsilon'_a) = G_{mnnm}(\bar{x}_a, \bar{x}_b, \bar{x}_b, \bar{x}_a; \varepsilon_a, \varepsilon_b, \varepsilon'_b, \varepsilon'_a) \exp[-ik_{\varepsilon_a ma}(x_a - \bar{x}_a) - ik_{\varepsilon_b nb}(x_b - \bar{x}_b) + ik_{\varepsilon'_b nb}(x'_b - \bar{x}_b) + ik_{\varepsilon'_a ma}(x'_a - \bar{x}_a)], \quad (44)$$

which must be compared with the similar relation (A18) for the single particle Green's function. To justify Eq. (44) we must consider first the phonon-free case, in which the two-particle Green's function is given by the product of the advanced ($G_0^{(-)}$) and the retarded ($G_0^{(+)}$) one-particle Green's functions. More specifically, in the absence of phonons,

$$G^0_{mnnm}(x_a, x_b, x'_b, x'_a; \varepsilon_a, \varepsilon_b, \varepsilon'_b, \varepsilon'_a) = (2\pi)^2\, \delta(\varepsilon_a - \varepsilon_b)\, \delta(\varepsilon'_a - \varepsilon'_b)\, G^{0(-)}_{mn}(x_a, x_b; \varepsilon_a)\, G^{0(+)}_{nm}(x'_b, x'_a; \varepsilon'_a), \quad (45)$$

where

$$G_{nm}^{0(\pm)}(x_b, x_a; \varepsilon) = \int \frac{dt}{\hbar} e^{i\varepsilon t/\hbar} G_{nm}^{0(\pm)}(x_b, x_a; t)$$
$$G_{nm}^{0(\pm)}(x_b, x_a; t) = \mp i\theta(\pm t)\langle \psi_n(x_b, t)\, \psi_m^{+}(x_a, 0)\rangle_0, \tag{46}$$

where $\langle A\rangle_0 \equiv \langle 0|\, A\, |0\rangle$ and $|0\rangle$ is the electron vacuum. It is easy to show that the definitions (46) and (2) are equivalent. From (A18) it is clear that Eq. (44) is obeyed in the absence of phonons. Since the relation (44) is a property of the asymptotic propagation in the leads, where the electron does not interact with phonons, it should hold regardless of the presence of phonons in the sample region. Equation (44) provides the crucial link between spatial and temporal (through the energy variable) dependence to which we referred before.

If (44) is introduced in (43b) and (42), the space integrals can be trivially performed. They yield the product of energy delta functions $\delta(\varepsilon_a - \varepsilon)\ \delta(\varepsilon_b - E_f)\ \delta(\varepsilon_b' - E_f)\ \delta(\varepsilon_a' - \varepsilon')$ and with proper account of all the factors involved, one obtains

$$T_{nm,ba}(E_f, E_i) = \left(\frac{\hbar}{2\pi}\right)^2 v_{E_f nb} \iint d\varepsilon\, d\varepsilon' \frac{1}{\Delta\varepsilon} \Phi^*\left(\frac{\varepsilon - E_i}{\Delta\varepsilon}\right) \Phi\left(\frac{\varepsilon' - E_i}{\Delta\varepsilon}\right) (v_{\varepsilon ma} v_{\varepsilon' ma})^{1/2}$$
$$\times G_{mnnm}(\bar{x}_a, \bar{x}_b, \bar{x}_b, \bar{x}_a; \varepsilon, E_f, E_f, \varepsilon')\, e^{i(k_{\varepsilon ma} - k_{\varepsilon' ma})\bar{x}_a}, \tag{47}$$

where the time-dependent phase factors have canceled.

Now we can Fourier transform back but, instead of returning to the former time variables $t_a, t_b, t_b', t_a'$ (see Eq. (43)), we introduce new time variables

$$t_a = t_0 + \tau - s, \qquad t_b = t_0 + \tau, \qquad t_b' = t_0 + t, \qquad t_a' = t_0. \tag{48}$$

We have (the bars are removed from the $x$'s)

$$G_{mnnm}(x_a, x_b, x_b, x_a; \varepsilon, E_f, E_f, \varepsilon')$$
$$= \frac{1}{\hbar^4} \iiiint dt\, ds\, d\tau\, dt_0 G_{mnnm}(x_a, x_b, x_b, x_a; t_0 + \tau - s, t_0 + \tau, t_0 + t, t_0)$$
$$\times e^{i[(\varepsilon' - \varepsilon)t_0 + (\varepsilon - E_f)\tau + E_f t - \varepsilon s]/\hbar}. \tag{49}$$

Due to time-translational symmetry the $G$ in (49) is independent of the variable $t_0$ whose integration therefore yields $2\pi\hbar\, \delta(\varepsilon - \varepsilon')$. If we now take the limit $\Delta\varepsilon \to 0$, the weight function becomes $\delta(\varepsilon - E_i)$ (see Eq. (A2)) and the final result is

$$T_{nm,ba}(E_f, E_i) = \frac{v_f v_i}{2\pi\hbar} \iiint_{-\infty}^{\infty} d\tau\, dt\, ds\, e^{i[(E_i - E_f)\tau + E_f t - E_i s]/\hbar}$$
$$\times G_{mnnm}(x_a, x_b, x_b, x_a; \tau - s, \tau, t, 0), \tag{50}$$

which is exactly the result we obtained in the previous section (see Eq. (14) and the definition (43a)).

A similar analysis can be performed for the reflection probability. However, like in the elastic case studied in Appendix A, the propagation of the purely reflected wave has to be properly isolated in order to apply a relation similar to (44). In the dissipative case studied here, the separation between direct and reflected components is slightly more subtle due to the presence of crossed terms. The most convenient procedure is to consider the phonon-free case and perform an appropriate extrapolation to the dissipative case. Apart from this delicate step, the rest of the derivation runs analogous to that of the transmission seen above. In this way one can rederive Eq. (16).

## 4. Diagrammatic Perturbation Theory

In this section we derive the rules for a diagrammatic perturbation theory in the electron–phonon interaction, which we take of the rather general form

$$V=\sqrt{\lambda}\sum_q \int d\mathbf{x}\, M_q(\mathbf{x})\,\rho(\mathbf{x})\,A_q, \tag{51}$$

where $\rho(\mathbf{x})\equiv\psi^+(\mathbf{x})\,\psi(\mathbf{x})$ is the electron density operator, $A_q\equiv a_q+a^+_{-q}$ is the phonon field operator, $a_q(a_q^+)$ being the destruction (creation) operator of phonon mode $q$, and $\lambda$ is a dimensionless coupling constant which we introduce for convenience. The only restriction on the function $M_q(\mathbf{x})$ is that it must be nonzero only in a finite region of space. The Hermiticity of $V$ implies $M_q(\mathbf{x})=M^*_{-q}(\mathbf{x})$, where $-q$ is the time-reversed of phonon mode $q$. Typically both modes are identical if (as we actually assume here) they are localized. Throughout this section, we assume that the electron motion in the absence of phonons (given by the Hamiltonian (3) and the Green's functions (2)) is known exactly. The Hamiltonian for the isolated phonon system is of course $H_B=\sum_q \hbar\omega_q a_q^+ a_q$.

### A. *Preservation of Unitarity in Perturbation Theory*

Before we develop explicitly a perturbation theory in $V$, we show that unitarity will be preserved to all orders in the coupling constant $\lambda$. In our problem, the condition of conservation of probability can be stated as

$$F_{ma}(E_i)\equiv\int\left[\sum_{nb} T_{nm,ba}(E_f,E_i)+\sum_n R_{nm,aa}(E_f,E_i)\right]dE_f=1 \tag{52}$$

for all energies $E_i$ and channels $ma$.

If the scattering probabilities are calculated in perturbation theory, one should be able to expand $F_{ma}(E)$ in powers of the coupling constant

$$F_{ma}(E)=F^{(0)}_{ma}(E)+\lambda F^{(1)}_{ma}(E)+\lambda^2 F^{(2)}_{ma}(E)+\cdots \tag{53}$$

(the coefficients of the odd powers in $\sqrt{\lambda}$ are zero for trivial reasons). The zeroth

order term $F^{(0)}_{ma}(E)$ is given by (52) in the particular case were $\lambda = 0$. This corresponds to the scattering of one electron in the absence of phonons, where unitarity must also be satisfied. Thus, $F^{(0)}_{ma}(E) = 1$. Since, on the other hand, $F_{ma}(E) = 1$ for all values of $\lambda$, then we must have $F^{(k)}_{ma}(E) = 0$ for $k \geqslant 1$. In other words, unitarity is satisfied to all orders in perturbation theory. The situation is similar to that which we encounter in standard scattering theory where the unitary condition $S^+S = 1$, must be fulfilled for any value of the coupling constant [41]. However, it is very common to develop perturbation theories for probability amplitudes. In those cases, unitarity is only satisfied after the amplitudes have been squared and only the terms that contribute to a given order are selected. In our approach, we develop a perturbation theory for scattering probabilities and unitarity is thus automatically satisfied within each order if all the corresponding diagrams are calculated. An explicit check of unitarity is presented in the next section for a simple case.

B. *Real Time Description*

It is clear from (14) and (50) that the reduced scattering probabilities can be obtained from the dressed two-particle Green's function defined in (43). In order to develop a diagrammatic perturbation theory in the electron–phonon interaction, we would like to write the field operators of (14) in a time-ordered form, so that Wick's theorem can be directly applied. To that end, we note that the two-particle Green's function in (14) can be written

$$\begin{aligned} &G_{mnnm}(x_a, x_b, x_b, x_a; t_a, t_b, s_b, s_a) \\ &\quad \equiv \theta(t_b - t_a)\,\theta(s_b - s_a)\langle \psi_m(x_a, t_a)\,\psi_n^+(x_b, t_b)\,\psi_n(x_b, s_b)\,\psi_m^+(x_a, s_a)\rangle \\ &\quad = \langle T_\gamma \psi_m(x_a, t_a)\,\psi_n^+(x_b, t_b)\,\psi_n(x_b, s_b)\,\psi_m^+(x_a, s_a)\rangle, \end{aligned} \tag{54}$$

where $T_\gamma$ indicates time ordering in the time contour $\gamma$ shown in Fig. 2, sometimes called the Keldysh contour. To obtain (54), we have used the fact that, by definition, the times $t_a$ and $t_b$ always are later in $\gamma$ than $s_a$ and $s_b$ and that, in the absence of other electrons, (54) vanishes if $s_b < s_a$ or $t_b < t_a$ (equivalent to $t_b >_\gamma t_a$ in the contour $\gamma$), since in those cases a destruction operator is on the right or a creation operator is on the left.

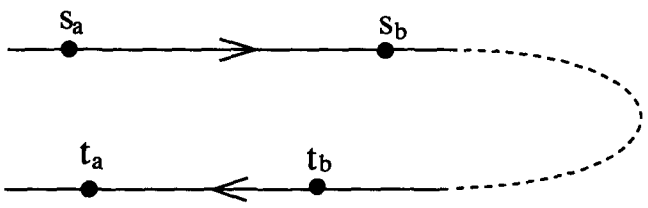


FIG. 2. Time ordering in the Keldysh contour.

To obtain a more symmetric notation we will introduce some changes. First, we adopt a position representation for both the $x$ and $y$ coordinates:

$$\psi_m^+(x_a) = \int dy_a \chi_m(y_a)\, \psi^+(\mathbf{x}_a), \tag{55}$$

where $\mathbf{x}_a \equiv (x_a, y_a)$. Equation (54) becomes

$$\begin{aligned} &G_{mnnm}(x_a, x_b, x_b, x_a; t_a, t_b, s_b, s_a) \\ &\quad = \iiiint dy_a\, dy_b\, dy'_b\, dy'_a \chi_m^*(y_a)\, \chi_n(y_b)\, \chi_n^*(y'_b)\, \chi_m(y'_a) \\ &\qquad \times G(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}'_b, \mathbf{x}'_a; t_a, t_b, s_b, s_a), \end{aligned} \tag{56}$$

where $\mathbf{x}'_b = (x_a, y'_a)$

$$\begin{aligned} &G(\mathbf{x}_a, \mathbf{x}'_b, \mathbf{x}'_b, \mathbf{x}'_a; t_a, t_b, s_b, s_a) \\ &\quad \equiv \theta(t_b - t_a)\, \theta(s_b - s_a) \langle \psi(\mathbf{x}_a, t_a)\, \psi^+(\mathbf{x}_b, t_b)\, \psi(\mathbf{x}'_b, s_b)\, \psi^+(\mathbf{x}'_a, s_a) \rangle \\ &\quad = \langle T_\gamma \psi(\mathbf{x}_a, t_a)\, \psi^+(\mathbf{x}_b, t_b)\, \psi(\mathbf{x}'_b, s_b)\, \psi^+(\mathbf{x}'_a, s_a) \rangle. \end{aligned} \tag{57}$$

Now we introduce the interaction picture, in which

$$\hat{A}(t) \equiv e^{i(H_0 + H_B)t/\hbar}\, A\, e^{-i(H_0 + H_B)t/\hbar}. \tag{58}$$

The operators in the Heisenberg and interaction picture are related by

$$A(t) = \hat{U}(0, t)\, \hat{A}(t)\, \hat{U}(t, 0), \tag{59}$$

where

$$\hat{U}(t, t_0) \equiv T \exp\left\{ \frac{-i}{\hbar} \int_{t_0}^{t} dt' \hat{V}(t') \right\} \tag{60}$$

is the evolution operator in the interaction picture. Equation (57) can then be written

$$\begin{aligned} &\langle T_\gamma \hat{U}(0, t_a)\, \hat{\psi}(\mathbf{x}_a, t_a)\, \hat{U}(t_a, t_b)\, \hat{\psi}^+(\mathbf{x}_b, t_b)\, \hat{U}(t_b, s_b)\, \hat{\psi}(\mathbf{x}'_b, s_b) \\ &\quad \hat{U}(s_b, s_a)\, \hat{\psi}^+(\mathbf{x}'_a, s_a)\, \hat{U}(s_a, 0) \rangle. \end{aligned} \tag{61}$$

Note that here $\hat{U}(0, t_a)$ and $\hat{U}(s_a, 0)$ can be replaced by the identity, since they are acting on states without electrons, but for the same reason they can be replaced by $\hat{U}(-\infty, t_a)$ and $\hat{U}(s_a, -\infty)$. On the other hand, $\hat{U}(t_b, s_b)$ is equivalent to $\hat{U}(t_b, \infty)\, \hat{U}(\infty, s_b)$ and (57) can thus be written formally as

$$\begin{aligned} &G(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}'_b, \mathbf{x}'_a; t_a, t_b, s_b, s_a) \\ &\quad = \langle T_\gamma \hat{\psi}(\mathbf{x}_a, t_a)\, \hat{U}(-\infty, \infty)\, \hat{\psi}^+(\mathbf{x}_b, t_b)\, \hat{\psi}(\mathbf{x}'_b, s_b)\, \hat{U}(\infty, -\infty)\, \hat{\psi}^+(\mathbf{x}'_a, s_a) \rangle. \end{aligned} \tag{62}$$

On the other hand, due to time-translational invariance, the Green's function (57) remains invariant under a global time shift:

$$G(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}'_b, \mathbf{x}'_a; \tau - s, \tau, t, 0) = G(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}'_b, \mathbf{x}'_a; t_0 + \tau - s, t_0 + \tau, t_0 + t, t_0). \quad (63)$$

If, instead of $T_{nm,ba}(E_f, E_i)$, we decide to compute

$$P_{nm,ba}(E_f; E_i, E'_i) \equiv T_{nm,ba}(E_f, E_i)\, \delta(E_i - E'_i), \quad (64)$$

the resulting expression is more symmetric in the four time variables since, due to (63), the delta function can be replaced by

$$\delta(E_i - E'_i) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt_0\, e^{i(E_i - E'_i)t'_0/\hbar}. \quad (65)$$

Once $P_{nm,ba}(E_f; E_i, E'_i)$ is known, the interesting quantity $T_{nm,ba}(E_f, E_i)$ can be trivially obtained from the relation

$$T_{nm,ba}(E_f, E_i) = \int P_{nm,ba}(E_f; E_i, E'_i)\, dE'_i. \quad (65a)$$

By introducing some obvious changes of variables, one obtains

$$P_{nm,ba}(E_f; E_i, E'_i) = \frac{v_f v_i}{(2\pi\hbar)^2} \int\int\int\int_{-\infty}^{\infty} ds_a\, ds_b\, dt_b\, dt_a \times e^{i[E'_i t_a - E_i s_a - E_f(t_b - s_b)]/\hbar} G_{mnnm}(x_a, x_b, x_b, x_a; t_a, t_b, s_b, s_a). \quad (66)$$

It is preferable to compute (66) instead of (14) because when (56) and (62) are introduced in (66) and the $\hat{U}$'s in (62) are expanded in powers of the interaction and Wick's theorem is applied to each term, the resulting contractions will depend on the time differences and, after Fourier transforming, the time integrals in (66) will be evaluated exactly and then we will be able to formulate the Feynman rules for the calculation of (66) directly in the energy space.

By expanding the evolution operators in (62), we obtain

$$\begin{aligned} G(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}'_b, \mathbf{x}'_a; t_a, t_b, s_b, s_a) &= \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} i^{k-j} \frac{(\lambda/\hbar)^{k+j}}{k!\, j!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_k \int_{-\infty}^{\infty} ds_j \cdots \int_{-\infty}^{\infty} ds_1 \\ &\times \int d\mathbf{x}_1 \cdots d\mathbf{x}_k\, d\mathbf{x}'_j \cdots d\mathbf{x}'_1 \sum_{p_1} \cdots \sum_{p_k} \sum_{q_j} \cdots \sum_{q_1} \\ &\times M_{p_1}(\mathbf{x}_1) \cdots M_{p_k}(\mathbf{x}_k)\, M_{q_j}(\mathbf{x}'_j) \cdots M_{q_1}(\mathbf{x}'_1) \\ &\times \langle T_\gamma \hat{A}_{p_1}(t_1) \cdots \hat{A}_{p_k}(t_k)\, \hat{A}_{q_j}(s_j) \cdots \hat{A}_{q_1}(s_1) \rangle \\ &\times \langle T_\gamma \hat{\psi}(\mathbf{x}_a, t_a)\, \hat{\rho}(\mathbf{x}_1, t_1) \cdots \hat{\rho}(\mathbf{x}_k, t_k)\, \hat{\psi}^+(\mathbf{x}_b, t_b)\, \hat{\psi}(\mathbf{x}'_b, s_b) \\ &\times \hat{\rho}(\mathbf{x}'_j, s_j) \cdots \hat{\rho}(\mathbf{x}_1, s_1)\, \hat{\psi}^+(\mathbf{x}_a, s_a) \rangle. \end{aligned} \quad (67)$$

Now we apply the statistical Wick's theorem to the expectation value of the time-ordered product of field operators [42]. One can easily convince oneself that, in the absence of a many-body background, the only nonvanishing contractions are those that pair electron operators in the same time branch, since for each contraction of the type $\langle T_\gamma \psi(t)\, \psi^+(s)\rangle = \langle \psi(t)\, \psi^+(s)\rangle$, there must be in the same term another contraction of the type $\langle T_\gamma \psi^+(t)\, \psi(s)\rangle = 0$. This is not the case for the phonon operators, for which we can have contractions within the same time branch, giving rise to terms of the type $\langle TA_q(s)\, A_q^+(s')\rangle$ or $\langle \tilde{T}A_q(t)\, A_q^+(t')\rangle$ ($\tilde{T}$ stands for anti-time ordering), or between the two branches, $\langle A_q(t)\, A_q^+(s)\rangle$.

Thus, the expectation value of the time-ordered product of electron operators can be effectively replaced by

$$k!\, j!\, i^{j-k} G_0^{(-)}(\mathbf{x}_a, \mathbf{x}_1; t_a - t_1) \cdots G_0^{(-)}(\mathbf{x}_k, \mathbf{x}_b; t_k - t_b) \times G_0^{(+)}(\mathbf{x}_b, \mathbf{x}_j'; s_b - s_j) \cdots G_0^{(+)}(\mathbf{x}_1', \mathbf{x}_a; s_1 - s_a), \tag{68}$$

where

$$\begin{aligned} G_0^{(+)}(\mathbf{x}, \mathbf{x}'; t) &= -i\langle T\hat{\psi}(\mathbf{x}, t)\, \hat{\psi}^+(\mathbf{x}', 0)\rangle \\ G_0^{(-)}(\mathbf{x}, \mathbf{x}'; t) &= i\langle \tilde{T}\hat{\psi}(\mathbf{x}, t)\, \hat{\psi}^+(\mathbf{x}', 0)\rangle \end{aligned} \tag{69}$$

are the time-ordered and anti-time-ordered unperturbed Green's function. In the absence of other electrons, we can write

$$\begin{aligned} G_0^{(\pm)}(\mathbf{x}, \mathbf{x}'; t) &= \mp i\theta(\pm t)\langle \hat{\psi}(\mathbf{x}, t)\, \hat{\psi}^+(\mathbf{x}', 0)\rangle \\ &= \langle \mathbf{x}|\, [\mp i\theta(\pm t)\, e^{-iH_0 t/\hbar}\, e^{-\eta|t|}]\, |\mathbf{x}'\rangle \\ &= \int \frac{dE}{2\pi} G_0^{(+)}(\mathbf{x}, \mathbf{x}', E)\, e^{-iEt/\hbar} \end{aligned} \tag{70}$$

$$G_0^{(\pm)}(\mathbf{x}, \mathbf{x}', E) \equiv \langle \mathbf{x}|\, (E - H_0 \pm i\eta)^{-1}\, |\mathbf{x}'\rangle \tag{71}$$

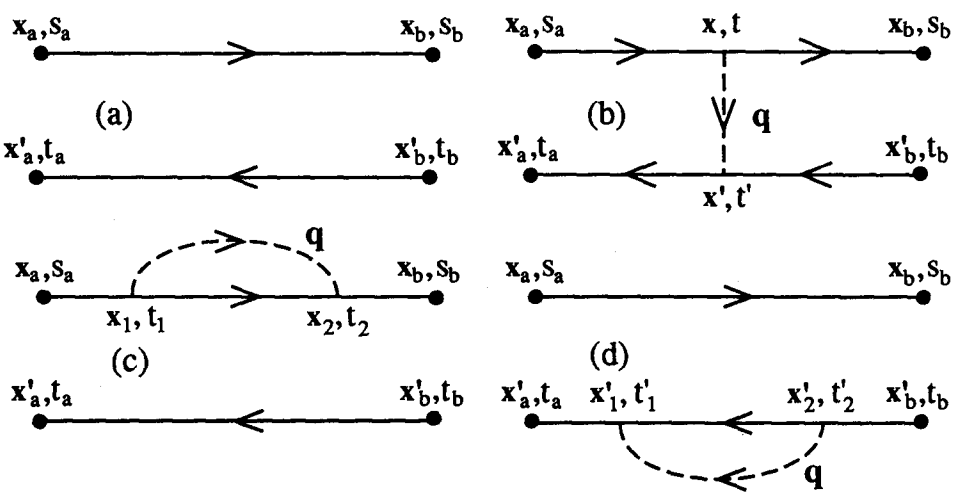


FIG. 3. Lowest order diagrams in the perturbative expansion of the dressed two-particle Green's function.

which should be compared with the definition (2). We shall often use the property

$$G_0^{(+)}(\mathbf{x}, \mathbf{x}'; E) = [G_0^{(-)}(\mathbf{x}', \mathbf{x}; E)]^*. \tag{72}$$

It is not entirely surprising that we cast our results in terms of quantum-mechanical one-particle Green's functions, since the field-theoretical notation for the electron was introduced for pure convenience.

The contraction of the phonon operators yields three types of phonon Green's functions, depending on whether the contraction takes place (a) within the positive time branch, (b) within the negative branch, or (c) between the two branches. The corresponding expressions are

$$\langle T\hat{A}_q(s)\,\hat{A}_q^+(s')\rangle = iD_q(s-s') = (N_q+1)\,e^{-i\omega_q|s-s'|} + N_q e^{i\omega_q|s-s'|} \tag{73a}$$

$$\langle \tilde{T}\hat{A}_q(t)\,\hat{A}_q^+(t')\rangle = i\tilde{D}_q(t-t') = [iD_q(t'-t)]^* \tag{73b}$$

$$\langle \hat{A}_q(t)\,\hat{A}_q^+(s)\rangle = iD_q^>(t-s) = (N_q+1)\,e^{-i\omega_q(t-s)} + N_q\,e^{i\omega_q(t-s)}, \tag{73c}$$

where $N_q$ is the Bose–Einstein occupation factor (we have used $N_q = N_{-q}$).

As a result of Wick's theorem, the perutbative expansion (67) admits a natural diagrammatic representation. One has to dress with phonon lines a double electron propagator. The diagrams for the lowest order terms are shown in Fig. 3. The sign of the arrows is important because it indicates the convention for the sign of the time arguments. The most generic diagram will be of the type shown in Fig. (4a), while the approximation (18) is represented by the diagram (4b), where the dressed one-electron propagators are decoupled.

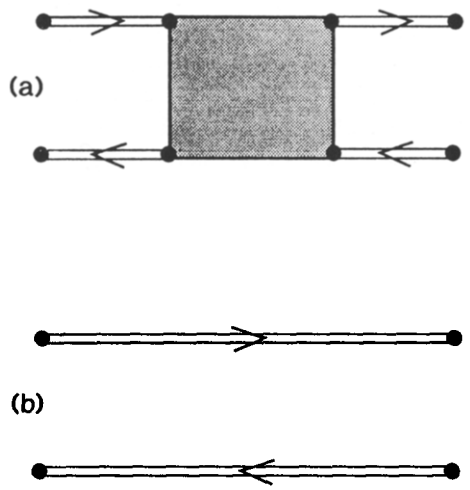


FIG. 4. (a) Most general representation of the two-particle Green's function. The double line represents the dressed one-particle propagator. (b) Most general diagram in the approximation of decoupled dressed one-electron Green's function (see Eq. (18) of the text).

C. *Energy Space Formulation*

When inserting an appropriate combination of (67)–(73) into (66), we are left with a multi-dimensional time integral of a function that depends only on the differences between the various times variables. It seems natural to expand these propagators in terms of their Fourier transforms and evaluate the time integrals exactly. We will need the Fourier transforms,

$$iD_q(\omega) \equiv \int dt\, e^{i\omega t} iD_q(t) = 2i\omega_q \left[ \frac{N_q + 1}{\omega^2 - \omega_q^2 + i\eta} - \frac{N_q}{\omega^2 - \omega_q^2 - i\eta} \right] \tag{74a}$$

$$i\tilde{D}_q(\omega) = [iD_q(\omega)]^* \tag{74b}$$

$$iD_q^>(\omega) = 2\pi[(N_q + 1)\,\delta(\omega - \omega_q) + N_q\,\delta(\omega + \omega_q)], \tag{74c}$$

where $\omega_q > 0$ and $\eta \to 0^+$.

At each vertex, there is a time integration whose evaluation yields a delta function that guarantees the conservation of energy. For example, the vertex of Fig. 5 corresponds to

$$\int dt\, e^{-iEt/\hbar}\, e^{iE't/\hbar}\, e^{i\omega t} = 2\pi\hbar\,\delta(\hbar\omega - E + E'). \tag{75}$$

We have adopted an arrow convention in which a given vertex accommodates both the absorption and the emission of phonons, as can be seen by inspection of (74). By comparing the phonon propagator (74c) that connects the two time branches with the propagators (74a) and (74b) which remain within the same branch, it becomes clear that the former corresponds to the real excitation of phonons (and requires conservation of energy, which is guaranteed by the delta functions) while the latter correspond to virtual phonons that renormalize the particle motion. This is a confirmation of the interpretation that was given in Section 2.B.

The Feynman rules for the calculation of $P(E_f; E_i, E_i')$ are in many ways similar to those found in textbooks of many-body theory (see, for instance, Refs. [28, 42]). There are, however, several rules that are specific of our perturbation theory. The "common" rules consist in drawing all topologically distinct diagrams that result

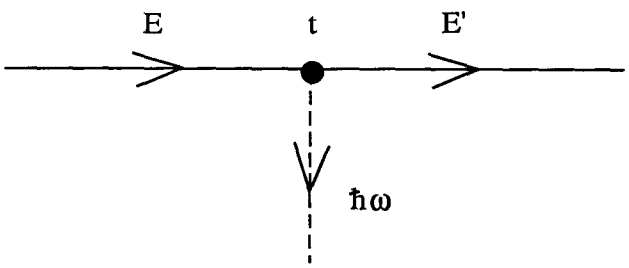


FIG. 5. A typical electron–phonon vertex where time is integrated out exactly.

from dressing the double electron propagator with phonon lines assigning positions and couplings to each vertex, labeling internal electron and phonon lines with energy and mode indices, and summing over these variables while conserving energy at all vertices. $G_0^{(+)}$ ($G_0^{(-)}$) must be assigned to the electron lines in the positive (negative) branch. Unlike in more standard cases, the phonon line must be assigned the propagator $iD_q$, $i\tilde{D}_q$, or $iD_q^>$, depending on whether the line remains in the positive or negative branch or connects them both. Energies $E_f$, $E_i$, and $E_i'$ must be assigned to the external propagators (see, e.g., Fig. 6). The external vertices must be labeled with points $\mathbf{x}_a$, $\mathbf{x}_b$, $\mathbf{x}_a'$, and $\mathbf{x}_b'$ (see also Fig. 6) and projection over the transverse modes has to be performed (see Eqs. (50) and (56)). The final result must be multiplied by $\hbar v_f v_i (\lambda/2\pi)^{(j+k)/2}$, where $j(k)$ is the number of phonon insertions in the upper (lower) particle propagator. Finally, the relevant quantity $T_{nm,ba}(E_f, E_i)$ can be obtained from the relation (65a).

The factor $\hbar v_f v_i (\lambda/2\pi)^{(j+k)/2}$ deserves some explanation. The factor $j!\,k!\,i^{j-k}$ that appears in (68) cancels exactly with the $i^{k-j}/(j!\,k!)$ of (67). There are $(j+k)$ electron–phonon vertices, which yields a factor $(\sqrt{\lambda})^{j+k}$. At each of these vertices, a time integral of the type (75) is carried out. There are four additional integrals corresponding to the four external time variables $t_a$, $t_b$, $s_b$, and $s_a$ (see Eq. (66)). Thus, there is a factor $(2\pi\hbar)^{j+k-4}$ coming from the time integrals. The $\hbar^{j+k}$ factor cancels with its inverse in the expansion (67), yielding $\hbar^4(2\pi)^{j+k+4}$. The expansion of the real time propagators in their energy dependent Fourier transforms introduces some $(1/2\pi)$ factors (note the conventions in (74) and (46)). There are $(j+k)/2$ phonon propagators ($iD$) and $(k+1)$ and $(j+1)$ electron Green's functions in the upper and lower branch, respectively. This gives a factor of $(2\pi)^{-3(j+k)/2-2}$. Combining all these numbers, we obtain $(\sqrt{\lambda})^{j+k}\hbar^4(2\pi)^{2-(j+k)/2}$, which when multiplied by the $v_f v_i/(2\pi\hbar)^2$ of Eq. (66), gives rise to the factor $\hbar^2 v_f v_i (\lambda/2\pi)^{(j+k)/2}$ that has been presented in the rules above. We note in addition that, given the way the diagram rules have been formulated, only an energy conserving delta function (without any accompanying factor) has to be effectively introduced at each vertex. This means that, according to convenience, one can explicitly introduce a delta function or directly include conservation of energy in the assignment of energy variables.

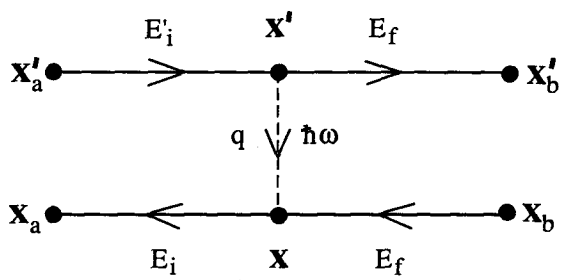


FIG. 6. Diagram representing the real emission or absorption of one phonon. Since the electron lines may contain elastic scattering exactly, this diagram represents the distorted wave Born approximation.

## 5. Applications

In this section, we illustrate the use of the Feynman rules derived above by applying them to some simple cases. We will compute all the one-phonon diagrams and some of the two-phonon diagrams in one dimension (only two leads, each of them supporting only one mode). An explicit check of unitarity is performed in the former case.

### A. *One-Phonon Processes*

Let us calculate the contribution of the diagram in Fig. 6 to the transmission probability. This diagram describes the absorption or emission of one phonon. By applying the rules derived in the previous section, we readily obtain

$$\begin{aligned} T^{(a)}(E_f, E_i) &= \hbar^2 v_f v_i \lambda \sum_q \iint dx\, dx'\, M_q(x)\, M_q^*(x') \\ &\quad \times [(N_q+1)\,\delta(E_f - E_i + \hbar\omega_q) + N_q\,\delta(E_f - E_i - \hbar\omega_q)] \\ &\quad \times G_0^{(-)}(x_a, x; E_i)\, G_0^{(-)}(x, x_b; E_f)\, G_0^{(-)}(x'_b, x', E_f)\, G_0^{(+)}(x', x'_a; E_i) \\ &= \hbar^2 v_f v_i \lambda \sum_q \left| \int dx\, G_0^{(+)}(x_b, x; E_f)\, M_q^*(x)\, G_0^{(+)}(x, x_a; E_i) \right|^2 \\ &\quad \times [(N_q+1)\,\delta(E_f - E_i + \hbar\omega_q) + N_q\,\delta(E_f - E_i - \hbar\omega_q)], \end{aligned} \tag{76}$$

where, in the second equation, $x'_a = x_a$ and $x'_b = x_b$ has been taken, since there is no transverse component. Clearly, the first term in square brackets corresponds to one phonon emission, while the second is due to phonon absorption.

We remark that although (76) includes the electron–phonon interaction only to the lowest order, it may well contain the elastic scattering to all orders through the electron Green's functions $G_0^{(+)}$ and $G_0^{(-)}$, which can often be calculated exactly by a variety of methods. Thus, Eq. (76) represents the so-called distorted wave Born approximation (DWBA) [41].

In the case where there is no elastic scattering [43],

$$G_0^{(+)}(x, x'; E) = \frac{e^{ik_E|x-x'|}}{i\hbar v_E} \tag{77}$$

(where $v_E = (2E/M)^{1/2} = \hbar k_E/M > 0$) and (76) takes the simpler form

$$\begin{aligned} T^{(a)}(E_f, E_i) &= \frac{\lambda}{\hbar^2 v_f v_i} \sum_q \left| \int dx\, M_q^*(x)\, e^{i(k_i - k_f)x} \right|^2 \\ &\quad \times [(N_q+1)\,\delta(E_f - E_i + \hbar\omega_q) + N_q\,\delta(E_f - E_i - \hbar\omega_q)]. \end{aligned} \tag{78}$$

Below we show that this particular result could have also been obtained through

the Fermi golden rule in the Born approximation: the (thermal) average scattering rate for the electron to go from plane wave $|k_i\rangle$ to $|k_f\rangle$ is given by

$$\tau^{-1}_{k_i \to k_f} = \frac{2\pi}{\hbar} \sum_\alpha P_\alpha \sum_\beta |\langle k_f, \beta | V | k_i, \alpha \rangle|^2 \, \delta(E_f - E_i + \varepsilon_\alpha - \varepsilon_\beta)$$

$$= \frac{2\pi\lambda}{\hbar L^2} \sum_q \left| \int dx \, M_q^*(x) \, e^{i(k_i - k_f)x} \right|^2$$

$$\times [(N_q + 1) \, \delta(E_f - E_i + \hbar\omega_q) + N_q \, \delta(E_f - E_i - \hbar\omega_q)], \tag{79}$$

where, $\langle x | k \rangle = L^{-1/2} \exp(ikx)$ $(L \to \infty)$ has been taken. If we divide (79) by the flux of incoming particles, $v_i/L$, we obtain the probability that the particle is scattered from $k_i$ to $k_f$ or, treating $k$ as a continuous variable, the probability of being scattered into the interval $(k_f, k_f + dk_f)$, where $dk_f \equiv 2\pi/L$. Since we are interested in the probability $T(E_f, E_i)\, dE_f$ of scattering into $(E_f, E_f + dE_f)$, we multiply the former probability by $(dk_f/dE_f)/(2\pi/L) = L/2\pi\hbar v_f$ and obtain for the inelastic transmission probability in the Born approximation

$$T^{(B)}(E_f, E_i) = \frac{L^2}{2\pi\hbar v_i v_f} \tau^{-1}_{k_i \to k_f}, \tag{80}$$

which exactly reproduces (78). Thus, $T^{(B)}(E_f, E_i) = T^{(a)}(E_f, E_i)$.

In more general cases, like those in which there is additional scattering by barriers or impurities, our method is much more advantageous than the simple use of the Fermi golden rule. First, it provides us with an unambiguous and systematic way of calculating corrections to the unperturbed scattering probabilities in which all the flux factors are automatically taken into account and, second, in this method, elastic and inelastic scattering are treated on the same footing, in such a way that unitarity is automatically satisfied to all orders in perturbation theory. An application of Eq. (76) to the problem of a tight-binding chain with phonons localized in a lateral stub (which already causes elastic scattering) is given in Refs. [44, 45].

Now we calculate the first-order corrections to the elastic scattering, which are given by the diagrams in Figs. (3b) and (3c). One obtains

$$T^{(b)}(E_f, E_i) = [T^{(c)}(E_f, E_i)]^* = T^{(b)}(E_i) \, \delta(E_f - E_i), \tag{81}$$

where

$$T^{(b)}(E) = \frac{\hbar^2 v^2}{2\pi} \lambda G_0^{(-)}(x_a, x_b; E) \sum_q \int d\omega \iint dx \, dx' \, M_q^*(x) \, M_q(x')$$

$$\times G_0^{(+)}(x_b, x'; E) \, G_0^{(+)}(x', x; E - \hbar\omega) \, G_0^{(+)}(x, x_a; E) \, iD_q(\omega). \tag{82}$$

In the case of free unperturbed motion, where $G_0^{(+)}$ is given by (77), unitarity can be easily checked. If the spectral decomposition

$$G_0^{(+)}(x, x'; E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ik(x-x')}}{E - E_k + i\eta} \tag{83}$$

(where $E_k \equiv \hbar^2 k^2/2M$) and Eq. (74a) are introduced in (82), the correction to the elastic transmission becomes

$$T^{(b)}(E) = -\frac{\lambda}{\hbar v_E} \sum_q \int_{-\infty}^{\infty} dk \left| \int dx\, M_q(x)\, e^{i(k-k_E)x} \right|^2 \times [(N_q + 1)\, \delta(E - E_k - \hbar\omega_q) + N_q\, \delta(E - E_k + \hbar\omega_q)]. \tag{84}$$

In order to perform a unitarity check, the reflection channels must also be included. The reflection probability in the presence of dissipation is given by Eq. (16), where only the first term contributes to inelastic scattering. This term is formally identical to expressions for the transmission probability and the same Feynman rules can be readily applied. The contribution from diagram (a) (where $x_b$ must be replaced by $x_a$) is

$$R^{(a)}(E_f, E_i) = \frac{\lambda}{\hbar^2 v_f v_i} \sum_q \left| \int dx\, M_q(x)\, e^{-i(k_i + k_f)x} \right|^2 \times [(N_q + 1)\, \delta(E_f - E_i + \hbar\omega_q) + N_q\, \delta(E_f - E_i - \hbar\omega_q)]. \tag{85}$$

By comparing with Eq. (78), we obtain the rather intuitive result that the expression for the inelastic reflection probability can be obtained from its transmission counterpart by substituting $-k_f$ for $k_f$ ($k_f > 0$, by definition).

To order $\lambda$ in perturbation theory, the elastic reflection probability is entirely given by the decoupled contribution from the first term of Eq. (16) plus the interference terms (second and third terms of Eq. (16)). Therefore, we can apply the result (22b) and conclude that, in the absence of unperturbed elastic reflection ($r = 0$), there is no phonon correction to the elastic reflection probability to order $\lambda$. Thus, using a notation analogous to that of Eqs. (81) and (82), we can assert that $R^{(b)}(E) = 0$.

By comparing Eqs. (78), (84), and (85) it is easy to show that unitarity is indeed satisfied. The expression (84) for $T^{(b)}(E)$ contains a sum over intermediate states $|k\rangle$ that exactly cancels the contribution from the inelastic transmission ($k > 0$) and reflection ($k < 0$) channels. In conclusion,

$$\int [T^{(a)}(E', E) + R^{(a)}(E', E)]\, dE' + T^{(b)}(E) + R^{(b)}(E) = 0, \tag{86}$$

which means that there is no correction to unitarity within order $\lambda$, as expected. The generalization of this result leads to the realization that, at any given order in

perturbation theory, the decoupled diagrams yield a correction to the elastic scattering probability that exactly cancels the probability contribution from the (mostly inelastic) channels that are represented by the irreducible diagrams. This statement can ve viewed as a generalization of the optical theorem to dissipative scattering in multilead structures.

### C. *Two-Phonon Processes*

In this subsection we calculate a selected group of two-phonon diagrams. In particular, we study the diagrams shown in Fig. 7, since, as will be seen below, they contain some similarities that allow us to understand better the interplay between reducible and irreducible contributions to elastic scattering (in the notation of Section 2.C, $T^0$ and $(T^{el} - T^0)$, respectively). For simplicity, we restrict ourselves

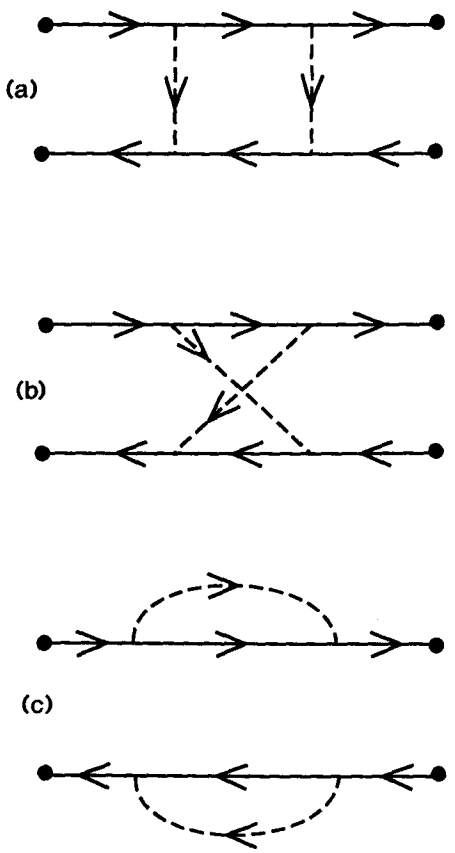


FIG. 7. A group of two-phonon diagrams. Diagrams (a) and (b) correspond to two real processes of phonon creation or destruction. Diagram (c) is a particular case of diagram 4(b).

to the transmission channel in one-dimensional scattering. The contribution form diagram 7a is

$$T^{(a)}(E_f, E_i) = \frac{\hbar^2\lambda^2 v_f v_i}{(2\pi)^2} \sum_{q,p} \iint d\omega_1\, d\omega_2 \iiiint dx_1\, dx_2\, dx_1'\, dx_2' \times M_q^*(x_1)\, M_q(x_1')\, M_p^*(x_2)\, M_p(x_2')\, iD_q^>(\omega_1) \times iD_p^>(\omega_2)\, \delta(E_i - E_f - \hbar\omega_1 - \hbar\omega_2) \times G_0^{(-)}(x_a, x_1'; E_i)\, G_0^{(-)}(x_1', x_2'; E_i - \hbar\omega_1)\, G_0^{(-)}(x_2', x_b; E_f) \times G_0^{(+)}(x_b, x_2; E_f)\, G_0^{(+)}(x_2, x_1; E_i - \hbar\omega_1)\, G_0^{(+)}(x_1, x_a; E_i), \quad (87)$$

which, from (72) and definition (74), becomes

$$T^{(a)}(E_f, E_i) = \hbar^2\lambda^2 v_f v_i \sum_{q,p} \Big\{ (N_q+1)(N_p+1)\, |t_{pq}(E_f, E_i - \hbar\omega_q, E_i)|^2 \times \delta(E_f - E_i + \hbar\omega_q + \hbar\omega_p) + (N_q+1)\, N_p\, |t_{pq}(E_f, E_i - \hbar\omega_q, E_i)|^2\, \delta(E_f - E_i + \hbar\omega_q - \hbar\omega_p) + N_q(N_p+1)\, |t_{pq}(E_f, E_i + \hbar\omega_q, E_i)|^2\, \delta(E_f - E_i - \hbar\omega_q + \hbar\omega_p) + N_q N_p\, |t_{pq}(E_f, E_i + \hbar\omega_q, E_i)|^2\, \delta(E_f - E_i - \hbar\omega_q - \hbar\omega_p) \Big\}, \quad (88)$$

where

$$t_{pq}(E_f, E, E_i) \equiv \iint dx_1\, dx_2 G_0^{(+)}(x_b, x_2; E_f)\, M_p^*(x_2)\, G_0^{(+)}(x_2, x_1; E) \times M_q^*(x_1)\, G_0^{(+)}(x_1, x_a; E_i). \quad (89)$$

A similar analysis for the contribution of diagram 7b yields

$$T^{(b)}(E_f, E_i) = \hbar^2\lambda^2 v_f v_i \sum_{q,p} \Big\{ (N_q+1)(N_p+1)\, t_{pq}(E_f, E_i - \hbar\omega_q, E_i) \times t_{qp}^*(E_f, E_i - \hbar\omega_p, E_i)\, \delta(E_f - E_i + \hbar\omega_q + \hbar\omega_p) + (N_q+1)\, N_p\, t_{pq}(E_f, E_i - \hbar\omega_q, E_i)\, t_{qp}^*(E_f, E_i + \hbar\omega_p, E_i) \times \delta(E_f - E_i + \hbar\omega_q - \hbar\omega_p) + N_q(N_p+1)\, t_{pq}(E_f, E_i + \hbar\omega_q, E_i)\, t_{qp}^*(E_f, E_i - \hbar\omega_p, E_i) \times \delta(E_f - E_i - \hbar\omega_q + \hbar\omega_p) + N_q N_p\, t_{pq}(E_f, E_i + \hbar\omega_q, E_i)\, t_{qp}^*(E_f, E_i + \hbar\omega_p, E_i) \times \delta(E_f - E_i - \hbar\omega_q - \hbar\omega_p) \Big\}. \quad (90)$$

(These transmissions are not be confused with those computed in the previous subsection.)

Clearly, both in (88) and in (90), the first and fourth terms within brackets correspond to the emission and absorption of two phonons, respectively, while the second and third terms stem from processes in which one phonon is emitted and another one is absorbed. If the same phonon is first emitted and then absorbed (or vice versa), an effective elastic process takes place that is not included in the diagrams obtained from the product of decoupled one-electron propagators, like that of Fig. 7c. We wish to focus now on this elastic contribution arising from the case $p=q$ in the second and third terms of (88) and (90).

To simplify the analysis, we explicitly assume that modes $q$ and $-q$ are identical and thus $M_q(x)=M_q^*(x)$. This is consistent with the initial assumption of localized phonons. If $T^{(a)}(E)$ and $T^{(b)}(E)$ are defined as the contributions from diagrams 7a and b to the elastic transmission probability, one obtains

$$T^{(a)}(E)=\hbar^2 v^2\lambda^2\sum_q (N_q+1)\,N_q[|f_{q-}(E)|^2+|f_{q+}(E)|^2] \tag{91}$$

$$T^{(b)}(E)=\hbar^2 v^2\lambda^2\sum_q (N_q+1)\,N_q[f_{q-}^*(E)\,f_{q+}(E)+f_{q+}(E)\,f_{q-}^*(E)], \tag{92}$$

where

$$f_{q\pm}(E)\equiv t_{qq}(E, E\pm\hbar\omega_q, E). \tag{93}$$

As we saw in Section 2.C, diagram 7c can only contribute to elastic scattering. One obtains

$$T^{(c)}(E)=\hbar^2 v^2\lambda^2\left|\sum_q [(N_q+1)\,f_{q-}(E)+N_q f_{q+}(E)]\right|^2. \tag{94}$$

The sum of the three contributions is

$$\begin{aligned}
&T^{(a)}(E)+T^{(b)}(E)+T^{(c)}(E)\\
&\quad=\hbar^2 v^2\lambda^2\Bigg\{\sum_{q,p}{}' [(N_q+1)(N_p+1)f_{q-}f_{p-}^* + N_q N_p f_{q+}f_{p+}^*\\
&\qquad+(N_q+1)\,N_p f_{q-}f_{p+}^* + N_q(N_p+1)\,f_{q+}f_{p-}^*]\\
&\qquad+\sum_q [(N_q+1)(2N_q+1)\,|f_{q-}|^2 + N_q(2N_q+1)\,|f_{q+}|^2\\
&\qquad+2N_q(N_q+1)(f_{q-}f_{q+}^* + f_{q+}f_{q-}^*)]\Bigg\},
\end{aligned} \tag{95}$$

where the prime in the first sum implies exclusion of the case $q=p$.

It is interesting to compare this result with what one would have obtained by analyzing directly the expression for the total elastic probability given in (25). By inspection of Eqs. (91)–(94), one can easily convince oneself that the elastic contribution contained in diagrams 7 a–c correspond to those terms in the general

expression (25) in which both $G_{\alpha\alpha}(x_b, x_a; E)$ and its complex conjugate contain terms of order $\lambda$. The sum of such terms in (25) is

$$T^{(d)}(E) = \hbar^2 v^2 \lambda^2 \sum_{\alpha} P_\alpha \left| \sum_q [(N_{q\alpha} + 1) f_{q-} + N_{q\alpha} f_{q+}] \right|^2, \tag{96}$$

where $N_{q\alpha}$ is defined as the occupation number of phonon mode $q$ in the bath state $|\alpha\rangle$. It is such that

$$N_q = \sum_{\alpha} P_\alpha N_{q\alpha} = \langle \hat{N}_q \rangle \tag{97}$$

is the usual Bose–Einstein occupation factor. The algebraic steps leading to Eq. (96) are very similar to those needed to calculate the lowest order phonon contribution to the one-electron propagator (see, e.g., the single propagators of Fig. 7c). The only difference is that the thermal average is formally replaced by the expectation value in the particular bath state $|\alpha\rangle$ and the final result is eventually thermally averaged over all the possible bath states. In this way, one obtains Eq. (96), which can be written as

$$T^{(d)}(E) = \hbar^2 v^2 \lambda^2 \sum_{q,p} [\langle (\hat{N}_q + 1)(\hat{N}_p + 1) \rangle f_{q-} f_{p-}^* + \langle \hat{N}_q \hat{N}_p \rangle f_{q+} f_{p+}^* + \langle (\hat{N}_q + 1) \hat{N}_p \rangle f_{q-} f_{p+}^* + \langle \hat{N}_q (\hat{N}_p + 1) \rangle f_{q+} f_{p-}^*].$$

If one notes that

$$\langle \hat{N}_q \hat{N}_p \rangle = N_q N_p + \delta_{qp} N_q (N_q + 1) \tag{98}$$

it becomes clear that

$$T^{(d)}(E) = T^{(a)}(E) + T^{(b)}(E) + T^{(c)}(E), \tag{99}$$

as expected. Thus, we have explicitly seen within a selected group of diagrams how both reducible and irreducible diagrams give corrections to the elastic transmission, defined here as the scattering channel in which the bath does not change state. Irreducible diagrams generally correspond to inelastic processes where real emission or absorption of phonons take place. However, a marginally effective contribution to the elastic scattering can arise from those processes in which the same phonon is "really" created and then destroyed or vice versa. These types of processes are known to sometimes give important corrections to the conductivity [28].

## 6. Computation of the Current

Once the inelastic transmission probabilities are known one may attempt to calculate the net current in a given lead as a function of the voltages in the various leads. A simple counting argument suggests that the net flux of electrons entering

the sample through lead $a$ must be given by the number of electrons that are transmitted per unit time from lead $a$ to all other leads $b \neq a$, minus the electron flux entering lead $a$ from those other leads. In quantitative terms,

$$I_a^{\mathrm{A}} = \frac{e}{h} \sum_b{}' \iint dE\, dE' \times \{T_{ba}(E, E') f_a(E')[1 - f_b(E)] - T_{ab}(E', E) f_b(E)[1 - f_a(E')]\}, \quad (100)$$

where

$$T_{ba}(E, E') \equiv \sum_{nm} T_{nm,ba}(E, E'), \quad (101)$$

$f_i(E) \equiv f(E - \mu_i) = [\exp((E - \mu_i)/kT) + 1]^{-1}$ is the Fermi–Dirac distribution, and the prime indicates exclusion of the case $b = a$. In (100), the well-known cancellation between the electron group velocity, $\hbar^{-1}\, dE/dk$, and the density of states in a one-dimensional channel, $dn/dE = (1/2\pi)(dk/dE)$ has already been included. The factors $(1 - f(E'))$ account for the fact that the electron can only effectively jump to another lead if the final state is initially empty. However, one might argue that this factor is not necessary since the Fermi statistics only enter through the energy distributions of the incoming channels and should not appear explicitly in the outgoing channels, which in principle should always be available. Thus, a second possible formula for the current (which we will label with a different superscript) is

$$I_a^{\mathrm{B}} = \frac{e}{h} \sum_b{}' \iint dE\, dE' \{T_{ba}(E, E') f_a(E') - T_{ab}(E', E) f_b(E)\}. \quad (102)$$

Before we embark on a discussion of the relative merits of ansätze A and B (Eqs. (100) and (102), respectively), let us see in what cases they are different. If we subtract Eq. (102) from Eq. (100), we obtain

$$\Delta I_a \equiv I_a^{\mathrm{A}} - I_a^{\mathrm{B}} = \frac{e}{h} \sum_b{}' \iint dE\, dE' f_a(E')\, f_b(E)[T_{ab}(E', E) - T_{ba}(E, E')]. \quad (103)$$

The symmetry relation (27) can be rewritten as

$$T_{ba}(E, E'; \mathbf{B}) = e^{\beta(E' - E)} T_{ab}(E', E; -\mathbf{B}), \quad (104)$$

where the definition (101) has been used and the possibility of a nonzero magnetic field $\mathbf{B}$ has been introduced. It is clear from (104) that, in the presence of inelastic scattering, $\Delta I_a \neq 0$ even if $\mathbf{B} = 0$.

In the elastic limit (103) becomes

$$\Delta I_a = \frac{e}{h} \sum_b{}' \int dE\, f_a(E)\, f_b(E)[T_{ab}(E) - T_{ba}(E)] \quad (105)$$

and then $\Delta I_a = 0$, provided that $\mathbf{B} = 0$. There is one particular case of the elastic regime in which $\Delta I_a = 0$, even if $\mathbf{B} \neq 0$, and this is the case where only two leads are coupled to the sample ($N_L = 2$). In such a case, one can express unitarity with two different equations

$$T_{ba}(E) + R_{aa}(E) = T_{ab}(E) + R_{aa}(E) = N_a, \qquad N_L = 2, \tag{106}$$

where $N_a$ is the number of both incoming and outgoing channels in lead $a$ (when $\mathbf{B} \neq 0$, channels always appear in pairs of edge states moving in oppposite directions; thus the number of incoming and outgoing channels is always the same [46]). Equation (106) immediately leads to $T_{ab} = T_{ba}$, which implies $\Delta I_a = 0$. The fact that, in the elastic limit, both current ansätze are equivalent if $\mathbf{B} = 0$ or $\mathbf{B} \neq 0$ but $N_L = 2$ probably explains why the ambiguity in the choice of current formula has been long neglected, or at least underestimated.

It is clear that, in the presence of inelastic scattering, ansätze A and B yield different results and a more careful assessment is required. Since we lack at present a rigorous formulation, we have to base our arguments on as careful physical considerations as possible. First of all, we point out that there is a small inconsistency which is common to both options if, in Eq. (100) or (102), one uses an inelastic transmission probability that has been calculated with the methods presented in the previous sections, since there the presence of other electrons has been neglected. In Eqs. (100) and (102) we are remedying this previous neglect of the Fermi statistics by introducing statistical factors in the initial and (only in case A) final states. However, quantum statistics is still being neglected in the intermediate (virtual) states which appear if one goes beyond order $\lambda$ in perturbation theory. We think nevertheless that this is not going to be a major source of error, since quantum statistics has its most important effect through the restrictions it imposes on the initial and final phase space. Furthermore, the neglect of statistical factors in the intermediate states is a long standing practice in the literature on the Boltzmann equation, where analogous expressions for the current are considered (the main difference lies in the use of scattering rates instead of the scattering probabilities of Eqs. (100) and (102)). We note incidentally that a more careful study of the inclusion of quantum statistics in Boltzmann equation approaches (particular in the "in" and "out" states) which contemplate phonon scattering may also be necessary and that the conclusion does not have to be necessarily directly analogous to the one we (eventually) obtain for the conductance (see below).

Let us now discuss the elastic limit of Eqs. (100) and (102). We obtain

$$I_a^{\mathrm{A}} = \frac{e}{h} \sum_b{}' \int dE \{ T_{ba}(E) f_a(E)[1 - f_b(E)] - T_{ab}(E) f_b(E)[1 - f_a(E)] \} \tag{107}$$

$$I_a^{\mathrm{B}} = \frac{e}{h} \sum_b{}' \int dE \{ T_{ba}(E) f_a(E) - T_{ab}(E) f_b(E) \}. \tag{108}$$

The condition of unitarity can be expressed as

$$N_a = \sum_b{}' T_{ba} + R_{aa} = \sum_b{}' T_{ab} + R_{aa}, \tag{109}$$

where $N_a$ is the number of incoming (or outgoing) channels in lead $a$. This implies

$$\sum_b{}' T_{ab} = \sum_b{}' T_{ba} \tag{110}$$

but note that this type of identity holds only in the elastic case. To calculate conductances, we linearize around a reference chemical potential $\mu_0$:

$$f_i(E) \simeq f_0(E) - f_0'(E)(\mu_i - \mu_0). \tag{111}$$

Introducing (111) in (107) and (108) and using (110), we obtain

$$I_a^{\mathrm{A}} = \frac{e}{h} \sum_b{}' \frac{1}{2} (T_{ab} + T_{ba})(\mu_a - \mu_b) \tag{112}$$

$$I_a^{\mathrm{B}} = \frac{e}{h} \sum_b{}' T_{ab}(\mu_a - \mu_b). \tag{113}$$

Thus we see that ansatz B correctly reproduces the Landauer–Büttiker equations [19, 37], while option A gives rise to a different result for nonzero magnetic fields. Recently, Eq. (113) has been successfully applied to a number of problems, particularly to the study of symmetry properties of the conductance [19, 37] and to the quantum Hall effect in microstructures [46]. The predictions of ansatz A can be easily obtained from those of ansatz B by everywhere replacing $T_{ab}$ by its symmetrized form $(T_{ab} + T_{ba})/2$. Equation (112) gives rise to a four-lead resistance formula $R_{ab,cd} \equiv (V_c - V_d)/I_a$ which markedly differs from the prediction of Eq. (113) [19, 37]. Among the many discrepancies that follow from the difference between $I_a^{\mathrm{A}}$ and $I_a^{\mathrm{B}}$ we remark that ansatz A predicts the symmetries

$$R_{ab,cd}^{\mathrm{A}}(\mathbf{B}) = R_{ab,cd}^{\mathrm{A}}(-\mathbf{B}) = R_{cd,ab}^{\mathrm{A}}(\mathbf{B}), \tag{114}$$

which have not been observed [47] (in particular, it would predict that $(R_{12,43} - R_{43,12})/2 = 0$).

There is another reason why Eq. (102) should be preferable to Eq. (100) and it is that current conservation is not clearly satisfied if, as is the case in both equations, $T_{ba}(E, E')$ represents the probability for a particular outcome in a one-attempt scattering process. These probabilities have been calculated in such a way that the unitarity condition is expressed by (52). The factor $(1 - f)$ describes an inhibition of the transmission process due to the Pauli exclusion principle. But if an electron is not transmitted from lead $a$ to lead $b$ because the state to which it would jump is occupied, then it is not clear how the scattering should evolve. Obviously, the electron should go to another lead or be reflected, but these alternative events

appear in (52) weighted by the same factors and the "rebounce" possibility is not considered in the calculation of their probabilities. Clearly, the unitarity condition (52), which was formulated for a single electron, excludes any possible restrictions on the availability of final states. In summary, current conservation may well be violated if one uncritically introduces $(1-f)$ factors in the final states, particularly if the probabilities have been calculated within a single particle approximation. We wish to remark here that this objection would not readily apply to a Boltzmann type equation in which (the equivalent of) $T_{ba}(E, E')$ would correspond to transition rates between plane wave states [28, 48]. In such a case, the factor $(1-f)$ simply gives rise to a longer waiting period in the initial state but does not lead to any obvious violation of current conservation. A very similar situation presents itself in tunneling studies based on the Bardeen Hamiltonian (see, for example, Ref. [41]), where one is essentially dealing with transition rates between stationary waves in each lead. The results obtained from such studies seem to favor the presence of $(1-f)$ factors. However, we use the formal analogy to the Boltzmann equation, where these factors are less problematic. The generalization of the Bardeen approach to the study of dissipative magnetotransport in multilead structures would probably shed light on the question discussed here.

After all these considerations, it is clear that Eq. (100) for the current cannot be correct, since it leads to results that grossly contradict experimental observations and seems to violate current conservation. One may readily conclude that Eq. (102) is the correct formula for the current. However, as we argue below, Eq. (102) is not completely free of contradictions, although is probably the best expression that we can use in the present circumstances. So far we have based the comparison of Eq. (100) and (102) solely on their performance in the elastic limit and on some considerations about current conservation, and we have seen that ansatz B clearly fares better. The situation becomes slightly more disturbing when one pays attention to another set of considerations related to the state of equilibrium in which all chemical potentials are equal. If the energy distributions in the leads are taken to be equal, we obtain

$$I_a^{\mathrm{A}} = \frac{e}{h} \sum_b{}' \iint dE\, dE' \{ T_{ba}(E, E')\, f(E')[1-f(E)] - T_{ab}(E', E)\, f(E)[1-f(E')] \} \tag{115}$$

$$I_a^{\mathrm{B}} = \frac{e}{h} \sum_b{}' \iint dE\, dE' \{ T_{ba}(E, E')\, f(E') - T_{ab}(E', E)\, f(E) \}. \tag{116}$$

In the absence of a magnetic field, the symmetry relation (104) leads immediately to $I_a^{\mathrm{A}} = 0$. However, it does not lead to $I_a^{\mathrm{B}} = 0$, unless the energy distribution $f(E)$ is taken of the Boltzmann type ($\sim e^{-\beta E}$), something which would correspond to a strictly consistent use of the single particle picture. In the case of nonzero magnetic field, detailed balance arguments cannot be applied. However, as we know from the elastic case with $B \neq 0$, detailed balance is not strictly ncessary to achieve zero

current at equilibrium and, as we see below, the model also fails for reasons that have to do with unitarity. To see this, we first note that the unitarity condition

$$N_a(E) = \int dE' \left[ R_{aa}(E', E) + \sum_b{}' T_{ba}(E', E) \right]$$
$$= \int dE' \left[ R_{aa}(E, E') + \sum_b{}' T_{ab}(E, E') \right] \tag{117}$$

allows us to rewrite $I_a^{\mathrm{B}}$ as (we focus directly on the equilibrium case $f_a = f_b$)

$$I_a^{\mathrm{B}} = \frac{e}{h} \int dE\, f(E) \left\{ N_a(E) - \int dE'\, R_{aa}(E', E) - \sum_b{}' \int dE'\, T_{ab}(E', E) \right\}. \tag{118}$$

However, neither of the two equations in (117) leads to the vanishing of $I_a^{\mathrm{B}}$ as expressed in (118), and this is due to the presence of the Fermi distribution $f(E)$. We note in passing that if ansatz A for the current is rewritten in a form analogous to (118) but with $f_a \neq f_b$ and with the $(1-f)$ factors, the resulting expression would not be, in general, equivalent to (100). This is related to the problem of current conservation commented upon above and further suggests the inadequacy of Eq. (100). Thus we see that regarding charge balance, neither of the two ansätze gives entirely satisfactory answers.

The upshot of this discussion is that, in the presence of dissipation, it may not be completely consistent to use formulae for the current like Eqs. (100) and (102), when the transmission probabilities have been obtained within a single particle picture, no matter how intuitively appealing these equations may be. This conclusion underlies the need for global transport equations in which the effects of quantum statistics and of dynamic electron interactions (either Coulomb or phonon mediated) are rigorously or at least consistently taken into account. However, as long as we lack a complete and satisfactory treatment, choice B for the current equation is probably much more adequate than the option A, since it correctly reproduces the elastic limit and is more consistent with current conservation considerations. We finally remark that these arguments should not be uncritically applied to the (in many regards analogous) context of the Boltzmann equation [28, 48], where the introduction of the factor $(1-f)$ in the final state is probably much more adequate and does not lead to obvious contradictions.

## 7. Conclusions

In this work we have developed a Green's function method to study dissipative transport in very small structures within the framework of single particle and localized phonon approximations. We have developed exact general expressions for the inelastic transmission and reflection probabilities in terms of dressed two-

particle Green's functions. We have obtained these results both by analyzing directly the scattering amplitudes and through a reduced density matrix approach. In both cases we have borrowed from the literature on dissipation in quantum machanics [35], particularly in regard to the tracing out of bath coordinates as a means of generating a description of dissipative dynamics. We have also developed a diagrammatic perturbation theory in the electron–phonon interaction that automatically preserves unitarity to all orders. The use of the corresponding Feynman rules has been illustrated with applications to some simple cases involving one- and two-phonon processes. Finally, we have discussed what is the correct method for calculating the current, once the inelastic scattering probabilities are known. There is an ambiguity in the way quantum statistics is introduced in the electron final states. We have shown that, although the absence of explicit statistical factors in the availability of final states provides a more correct picture, there is no obvious formula for the current that is entirely free of contradictions. These difficulties point out the need for a description of electron transport that incorporates both many-body and dissipation effects in a consistent fashion. It is our hope nevertheless that the formalism here presented will prove useful in quantitative studies of dissipative transport in mesoscopic systems, particularly in case where many-body effects do not play an essential role. For those systems where Fermi statistics is of primary importance, this work must be viewed as a useful preliminary step towards a complete treatment of dissipation in quantum transport within the scattering picture first advocated by Landauer [16].

## APPENDIX A: WAVE PACKET ANALYSIS OF THE RELATION BETWEEN GREEN'S FUNCTIONS AND THE SCATTERING MATRIX

The essence of the analysis which we present in this appendix is the following: we consider the evolution of an incident (normalized) wave packet which is in a single transverse mode and is eventually assumed to be arbitrarily monochromatic. This packet evolves with the full Hamiltonian $H_0$ and, at a much later time, it becomes a linear superposition of outgoing wave packets in the various leads and transverse modes with a relative weight given by the transmission and reflection coefficients. These can be calculated by projecting the total wave function at very long times on the different outgoing wave packets that can be defined in the various channels and which are formally similar to the incident one. In particular, they are also normalized to unity and are eventually assumed to be highly monochromatic. The resulting expression for the scattering coefficients is conveniently transformed and written in terms of the electron Green's function. In the derivation, some assumptions have to be made regarding time scales and wave packet properties. For the sake of clarity, we will only discuss their legitimacy and mutual compatibility after all of them have been introduced.

Let us consider a wave packet that approaches the sample (region $S$ of Fig. 2) from the semi-infinite lead $a$ (region $L_a$) in transverse mode $m$ with an average total

energy $E$. The wave function for such a wave packet in the remote past ($t \sim -T$, $T \to \infty$) is

$$\Psi^{-}_{Ema}(\mathbf{x}, t) = \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \xi^{-}_{\varepsilon ma}(\mathbf{x})\, e^{-i\varepsilon t/\hbar}, \tag{A1}$$

where $\Phi(u)$ is an amplitude weight function that is normalized to unity,

$$\int |\Phi(u)|^2\, du = 1, \tag{A2}$$

and

$$\xi^{\pm}_{\varepsilon ma}(\mathbf{x}) = (2\pi\hbar v_{\varepsilon ma})^{-1/2} \chi_m(y)\, e^{\pm i k_{\varepsilon ma} x} \tag{A3}$$

is a plane wave in the transverse mode $m$ of lead $a$ with total energy

$$\varepsilon = E_{ma} + \hbar^2 k^2_{\varepsilon ma}/2M \tag{A4}$$

and $v_{\varepsilon ma} = \hbar k_{\varepsilon ma}/M$ is the velocity of longitudinal propagation. The plane wave (A3) would be an eigenstate in the fictitious infinite perfect lead formed by $L_a$ and $L'_a$ ($L_a \cup L'_a$), $L'_a$ being an imaginary prolongation of the semiinfinite perfect lead $L_a$ (see Fig. A1). In $L_a \cup L'_a$, the normalization is, of course,

$$\langle \xi^{\pm}_{\varepsilon ma} \mid \xi^{\pm}_{\varepsilon' m' a} \rangle = \delta_{mm'}\, \delta(\varepsilon - \varepsilon'). \tag{A5}$$

The center of the wave packet (A1) is assumed to be far enough from the sample region so that it is appreciably different from zero only within the lead $L_a$. We will

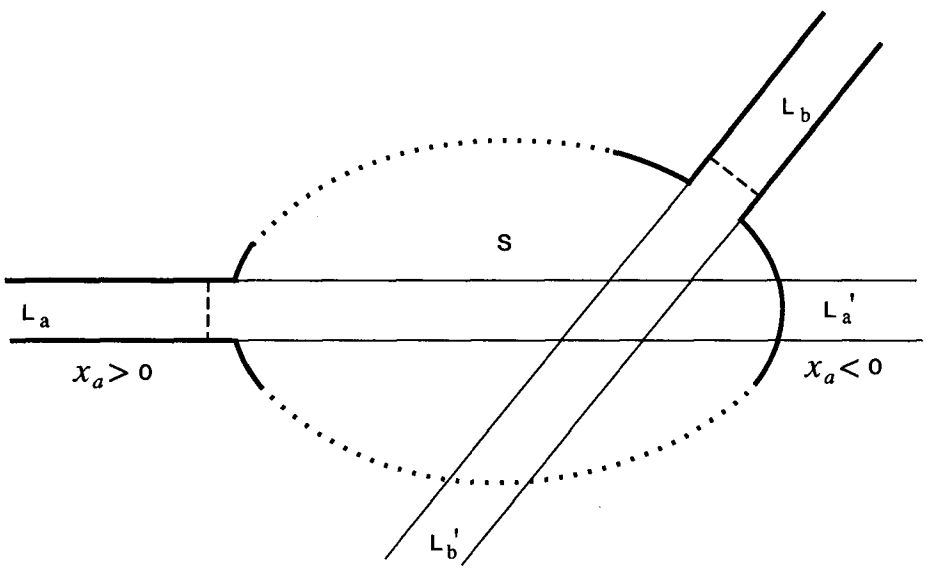


FIG. A1. Imaginary extensions $L'_a$ and $L'_b$ of semi-infinite leads $L_a$ and $L_b$. The combined regions $L_a \cup L'_a$ and $L_b \cup L'_b$ constitute infinite perfect leads.

comment later on the required numerical conditions for this assumption to be meaningful. From (A2) and (A5) it follows that $\langle \psi_{Ema}(t) \mid \psi_{Ema}(t) \rangle = 1$. At this point we can borrow from the analysis of three-dimensional wave packet scattering given in standard text books and show that, in Eq. (A1), the plane waves $\xi^{-}_{\varepsilon ma}(\mathbf{x})$ can be replaced by the *retarded* scattering states $\phi^{(+)}_{\varepsilon ma}(\mathbf{x}$, which satisfy $H_0 \phi^{(+)}_{\varepsilon ma} = \varepsilon \phi^{(+)}_{\varepsilon ma}$ and whose asymptotic behavior is

$$\phi^{(+)}_{\varepsilon ma}(\mathbf{x}) = \begin{cases} \xi^{-}_{\varepsilon ma}(\mathbf{x}) + \sum_n r_{nm,aa}(\varepsilon)\, \xi^{+}_{\varepsilon na}(\mathbf{x}), & \mathbf{x} \in L_a \\ \sum_n t_{nm,ba}(\varepsilon)\, \xi^{+}_{\varepsilon na}(\mathbf{x}), & \mathbf{x} \in L_b. \end{cases} \tag{A6}$$

We will argue later that what has been added to (A1) (the outgoing waves) gives a negligible contribution. Since all the plane waves defined by (A3) carry the same normalized flux $1/2\pi\hbar$, the set of transmission and reflection coefficients displayed in (A6) form a unitary discrete $S$-matrix. It can be shown that (A5) and (A6) imply [49]:

$$\langle \phi^{(+)}_{\varepsilon ma} \mid \phi^{(+)}_{\varepsilon' m' a'} \rangle = \delta(\varepsilon - \varepsilon')\, \delta_{mm'}\, \delta_{aa'}. \tag{A7}$$

(In regard to the content of Refs. [31, 49] we wish to emphasize that the energy delta function normalization (A7) is perfectly compatible with unitarity if, as is the case in (A6), the scattering states are defined in terms of constant flux plane waves that are related through a unitarity $S$-matrix. What is wrong is to take the normalization (A7) for the states $\bar{\phi}^{(+)}_{\varepsilon ma} \equiv (2\pi\hbar v_{\varepsilon ma})^{1/2} \phi^{(+)}_{\varepsilon ma}$ which, when written in terms of the plane waves $\bar{\xi}^{\pm}_{\varepsilon ma} \equiv (2\pi\hbar v_{\varepsilon ma})^{1/2} \xi^{\pm}_{\varepsilon ma}$, are related by coefficients $\bar{r}_{nm,aa}$ and $\bar{t}_{nm,ba}$ that do not form a unitary $S$-matrix. For these states, the correct normalization is $\langle \bar{\phi}^{(+)}_{\varepsilon ma} \mid \bar{\phi}^{(+)}_{\varepsilon' m' a'} \rangle = \delta(k - k')\, \delta_{mm'}\, \delta_{aa'}$, as has been explicitly shown by Kriman *et al.* [49], and which immediately leads to (A7). Thus, the work of Ref. [49], which deals with the normalization of the states $\bar{\phi}^{(+)}$, can be used as a constructive proof of (A7).) Once the wave function (A1) is written in terms of the eigenstates of $H_0$, we are in a position to study its time evolution:

$$\Psi^{-}_{Ema}(\mathbf{x}, t) = \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \phi^{(+)}_{\varepsilon ma}(\mathbf{x})\, e^{-i\varepsilon t/\hbar}. \tag{A8}$$

At a much later time $t \sim T$, it can be shown (see below) that the incident part of $\phi^{(+)}_{\varepsilon ma}$, as well as its portion within the sample $S$, gives a negligible contribution and all the amplitude is in the outgoing waves. Thus, at $t \sim T$ (the appropriate value of $T$ is to be specified later), one can write

$$\Psi^{-}_{Ema}(\mathbf{x}, t) = \begin{cases} \sum_n r_{nm,aa}(E) \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \xi^{+}_{\varepsilon na}(\mathbf{x})\, e^{-i\varepsilon t/\hbar}, & \mathbf{x} \in L_a, \\ \sum_n t_{nm,ba}(E) \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \xi^{+}_{\varepsilon nb}(\mathbf{x})\, e^{-i\varepsilon t/\hbar}, & \mathbf{x} \in L_b,\ b \neq a, \end{cases} \tag{A9}$$

where the $S$-matrix elements have been assumed to vary slowly in the scale of $\Delta\varepsilon$ and have been taken out of the integral sign. For reasons similar to those which lead from (A1) to (A8), we can replace the plane waves in (A9) by the *advanced* scattering states, $\phi_i^{(-)}(\mathbf{x}) \equiv [\phi_i^{(+)}(\mathbf{x})]^*$, which also obey the orthogonality relations (A7). Now we project (A9) onto the outgoing wave packet

$$\Psi_{Enb}^{+}(\mathbf{x}, t) \equiv \int d\varepsilon \frac{1}{\sqrt{\Delta\varepsilon}} \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \xi_{\varepsilon nb}^{+}(\mathbf{x})\, e^{-i\varepsilon t/\hbar}, \tag{A10}$$

where $\xi^+$ can also be replaced by $\phi^{(-)}$. By using (A9) and (A10) in combination with the orthonormality of the asymptotic wave packets (which can be obtained from (A2) and (A5) or (A7)) we arrive at

$$t_{nm,ba}(E) = \langle \Psi_{Enb}^{+}(t) \mid \Psi_{Ema}^{-}(t) \rangle, \tag{A11}$$

which can be more conveniently written as

$$t_{nm,ba}(E) = \langle \Psi_{Enb}^{+}(t) \mid iG_0^{(+)}(t - t') \mid \Psi_{Ema}^{-}(t') \rangle, \tag{A12}$$

where we remember that $t \sim T \sim -t'$ and that the limit $\Delta\varepsilon \to 0$ has to be taken. In (A12), $iG_0^{(+)}$ is the retarded evolution operator,

$$iG_0^{(+)}(t) = \Theta(t)\, e^{-iH_0 t/\hbar}\, e^{-\eta t} = \int \frac{dE}{2\pi} iG_0^{(+)}(E)\, e^{-iEt/\hbar}, \tag{A13}$$

where $G_0^{(+)}(E)$ is given by (2). Analogously,

$$r_{nm,aa}(E) = \langle \Psi_{Ena}^{+}(t) \mid iG_0^{(+)}(t - t') \mid \Psi_{Ema}^{-}(t') \rangle. \tag{A14}$$

Before we proceed further, let us discuss the legitimacy of the assumptions that have been made about the scattering process. Some of the arguments we give below can be found in standard textbooks [50]. However, the novel nature of multilead scattering and, in particular, the presence of asymptotic channels with different energy thresholds for propagation poses new difficulties that deserve a separate discussion. The assumptions are essentially three: (i) The packet has negligible spreading during the time interval in which the wave packet evolution is considered (from $-T$ to $T$); (ii) the wave packet is sufficiently localized, both at $T$ and $-T$, for the wave amplitude in the sample region to be negligible; and (iii) the wave packet is sufficiently monochromatic, so that the energy dependence of the $S$-matrix elements can be neglected. Below we show that the first two requirements impose conditions on the choice of $T$ that can always be met. In a given transverse mode, these two assumptions can be quantitatively formulated as (i) $\hbar(\Delta k)^2 T/M \ll 1$, and (ii) $\Delta x \ll vT$, where $\Delta k$ is the wavevector width, $\Delta x \sim 1/\Delta k$ is the spatial width, and $v = \hbar k/M$ is the average longitudinal vocity in the particular mode considered. Clearly, (i) is most stringent for the mode with the highest $\Delta k$, which will be that with the highest energy threshold $E_0$, since $E = E_0 + \hbar^2 k^2/2M$ is conserved and $\Delta E = \hbar k\, \Delta k/M$ is the same for all modes involved (remember that $\Delta E$ is assumed

small enough for the energy distribution not to be distorted by the energy dependence of the scattering amplitudes).

On the other hand, (ii) is equivalent to $\hbar/\Delta E \ll T$, which is independent of the mode. Thus, it is sufficient to meet requirements (i) and (ii) for the available mode with the highest $E_0$ at a given energy $E$. Both conditions can be combined into

$$\frac{\hbar}{\Delta E} \ll T \ll 2\hbar \frac{E_k}{(\Delta E)^2}, \tag{A15}$$

where $E_k = \hbar^2 k^2/2M$ is the longitudinal kinetic energy in the highest threshold mode. Given $\Delta E$, it is always possible to choose a time scale $T$ that satisfies the double requirement (A15), provided $\Delta E \ll E_k$. In particular, this implies that $\Delta E$ can be made arbitrarily small and thus condition (iii) can always be satisfied, even close to the threshold and at resonances, where the strongest energy dependence of the scattering amplitudes is expected.

When (i) is satisfied, it is possible to approximate

$$e^{\pm ik_{\varepsilon na}x}\, e^{-i\hbar k_{\varepsilon na}^2 t/2m} \simeq e^{i\hbar k_{Ena}^2 t/2M}\, e^{ik_{\varepsilon na}(\pm x - v_{Ena}t)} \tag{A16}$$

at all times $(-T < t < T)$ within the various energy integrals defining the wave packets. When (A16) is introduced in (A1), it becomes clearer that (A1) describes a wave packet centered around $x = -v_{Enm}t > 0$ in $L_a$ and the subsequent analysis becomes more transparent: (A1) can be replaced by (A8) because the added outgoing waves correspond to wave packets centered around the various $x = v_{Enb}t < 0$, which only have appreciable amplitude in the imaginary $L_b'$. As to the sample region contribution, $\phi_{\varepsilon ma}^{(+)}(\mathbf{x})$ can be assumed to be smoothly dependent on $\varepsilon$ for $\mathbf{x} \in S$ (see above) and the sample contribution in (A8) would be roughly equivalent to a wave packet centered in, e.g., $-v_{Enb}t$, but evaluated at $x \simeq 0$, where the amplitude is negligible.

At this point, we can resume our analysis and note that by introducing (A1), (A10), and (A3) into (A12) we can write

$$\begin{aligned} t_{nm,ba}(E) = \iint d\varepsilon\, d\varepsilon' \frac{1}{\Delta\varepsilon} \Phi^* \left(\frac{\varepsilon - E}{\Delta\varepsilon}\right) \Phi \left(\frac{\varepsilon' - E}{\Delta\varepsilon}\right) e^{i(\varepsilon t - \varepsilon' t')/\hbar} \\ \times \int \frac{dE'}{2\pi} \int_{L_b} dx \int_{L_a} dx' \frac{e^{-ik_{\varepsilon nb}x}}{(2\pi v_{\varepsilon nb})^{1/2}} \frac{e^{ik_{\varepsilon' ma}x'}}{(2\pi\hbar v_{\varepsilon' ma})^{1/2}} \\ \times iG_{nm,ba}^{0(+)}(x, x'; E')\, e^{-iE'(t-t')/\hbar}, \end{aligned} \tag{A17}$$

where the definition (2) has been used.

From the previous discussion on the properties of the wave packets, we know that the space integrals in (A17) only receive appreciable contributions from segments that lie well in the asymptotic regions. Thus, it is possible to find two reference points $\mathbf{x}_a \in L_a$ and $\mathbf{x}_b \in L_b$ such that $x > x_b$ and $x' > x_a$ for all $x$ and $x'$ that contribute significantly to (A17). One can then use the property [51]

$$G_{nm,ba}^{0(+)}(x, x'; E) = G_{nm,ba}^{0}(x_b, x_a; E)\, e^{ik_{Enb}(x - x_b)}\, e^{ik_{Ema}(x' - x_a)} \tag{A18}$$

and formally extend the spatial integrals to $L_a \cup L'_a$ and $L_b \cup L'_b$ (i.e., integrate $x$ and $x'$ from $-\infty$ to $+\infty$), so that they can be trivially performed. They yield $\delta(\varepsilon - E')\,\delta(\varepsilon' - E')$ with some factors. As a result,

$$t_{nm,ba}(E) = \int d\varepsilon \frac{1}{\Delta\varepsilon} \left| \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right)\right|^2 \times i\hbar (v_{\varepsilon nb} v_{\varepsilon ma})^{1/2} G^{0(+)}_{nm,ba}(x_b, x_a; \varepsilon)\, e^{-i(k_{\varepsilon nb} x_b + k_{\varepsilon ma} x_a)}. \tag{A19}$$

If we now take the limit of a very monochromatic wave packet,

$$\lim_{\Delta\varepsilon \to 0} \frac{1}{\Delta\varepsilon} \left| \Phi\left(\frac{\varepsilon - E}{\Delta\varepsilon}\right)\right|^2 = \delta(\varepsilon - E), \tag{A20}$$

Eq. (A17) becomes Eq. (1b) of the text, as we wanted to show.

A similar analysis can be performed for the reflection coefficient. However, in this case the replacement (A18) can only be made for the *purely reflected* part of the propagator,

$$F_{nm,aa}(x, x'; E) \equiv G^{0(+)}_{nm,aa}(x, x'; E) - \delta_{nm} \frac{e^{ik_{Ena}|x - x'|}}{i\hbar v_{Ena}}, \tag{A21}$$

for which

$$F_{nm,aa}(x, x'; E) = F_{nm,aa}(x_a, x'_a; E)\, e^{ik_{Ena}(x - x_a)}\, e^{ik_{Ema}(x' - x'_a)}, \tag{A22}$$

where we have used the fact that $x > x_a$ and $x' > x'_a$, and that they all lie in the asymptotic region $L_a$. It is important to note that in (A14) the full propagation $G_0^{(+)}$ can be replaced by the reflected component $F$, because the free propagator which has been subtracted makes $\Psi^-_{Ema}$ evolve into a wave packet that at $t \sim T$ is located far in $L'_a$, where no overlap with $\Psi^+_{Ena}$ exists, and thus gives a vanishing contribution to the matrix element. Once $G_0^{(+)}$ has been replaced by $F$, one uses (A22) and, following steps similar to those we studied for the transmission, one obtains (we take $x'_a \geqslant x_a$)

$$r_{nm,aa}(E) = i\hbar (v_{Ena} v_{Ema})^{1/2} \times \left[ G^{0(+)}_{mn,aa}(x_a, x'_a; E) - \delta_{nm} \frac{e^{ik_{Ena}(x'_a - x_a)}}{i\hbar v_{Ena}} \right] e^{-i(k_{Ena} x_a + k_{Ema} x'_a)} \tag{A23}$$

which immediately leads to Eq. (1a), as required.

## APPENDIX B: LATTICE FORMULATION

In a tight-binding structure the one-electron Hamiltonian is of the type

$$H_0 = \sum_{\mathbf{R}} \varepsilon_{\mathbf{R}} e^+_{\mathbf{R}} c_{\mathbf{R}} + \sum_{\mathbf{R}, \mathbf{R}'} \Delta_{\mathbf{R}\mathbf{R}'} c^+_{\mathbf{R}} c_{\mathbf{R}'}, \tag{B1}$$

where sites are labeled by its vector position $\mathbf{R}$, the operator $c_{\mathbf{R}}^{+}$ creates an electron in site $\mathbf{R}$, and the hopping matrix element $\Delta_{\mathbf{RR}'}$ is assumed to connect only nearest neighbors. The sites $\mathbf{R}$ can represent real atoms in a lattice or they can be fictitious entities filling a multilead structure with a sufficiently high density. The latter case corresponds to the replacement of a continuum problem by a lattice structure for numerical purposes, which is equivalent to the use of a finite difference method to solve the Schrödinger equation [11]. Hard-wall boundaries are simulated by the absence of sites and possible variations in the potential $U(\mathbf{x})$ are obtained by modulating the site energies $\varepsilon_{\mathbf{R}}$. The hopping term corresponds to the kinetic energy. In order to define the scattering problem, we assume that the tight-binding structure is formed by semi-infinite perfect stripes ($L_i$) that are connected through a central region (S) where scattering occurs, like in Fig. B1. This means that

$$\varepsilon_{\mathbf{R}} = \varepsilon_0, \qquad \Delta_{\mathbf{RR}'} = \Delta_0 < 0 \qquad \text{for} \quad \mathbf{R}, \mathbf{R}' \in L_i \tag{B2}$$

and nearest neighbors (in order to have a common energy reference for the lattice and continuum descriptions, it is convenient to take $\varepsilon_0 = 2d\Delta_0$, where $d$ is the dimension, cf. Ref. [11]).

The electron–phonon interaction will be of the form (see Eq. (51))

$$V = \sqrt{\lambda} \sum_{q} \sum_{\mathbf{R}} M_q(\mathbf{R})\, c_{\mathbf{R}}^{+} c_{\mathbf{R}} (a_q + a_{-q}^{+}). \tag{B3}$$

Below we give some of the most important transformations that are required to shift from a continuum to a lattice formulation (some of them are given for $d = 1$, then $\mathbf{R} \equiv l$)

$$|\mathbf{x}\rangle \to \frac{1}{a^{d/2}} |\mathbf{R}\rangle, \qquad \psi(\mathbf{x}) \to \frac{1}{a^{d/2}} c_{\mathbf{R}}, \qquad \int d^d\mathbf{x} \to a^d \sum_{\mathbf{R}},$$

$$G(\mathbf{x}, \mathbf{x}') \to \frac{1}{a^d} G(\mathbf{R}, \mathbf{R}'), \qquad kx \to \theta l, \qquad v \to -(2\Delta_0 a/\hbar) \sin\theta, \tag{B4}$$

$$E_k = \hbar^2 k^2 / 2M \to E_0 = 2\Delta_0(\cos\theta - 1), \qquad \int_{-\infty}^{\infty} dk \to \frac{1}{a} \int_{-\pi}^{\pi} d\theta.$$

As an illustration, we show that the analysis of Section 2 can be conveniently adapted to reproduce the result of Wingreen *et al.* [22] for $T(E_f, E_i)$ in a one-site model of a resonant tunneling structure which is essentially equivalent to the structure shown in Fig. B1. As in Ref. [22] the space between the barriers is described by a single relevant orbital, the weak tunneling through the barriers is given by the

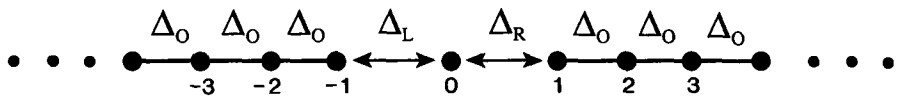


FIG. B1. Schematic representation of a resonant site ($l = 0$) coupled elastically to semi-infinite right ($l > 0$) and left ($l < 0$) leads which, for convenience, are described by tight-binding chains.

hopping energies $\Delta_L$ and $\Delta_R$, and phonons are assumed to couple only to the resonant site ($l=0$). Here we choose for convenience a tight-binding representation of the semi-infinite leads where the uniform hopping energy is $\Delta_0$ and $\varepsilon_0=0$. The results do not depend, of course, on this particular choice of lead description.

Most of the derivation runs completely analogous to the continuum analysis of Section 2. The starting point is the equivalent of Eq. (4) in a tight-binding language (see (B4)):

$$t_{\beta\alpha}(E)=2i\,|\Delta_0|\,(\sin\theta_{E\beta}\sin\theta_{E\alpha})^{1/2}\,e^{-i(\theta_{E\beta}l-\theta_{E\alpha}l')}G^{(+)}_{\beta\alpha}(l,l';E), \tag{B5}$$

where $l>0$ and $l'<0$ (note the change in sign convention for the left lead), where $v_{E\alpha}=-(2\,\Delta_0 a/\hbar)\sin\theta_{E\alpha}$ is the group velocity and $\theta_{E\alpha}=\cos^{-1}[(E-\varepsilon_\alpha)/2\,\Delta_0+1]$ is the dimensionless crystal momentum for motion in the chains when the bath is in state $\alpha$ and the total energy is $E$. In this particular problem, everything can be referred to the Green's function at the resonant site. This is due to the relation

$$G_{\beta\alpha}(l,l';E)=G^0_{\beta\beta}(l,1;E)\,\Delta_R G_{\beta\alpha}(0,0;E)\,\Delta_L G^0_{\alpha\alpha}(-1,l';E), \tag{B6}$$

which holds exactly if, as assumed, phonon coupling only takes place at $l=0$. The Green's function in the semi-infinite chains are known exactly:

$$G^{0(+)}_{\beta\beta}(l,1;E)=\frac{e^{i\theta_{E\beta}l}}{\Delta_0},\qquad G^{0(+)}_{\alpha\alpha}(-1,l';E)=\frac{e^{-i\theta_{E\alpha}l'}}{\Delta_0}. \tag{B7}$$

As a consequence,

$$G^{(+)}_{\beta\alpha}(l,l';E)=\frac{\Delta_R\,\Delta_L}{\Delta_0^2}\,e^{i(\theta_{E\beta}l-\theta_{E\alpha}l')}G^{(+)}_{\beta\alpha}(0,0;E), \tag{B8}$$

and we can write

$$t_{\beta\alpha}(E)=2i(\sin\theta_{E\beta}\sin\theta_{E\alpha})^{1/2}\,\frac{\Delta_R\,\Delta_L}{|\Delta_0|}\,G^{(+)}_{\beta\alpha}(0,0;E). \tag{B9}$$

From this point, the derivation is identical to that which leads from (4) to (14). The only difference lies in the replacement of $\hbar(v_f v_i)^{1/2}$ by $2(\Delta_R\Delta_L/|\Delta_0|)(\sin\theta_f\sin\theta_i)^{1/2}$ and of $x_a$ and $x_b$ by $l=0$. Before writing the final result (the equivalent of Eq. (14)), we note that the self-energies of the resonant site due to the presence of the leads (in the absence of phonons) are [11]

$$\Sigma_R(E)=\Delta_R^2 G_0^{(+)}(1,1;E)=\frac{\Delta_R^2}{\Delta_0}\,e^{i\theta_E}, \tag{B10}$$

and similarly for $\Sigma_L(E)$. The linewidths are thus

$$\Gamma_L(E_i)=-\frac{2\,\Delta_L^2}{\Delta_0}\sin\theta_i,\qquad \Gamma_R(E_f)=-\frac{2\,\Delta_R^2}{\Delta_0}\sin\theta_f. \tag{B11}$$

Collecting all the pieces together, the final expression for the transmission probability is

$$T(E_f, E_i) = \Gamma_L(E_i)\,\Gamma_R(E_f) \iiint \frac{d\tau\, dt\, ds}{2\pi\hbar^3} e^{i[(E_f - E_i)\tau + E_f t - E_i s]/\hbar} \theta(t)\,\theta(s) \times \langle c_0(\tau - s)\, c_0^+(\tau)\, c_0(t)\, c_0^+(0)\rangle \tag{B12}$$

which is the result first obtained by Wingreen *et al.* [22].

We note that the linewidths $\Gamma_L$ and $\Gamma_R$ are intrinsic properties of the system and do not depend on the particular choice of a tight-binding description for the leads. Our derivation of (B12) is therefore completely general. A similar analysis can be performed for the reflection probability $R(E_f, E_i)$, with results that agree also with those of Ref. [22].

## APPENDIX C: Explicit Proof of Unitarity

Unitarity is satisfied if

$$\int \left[ \sum_{nb} T_{nm,ba}(E_f, E_i) + \sum_{n} R_{nm,aa}(E_f, E_i) \right] dE_f = 1 \tag{C1}$$

for all $E$, $m$, and $a$. To show that (C1) can be obtained from Eqs. (14) and (16) in the text, let us rewrite these in a slightly different way:

$$T_{nm,ba}(E_f, E_i) = \delta_{ba}\,\delta_{nm}\,\delta(E_f - E_i) + T^{\mathrm{A}}_{nm,ba}(E_f, E_i) + T^{\mathrm{B}}_{nm,ba}(E_f, E_i) \tag{C2a}$$

$$T^{\mathrm{A}}_{nm,ba}(E_f, E_i) = \frac{v_f v_i}{2\pi\hbar} e^{ik_f(x_b - x_b')} \iiint_{-\infty}^{\infty} d\tau\, dt\, ds\, e^{i[(E_i - E_f)\tau + E_f t - E_i s]/\hbar} \theta(t)\,\theta(s) \times \langle \psi_m(x_a, \tau - s)\, \psi_n^+(x_b, \tau)\, \psi_n(x_b', t)\, \psi_m^+(x_a, 0)\rangle \tag{C2b}$$

$$T^{\mathrm{B}}_{nm,ba}(E_f E_i) = \delta_{ba}\,\delta_{nm}\,\delta(E_f - E_i)\, 2\hbar v_i\, \mathrm{Im}\, G^{(+)}_{nn}(x_a, x_a; E_i). \tag{C2c}$$

We have made use of the freedom to choose the reference points in Eq. (4) for $t_{nm,ba,\beta\alpha}(E)$. When squaring this expression in (8) we can choose different reference coordinates for $t_{nm,ba,\beta\alpha}$ and its complex conjugate. If $b = a$, we assume $x_b, x_b' > x_a$. Incoming and outgoing channels are formally treated now on the same footing, except for the presence of the term $T^{\mathrm{B}}$, which is nonzero only when the bath channels are identical ($nb = ma$). Equation (C1) can now be rewritten as the condition

$$F^{\mathrm{A}}_{ma}(E) = -F^{\mathrm{B}}_{ma}(E), \tag{C3}$$

where

$$F^{\mathrm{A(B)}}_{ma}(E_i) \equiv \sum_{nb} \int T^{\mathrm{A(B)}}_{nm,ba}(E_f, E_i)\, dE_f \tag{C4}$$

From the definition (70), it is easy to see that

$$F^{B}_{ma}(E) = -v_{Ema}\int_{-\infty}^{\infty} d\tau\, e^{iEt/\hbar}\, e^{-\eta|\tau|}\langle \psi_m(x_a, \tau)\, \psi_m^{+}(x_a, 0)\rangle. \tag{C5}$$

The transformation of $F^{A}_{ma}$ onto the negative of Eq. (C5) requires substantially more algebra. First we note that the freedom of choice of reference points can be phrased as

$$\frac{\partial}{\partial x_b} T^{A}_{nm,ba}(E_f, E_i) = \frac{\partial}{\partial x'_b} T^{A}_{nm,ba}(E_f, E_i) = 0, \tag{C6}$$

which implies that, in (C2b), we may replace $v_f$ by $(i\hbar/M)\,\partial/\partial x_b$ or $(-i\hbar/M)\,\partial/\partial x'_b$ acting on $\psi_n^{+}(x_b, \tau)$ or $\psi_n(x'_b, t)$, respectively. In particular, we choose the substitution

$$v_f \psi_n^{+}(x_b, \tau)\, \psi_n(x'_b, t) \to \frac{i\hbar}{2M}\left[\frac{\partial \psi_n^{+}(x_b, \tau)}{\partial x_b}\psi_n(x'_b, t) - \psi_n^{+}(x_b, \tau)\frac{\partial \psi_n(x'_b, t)}{\partial x'_b}\right] \tag{C7}$$

in Eq. (C2b). The explicit dependence on $v_f$ has now disappeared and, in (C4), the integral over $E_f$ yields $2\pi\hbar\,\delta(\tau - t)$. If $x'_b = x_b$ is taken again, we can write

$$F^{A}_{ma}(E) = v_{Ema}\int_0^{\infty} dt \int_0^{\infty} ds\, e^{iE(t-s)/\hbar}\, e^{-\eta(t+s)} \left\langle \psi_m(x_a, t-s) \times \left\{\sum_{nb} \frac{\hbar}{2Mi}\left[\psi_n^{+}(x_b, t)\frac{\partial \psi_n(x_b, t)}{\partial x_b} - \frac{\partial \psi_n^{+}(x_b, t)}{\partial x_b}\psi_n(x_b, t)\right]\right\} \psi_m^{+}(x_a, 0)\right\rangle. \tag{C8}$$

Obviously, the expression within curled brackets is the current flux leaking out of the sample region into the asymptotic leads. By applying the divergence theorem and invoking the continuity equation

$$\nabla \mathbf{j}(\mathbf{x}, t) + \frac{\partial \rho(\mathbf{x}, t)}{\partial t} = 0, \tag{C9}$$

the current flux can be written as

$$-\int_S dx \frac{\partial \rho(\mathbf{x}, t)}{\partial t}, \tag{C10}$$

where $\rho(\mathbf{x}, t) = \psi^{+}(\mathbf{x}, t)\,\psi(\mathbf{x}, t)$ is the electron density operator and the integration is performed over the sample region $S$. If (C10) is introduced in the curled brackets of (C8) and the times $t$ and $s$ are replaced by the variables $t$ and $\tau = t - s$, Eq. (C8) becomes

$$F^{\mathrm{A}}_{ma}(E) = -v_{Ema}\int_{-\infty}^{\infty} d\tau\, e^{iE\tau/\hbar}\int_{\tau_0}^{\infty} dt\, e^{-\eta(2t-\tau)}\int_S d\mathbf{x} \tag{C11}$$

$$\times\left\langle \psi_m(x_a,\tau)\frac{\partial\rho(\mathbf{x},t)}{\partial t}\psi^+_m(x_a,0)\right\rangle, \tag{C12}$$

where $\tau_0 \equiv \max(0,\tau)$. The integral over $t$ is performed by parts and then the limit $\eta \to 0^+$ is taken where needed. The result is

$$F^{\mathrm{A}}_{ma}(E) = v_{Ema}\int_S d\mathbf{x}\iint dy_a\, dy'_a \chi^*_m(y_a)\,\chi_m(y'_a)\int_{-\infty}^{\infty} d\tau\, e^{iE\tau/\hbar}\, e^{-\eta|\tau|}$$

$$\times\langle\psi(\mathbf{x}_a,\tau)\,\rho(\mathbf{x},\tau_0)\,\psi^+(\mathbf{x}'_a,0)\rangle, \tag{C13}$$

where $\mathbf{x}_a = (x_a, y_a)$, $\mathbf{x}'_a = (x_a, y'_a)$, and the decomposition (55) has been employed. Now we make use of the equal time commutation relations

$$[\rho(\mathbf{x},t),\psi^+(\mathbf{x},t)] = \psi^+(\mathbf{x},t)\,\delta(\mathbf{x}-\mathbf{x}') \tag{C14}$$

and its hermitian conjugate, which are satisfied by both Fermi and Bose field operators. We can apply them to our particular single electron problem, where the result must not depend on the choice of statistics. For $\tau<0$, $\tau_0=0$, and we have

$$\langle\psi(\mathbf{x}_a,\tau)\,\rho(\mathbf{x},0)\,\psi^+(\mathbf{x}'_a,0)\rangle$$

$$= \langle\psi(\mathbf{x}_a,\tau)\,\psi^+(\mathbf{x}'_a,0)\rangle\,\delta(\mathbf{x}-\mathbf{x}'_a) + \langle\psi(\mathbf{x}_a,\tau)\,\psi^+(\mathbf{x}_a,0)\,\rho(\mathbf{x},0)\rangle \tag{C15}$$

but the second term is identically zero, since the expectation value is taken over the electron vacuum. Analogously, for $\tau>0$, $\tau_0=\tau$, and

$$\langle\psi(\mathbf{x}_a,\tau)\,\rho(\mathbf{x},\tau)\,\psi^+(\mathbf{x}'_a,0)\rangle = \langle\psi(\mathbf{x}_a,\tau)\,\psi^+(\mathbf{x}'_a,0)\rangle\,\delta(\mathbf{x}-\mathbf{x}_a). \tag{C16}$$

Since the sample region $S$ can always be taken large enough to include the reference points $\mathbf{x}_a$ and $\mathbf{x}'_a$ (in fact, we assumed $x_b > x_a$ for $b=a$), the integral over $\mathbf{x}$ can be trivially performed. The result is

$$F^{\mathrm{A}}_{ma}(E) = v_{Ema}\iint dy_a\, dy'_a\chi^*_m(y_a)\,\chi_m(y'_a)$$

$$\times\int_{-\infty}^{\infty} d\tau\, e^{iE\tau/\hbar}\, e^{-\eta|\tau|}\langle\psi(\mathbf{x}_a,\tau)\,\psi^+(\mathbf{x}'_a,0)\rangle, \tag{C17}$$

which is obvious identical to $-F^{\mathrm{B}}_{ma}(E)$, as given in (C5).

Therefore, we have shown that the unitarity condition (C1) can be explicitly derived from the general expression (C2) (equivalent to (14) and (16)) by invoking the continuity equation (C9).

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