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Classical and quantum transport from generalized Landauer-Büttiker equations. II. Time-dependent resonant tunneling

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A generalization of the Landauer-Büttiker picture of transport applicable to time-dependent problems in the presence of dissipation is presented. Starting from the Schrödinger equation in the Keldysh formalism under appropriate boundary conditions and using a linear-response approximation, we find that an *ideal voltage probe* is described by a generalized Landauer-Büttiker equation (GLBE). Thus, the GLBE may be considered as a particular case of the Keldysh kinetic equation. The transmission probabilities become *retarded* functions of the elapsed time, and are evaluated in terms of the retarded and advanced Green's functions. The interpretation of the mathematical formalism is emphasized. The GLBE is applied to get the time-dependent dissipative resonant tunneling by considering a resonant dot coupled with (a) a dephasing process and (b) a finite side probe. For case (a), we find that the resonant-tunneling conductance G is associated with an inductance $L \approx \tau_q / G$ which accounts for the response in the low-frequency regime; G depends on the dissipation inside the resonant region, while τ_q, being twice the natural lifetime of the resonant state, does not. For case (b), we find an additional delay in the response accounting for the "inertia" of the side probe. This result clarifies the concepts of ideal voltage probe and *voltage source* as applied in the case of time-dependent transport.

I. INTRODUCTION

In recent years, many experimental works on transport in mesoscopic systems[1] found a good deal of inspiration in the Landauer-Büttiker picture[2] for *steady-state* conductance. The fundamental observation that leads to this picture is that a transport experiment is performed in an open system exchanging particles and energy with the external world. Therefore, this exchange can be viewed as a scattering problem in which particles injected through a given channel connected with the external world are found in some other channels after having interacted in some region called "the sample." These particles account for (boundary) conditions controlled externally (such as current, voltage, or temperature). While this picture was also believed[2] to apply to samples subject to dephasing and inelastic processes, it was not until the independent works of D'Amato and Pastawski[3] and Datta,[4] that a quantum description was obtained. Transport in the linear-response regime is then described by a generalized Landauer-Büttiker equation (GLBE). This expresses the transmission probabilities, which contain the dephasing processes, in terms of a model Hamiltonian in which both leads and dephasing processes are represented by the self-energy corrections they produce.[3,4] Works following related lines were soon successfully applied to a number of problems.[5] More recently, we have shown[6] that the GLBE is consistent with the known behavior of dc conductivity in macroscopic systems in a wide range of situations. The fundamental observation that led to these results is the connection between the transmission probabilities in the GLBE and a density propagator. The object of the present paper is to extend the GLBE to evaluate the *time-dependent conductance* in the presence of dephasing processes, making explicit the assumptions needed to make the mentioned connection. In so doing, we will need to extend our previous results[3,6] and those of Datta and collaborators[4,5(a)-5(c)] which considered exhaustively the steady-state problem. Besides, while our results in Ref. 6 point in the right direction as to how the Landauer-Büttiker picture could be extended to a time-dependent problem, the conditions under which this can be done were not clear. For example, in a steady state the local occupation is that measured by a weakly coupled voltage problem. Is that valid in a time-dependent situation? A voltage probe and an inelastic process are equivalent, within certain limitations, for the dc transport. Is that true in a time-dependent case? May the voltage probes manifest an "inertia"? A dephasing process affects the dc conductance. Does it also show up in the ac response? This work will answer these questions and establish a framework to answer further ones.

In order to show our main result in the simplest terms, let us consider the typical case described by a Landauer-Büttiker equation: a voltage probe α connected to a sample. If $T_{\alpha,\beta}$ ($T_{\beta,\alpha}$) are the transmission probabilities from (toward) all the leads β connected to the sample, the balance of currents at this lead is obtained from addition of these transmittances, weighted by $\delta\mu_\beta$ ($\delta\mu_\alpha$), the shift from equilibrium of the chemical potential in the outgoing channel. While the original Landauer-Büttiker equation and the GLBE describe the steady state, we will find a time-dependent equation which for an *ideal* voltage probe α is

$$0=\frac{2e}{\hbar}\left[\sum_{\beta}\int_{-\infty}^{t}T_{\alpha,\beta}(t-t_i)\delta\mu_{\beta}(t_i)dt_i\right.$$
$$\left.-[1-R_{\alpha}]\delta\mu_{\alpha}(t)\right]. \qquad (1.1)$$

Here we introduced the retarded transmission probabilities whose integral in time gives the usual steady-state coefficients $T_{\alpha,\beta}=\int dt_i T_{\alpha,\beta}(t-t_i)$. The total transmission probability, $[1-R_\alpha]=\sum_\beta T_{\alpha,\beta}$, is defined including the channel α in the sum.

The physical meaning of Eq. (1.1) is quite simple: It is the electric current leaving the sample at contact α. It results from the balance between the "out" and "in" contributions which gives zero net current at the ideal voltage probe α at *any* time t. The out current at α is the sum of all the incoherent electrons which having left the reservoir β at a previous time t_i, reach the reservoir α at time t. This sum also includes the electrons, which having left reservoir α at time t_i, return at time t without having a dephasing collision in its journey. The second term on the right is the in current, which describes the electrons that at time t are leaving the reservoir α to explore the sample and are absorbed somewhere at a later time.

Equation (1.1) generalizes that originally proposed by Büttiker because of the following: (a) The transmission probabilities are now *retarded* in time, representing the finite velocity of propagation of wave packets. (b) The chemical potentials are also generalized to describe a time-dependent problem. (c) In the general case the transmission probabilities will contain dephasing processes such as the electron-phonon interaction. (d) The chemical potential is not necessarily that of an external reservoir but can be a quantity characterizing the local density of electrons in a nonequilibrium state. This last point, as well as the meaning of an ideal voltage probe, will be clarified in this work.

Therefore, this work is devoted to show that Eq. (1.1) can be derived from the time evolution described by the Schrödinger equation of a system modeled by a precise Hamiltonian. This will give explicit forms for the time-dependent transmission coefficients and chemical potentials involved. With this purpose we will resort to the quantum evolution in the nonequilibrium quantum fields (Keldysh) formalism.[7] While the Keldysh technique has been extensively used[8] to treat quantum transport in various problems of nonlinear transport, its connection to the Landauer-Büttiker picture in the linear-response regime will shed light on how irreversibility and dissipation are introduced in quantum mechanics. The essential idea we advocate throughout this work is that the effect of the leads and the phase-breaking processes can be represented as boundary conditions on the closed system. This idea motivated the work of Refs. 3 and 6, and here it will be presented on formal grounds, making explicit the approximations used with that objective. Here the boundary conditions appear as time-dependent self-energies. The resulting evolution equations will then be cast in the form of the kinetic equation (1.1). Besides, the main features of the solution in some representative cases will be sketched. The time-dependent problem, in contrast with the steady-state situation, makes evident the difference between a real voltage lead and a dephasing process: they may produce a very different time response.

This paper is organized as follows: Section II presents an overview of the basic material used in the following sections, introducing a notation which will assist us in the development of the conceptual framework. We start with a brief discussion about open and closed systems (Sec. II A) and how they are accounted for in the Keldysh formalism (Sec. II B). In Sec. II C we develop a real-time formulation and obtain our main kinetic equation. In Sec. II D this is expressed in terms of measurable electronic densities. Section III shows explicitly how boundary conditions are introduced as self-energies in the case of leads (Sec. III A) and the electron-phonon interaction (Sec. III B). Section IV is the central part of the work; there we obtain a simplified time-dependent kinetic equation and show that it has a classical interpretation in terms of a density propagator. Section V has a practical intention as it shows how, from our knowledge of the electron densities of the system at previous times, one can evaluate electric currents in both nonlinear- and linear-response regimes. Then, we show that the kinetic equation is equivalent to the GLBE. Section VI addresses the important problem of time-dependent dissipative resonant tunneling, which represents a straightforward application of the formalism developed and it clarifies the conceptual elements involved. We start discussing the salient features of the steady-state situation (Sec. VI A) and two different mechanisms to achieve dephasing solved in the following sections, both of which are experimentally accessible. In Sec. VI B the resonant state interacts with a dephasing field. We find that the frequency-dependent tunneling conductance $G(\omega)$ (in the low-frequency limit) has an inductive component $L\approx\tau_q/G(0)$, where τ_q is twice the escape time τ_1 of the resonant state in the absence of dephasing processes. An interesting prediction of our kinetic equation is that this functional form is maintained even in the limiting case of completely incoherent tunneling. These results support the observation of the correspondent behavior in the differential conductance of a biased double-barrier resonant tunneling device (DBRTD). In Sec. VI C we solve a resonant region connected with a side dot. Since the side dot can be considered a model for a voltage probe, the results of Sec. VI C clarify the difference between an ideal and a real voltage probe. In the first case, as occurs with a dephasing field, the electrons cannot escape from the sample. In the last case, this restriction does not hold. Then, it appears an additional delay time which is proportional to the total density of states on the side probe and to $\tau_1+\tau_S$, the sequential composition of the escape time to the leads and to the side probe τ_S. Finally, a general discussion is presented in Sec. VII.

II. THE FORMAL FRAMEWORK

A. Closed and open systems

The behavior of a closed noninteracting electronic system in a state Ψ is described by the Hermitic Hamiltonian H^0, which contains the impurities potential and the external fields, according to the Schrödinger equation:

$$\left[i\hbar\frac{\partial}{\partial t} - H^0(\mathbf{r}) \right] |\Psi(\mathbf{r},t)\rangle \equiv [G^0(X)]^{-1} |\Psi(X)\rangle = 0 \ . \tag{2.1}$$

In the definition of the Schrödinger differential operator $[G^0(X)]^{-1}$, the variable $X=(\mathbf{r},t)$ is short for d-dimensional space and time coordinates. For any initial condition, there will be a finite time (Poincaré cycle) for which the state of the system returns arbitrarily close to this initial condition.[9] This situation changes when we couple the sample to the rest of the universe. Because of the increase in the number of quasidegenerate degrees of freedom (energy band), the Poincaré cycle becomes infinite and an irreversible behavior appears. In order to describe the opening to the external world while keeping the manageable Hilbert space spanned by the states of the noninteracting sample, it is possible to use the projection operator technique.[10] This allows us to downfold or decimate the external degrees of freedom generating an effective Hamiltonian:

$$H_{\mathrm{eff}} = H^0 + \Sigma \ , \tag{2.2}$$

where the added effective potential (or self-energy) accounts for the degrees of freedom left out of H^0. This scheme is quite convenient in various simple cases such as systems with few degrees of freedom or the description of the radiative decay. In the first case Σ can be obtained by an exact decimation procedure,[11] and it results in a nonlinear real function of the energy ε. The roots of the secular equation are the eigenenergies of the complete system. Evaluating the time evolution with Eq. (2.2), we see that the density is not conserved within the subspace spanned by H^0, but fluctuates quasiperiodically in time with the Poincaré cycle.[11] In the second case the self-energy can be evaluated[12] in a golden-rule approximation and it becomes a complex function of the energy, indicating that some density is irreversibly lost from the subspace spanned by H^0. However, the generation of an effective Hamiltonian becomes more convoluted for elaborated boundary conditions, particularly in cases where particles are being injected in the system, or when they lose their phase coherence as in inelastic processes. To the first situation corresponds the exchange of particles with some external reservoir identified by a chemical potential μ^{ext}. An example of the latter is the interaction with a phonon bath characterized by a Hamiltonian H_{ph} and a thermal energy k_BT. These are particularly complex when the system is far from equilibrium. Therefore we prefer to employ a Green's-function technique developed by Kadanoff and Baym and independently by Keldysh.[7] This is nothing else but the formulation of the Schrödinger equation in a quantum field formalism. This has the advantage that the boundary conditions can be introduced through the appropriate selection of the fields producing the self-energies and that the exclusion principle is already included in the formalism. Besides, another advantage is that it can deal with situations far from equilibrium. The fundamental objects of the theory are the electron and phonon field operators $\psi(X)$ and $\phi(X)$ in the Heisenberg representation, acting on their respective noninteracting ground states, $|\Psi_0\rangle$ and $|\Phi_0\rangle$, held in equilibrium at some very early time t_0.

B. The Keldysh formalism

The formalism[13,14] deals with the electron and hole distribution functions:

$$G^<(X_2,X_1) = \frac{i}{\hbar}\langle \Psi_0 | \psi^\dagger(X_1)\psi(X_2) | \Psi_0 \rangle \tag{2.3a}$$

and

$$G^>(X_2,X_1) = -\frac{i}{\hbar}\langle \Psi_0 | \psi(X_2)\psi^\dagger(X_1) | \Psi_0 \rangle \ . \tag{2.3b}$$

The phonons (bosons) are described by the distributions

$$D^<(X_2,X_1) = -\frac{i}{\hbar}\langle \Phi_0 | \phi(X_1)\phi(X_2) | \Phi_0 \rangle \tag{2.4a}$$

and

$$D^>(X_2,X_1) = -\frac{i}{\hbar}\langle \Phi_0 | \phi(X_2)\phi(X_1) | \Phi_0 \rangle \ . \tag{2.4b}$$

The usual retarded and advanced Green's functions as well as an additional Keldysh's function, are defined in terms of these distributions,

$$G^R(X_2,X_1) = \Theta(t_2-t_1)[G^>(X_2,X_1) - G^<(X_2,X_1)] \ , \tag{2.5a}$$

$$G^A(X_2,X_1) = \Theta(t_1-t_2)[G^>(X_2,X_1) - G^<(X_2,X_1)] \ , \tag{2.5b}$$

$$G^K(X_2,X_1) = G^>(X_2,X_1) + G^<(X_2,X_1) \ ; \tag{2.5c}$$

and

$$D^R(X_2,X_1) = \Theta(t_2-t_1)[D^>(X_2,X_1) - D^<(X_2,X_1)] \ , \tag{2.6a}$$

$$D^A(X_2,X_1) = \Theta(t_1-t_2)[D^>(X_2,X_1) - D^<(X_2,X_1)] \ , \tag{2.6b}$$

$$D^K(X_2,X_1) = D^>(X_2,X_1) + D^<(X_2,X_1) \ . \tag{2.6c}$$

These functions are arranged in a 2×2 matrix form:

$$\hat{G} = \begin{bmatrix} G^R & G^K \\ 0 & G^A \end{bmatrix} , \tag{2.7}$$

and

$$\hat{D} = \begin{bmatrix} D^R & D^K \\ 0 & D^A \end{bmatrix} . \tag{2.8}$$

Their equation of motion is given by the Dyson equation in the Keldysh space which is obtained, just as in the equilibrium theory, by considering the time evolution of the field operators. In the case of the electronic degrees of freedom it appears as

$$[G^0(X_2)]^{-1}\hat{G}(X_2,X_1)-\int dX_j\hat{\Sigma}(X_2,X_j)\hat{G}(X_j,X_1)=\delta(X_2-X_1)\hat{I}\ , \qquad (2.9)$$

which has been written in a form which makes explicit that it is a Schrödinger equation of the form (2.1) with H^0 replaced by an effective Hamiltonian (2.2). $\hat{I}$ is the identity matrix. The electronic self-energy operator $\hat{\Sigma}$ contains the interactions left out in H^0, and has the same matrix structure as given by Eq. (2.7). We will see that by tracing over the undesired Hilbert subspaces, we can obtain a $\hat{\Sigma}$ that represents a nonlocal effective potential as in Eq. (2.2). In particular, we will be interested in obtaining a self-energy of the form $\hat{\Sigma}={}^{\text{esc}}\hat{\Sigma}+{}^{\phi}\hat{\Sigma}$, adding the independent effects of the escape from the sample through the leads and the electron-phonon interactions.

While most of the approaches to transport deal with the differential equation (2.9) and transform it in a quantum Boltzmann equation, we attack the problem in a different way. We use the formal solution of Eq. (2.9), which can be written for each component of $\hat{G}$. The retarded Green's function is

$$G^R(X_2,X_1)=G^{0R}(X_2,X_1)+\int dX_j\int dX_k G^{0R}(X_2,X_j)\times\Sigma^R(X_j,X_k)G^R(X_k,X_1)\ , \qquad (2.10)$$

which is the integral form of the Dyson equation for the retarded Green's function. Its solution in the steady state does not offer much difficulty. The advanced Green's function satisfies an equivalent equation, while the Keldysh function results:[14]

$$G^K(X_2,X_1)=\int dX_j\int dX_k G^R(X_2,X_j)\times\Sigma^K(X_j,X_k)G^A(X_k,X_1)\ , \qquad (2.11)$$

also valid exchanging G^K by $G^<$ ($G^>$) and Σ^K by $\Sigma^<$ ($\Sigma^>$). In the above expression we have dropped a boundary term:

$$\int d\mathbf{r}_j\int d\mathbf{r}_k G^R(X_2,\mathbf{r}_j,t_0)G^K(\mathbf{r}_j,t_0,\mathbf{r}_k,t_0)\times G^R(\mathbf{r}_k,t_0,X_1)\ , \qquad (2.12)$$

which is negligible due to the damping in G^R and G^A originated by the inelastic processes inside the sample and the escape through the leads.

An equation similar to (2.9) holds for $\hat{D}$ in terms of a phonon self-energy $\hat{\Pi}$. In a general case $\hat{\Sigma}$ is a functional of $\hat{G}$ and $\hat{D}$ and this gives a nonlinear set of equations. Our purpose will be to reduce them to a system of equations which can be solved without much difficulty.

C. Time evolution

The solution of Eq. (2.9) contains all the information we need about the system. However, we want to express it in a more transparent form. Even when it is usual to keep $\hat{D}$ with its equilibrium value, we are still left with a nonlinear set of equations for $\hat{\Sigma}$ and $\hat{G}$. It is in this point where a deep physical insight of the problem must be used. The physics contained in the equations is more clearly expressed in the Wigner coordinates:

$$\begin{aligned} t&=\tfrac{1}{2}[t_2+t_1]\ ,\\ \mathbf{r}&=\tfrac{1}{2}[\mathbf{r}_2+\mathbf{r}_1]\ ,\\ \delta t&=t_2-t_1\ ,\\ \delta\mathbf{r}&=\mathbf{r}_2-\mathbf{r}_1\ . \end{aligned} \qquad (2.13)$$

The first two variables correspond to the macroscopic time and position, and therefore are conjugated to the external frequency ω and wave vector $\mathbf{q}$, respectively. The last two variables are uncertainties, and therefore are conjugated to the canonical energy ε and canonical momentum $\mathbf{p}$. For example, we will use

$$\hat{G}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)=\int\hat{G}\left[\mathbf{r}_2,t+\frac{\delta t}{2},\mathbf{r}_1,t-\frac{\delta t}{2}\right]\times\exp(i\varepsilon\delta t/\hbar)d\delta t\ . \qquad (2.14)$$

Let us use these variables in the simplification of the kinetic equation, by writing G^R, Σ^K, and G^A in terms of the energy variables:

$$\begin{aligned} \varepsilon_R/\hbar&\rightarrow t_2-t_j=(t+\delta t/2)-(t_i+\delta t_i/2)\ ,\\ \varepsilon_i/\hbar&\rightarrow t_j-t_k=\delta t_i\ ,\\ \varepsilon_A/\hbar&\rightarrow t_k-t_1=(t_i-\tfrac{1}{2}\delta t_i)-(t-\tfrac{1}{2}\delta t)\ . \end{aligned} \qquad (2.15)$$

The resulting equation is more clear if written in terms of the variables:

$$\begin{aligned} \vartheta&=\tfrac{1}{4}(\delta t+\delta t_i)\ ,\\ \varepsilon&=\tfrac{1}{2}(\varepsilon_R+\varepsilon_A)\ ,\\ \omega&=\frac{1}{\hbar}(\varepsilon_R-\varepsilon_A)\ . \end{aligned} \qquad (2.16)$$

Dropping the spatial variables for a while, we write (2.11) in the form

$$\begin{aligned} G^K(t+\tfrac{1}{2}\delta t,t-\tfrac{1}{2}\delta t)&=\int G^K(\varepsilon,t)\exp\left[-i\frac{\varepsilon\delta t}{\hbar}\right]\frac{d\varepsilon}{2\pi\hbar}\\ &=\int\int\int\int\int G^R(\varepsilon+\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i)+\vartheta)\Sigma^K(\varepsilon_i,t_i)\\ &\quad\times G^A(\varepsilon-\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i)-\vartheta)\left[\exp\left[-i\frac{(\varepsilon-\varepsilon_i)\delta t_i}{\hbar}\right]d\delta t_i\frac{d\varepsilon_i}{2\pi\hbar}\right]\\ &\quad\times\exp[-i\omega(t-t_i)]\frac{d\omega}{2\pi}dt_i\exp\left[-i\frac{\varepsilon\delta t}{\hbar}\right]\frac{d\varepsilon}{2\pi\hbar}\ . \end{aligned} \qquad (2.17)$$

This equation is more convenient than (2.11) because it is expressed in terms of macroscopic times and energies. No approximation has been done so far. We first notice that macroscopic transport occurs on a scale of time much longer than that given by the fast variables such as the absolute time uncertainty ϑ. This allows us to neglect the dependence of the retarded and advanced Green's functions on ϑ which appears shifting the macroscopic time $\frac{1}{2}(t+t_i)$. We will name this the *adiabatic spectrum approximation*, which implies that the probability of propagation between times t_i and t is evaluated using the dynamics of the spectrum at the intermediate time $\frac{1}{2}(t+t_i)$. In fact, we can expand the product $G^R G^A$ around $\vartheta=0$, and get the series

$$G^R G^A \left[1 + \left[G^R \frac{\partial}{\partial t}(1/G^R) - G^A \frac{\partial}{\partial t}(1/G^A) \right] \vartheta + \cdots \right] .$$

This approximation is good provided that we can drop the linear term as compared to 1 *or* if the product $G^R G^A$ is itself small. In words, it requires that, for the relevant transitions, the instantaneous spectrum of the system does not change much within the propagation time of those transitions. This should be checked using the self-consistent solutions of each particular problem. As an example we consider here the case of a classical potential dependent of time $U\cos(\omega t)$. This appears as an energy shift $\Delta(t)=U\cos(\omega t)$ in the energy scale of the retarded and advanced Green's functions and hence

$$\frac{\partial}{\partial t} \to -\left[\frac{\partial U}{\partial t} \right] \frac{\partial}{\partial \varepsilon} .$$

It will become clear after the discussion of Sec. IV that the term dropped is $\tilde{\tau}_q(\partial\Delta/\partial t)\vartheta/\hbar$, where $\tilde{\tau}_q$ is the minimum between the quantum propagation time (τ_q) and the dephasing time (τ_ϕ), the derivative represents the variation of the energy levels as a function of the absolute time (in the case of an oscillatory classical potential it would be $U\omega$), and an extreme upper bound for ϑ could be τ_ϕ. Therefore the approximation requires that $\tilde{\tau}_q U \omega \tau_\phi/\hbar \ll 1$, which can be achieved either if the potential is weak, or if the frequency is low or if the relaxation is fast. Besides although the propagation time might increase with some power of the distance, the overall factor $G^R G^A$ will decrease exponentially and therefore contributions with large $\tilde{\tau}_q$ are irrelevant to transport.

Therefore we are left with an integral on δt_i which provides a function $\delta(\varepsilon-\varepsilon_i)$. Because of this energy conservation the integral on ε_i is trivial. Writing again the space variables, we obtain

$$G^K(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t) = \int\int d\mathbf{r}_j d\mathbf{r}_k \int\int \frac{d\omega}{2\pi} \exp[-i\omega(t-t_i)] G^R(\mathbf{r}_2,\mathbf{r}_j,\varepsilon+\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i)) \times \Sigma^K(\mathbf{r}_j,\mathbf{r}_k,\varepsilon,t_i) G^A(\mathbf{r}_k,\mathbf{r}_1,\varepsilon-\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i)) dt_i , \tag{2.18}$$

also valid exchanging G^K by $G^<$ ($G^>$) and Σ^K by $\Sigma^<$ ($\Sigma^>$). We are not aware of any previous report of this expression. In order to proceed with the solution of Eq. (2.18), a self-consistent solution of Eq. (2.10) must be found.

When one wants to study the *linear response* to a perturbation in the density, as occurs in the semiclassical Boltzmann equation, it is not necessary to correct the transition probabilities. This correction would give a higher-order effect. For a discussion of this regime in the Keldysh formalism see Refs. 4(c) and 5(a). The role of transition probabilities is played by the product of retarded and advanced Green's functions, together with the density of states and the interaction rates. Thus, we can drop their dependence on the fluctuations in the occupation which in turn depends on time. We will call this the *steady-spectrum* approximation and it results as a natural consequence of the linear-response regime. Out of this regime, we can still use this approximation provided that

$$\left[G^R \frac{\partial}{\partial t}(1/G^R) + G^A \frac{\partial}{\partial t}(1/G^A) \right] \tau_\phi$$

is a small parameter. This is evaluated similarly to what we did above. Obviously, this is small when the Green's functions have a weak dependence on the absolute time or when the dephasing time is very short. In this work, whenever the linear-response regime is invoked the transition probabilities will be evaluated in the steady-spectrum approximation. This is the regime that leads to a transport equation of the form of Eq. (1.1).

Notice that if the self-energy depends on the absolute time t_i, the integral over ω must be performed first, and we will see that this provides a retarded dependence on $t-t_i$. However, in the *steady-state* $\Sigma^K(\varepsilon)$ is constant in time. The Green's functions are also time independent and we can integrate t_i first, obtaining a $\delta(\omega)$ function which leads to the kinetic equation for the steady state:

$$G^K(\mathbf{r}_2,\mathbf{r}_1,\varepsilon) = \int\int d\mathbf{r}_j d\mathbf{r}_k G^R(\mathbf{r}_2,\mathbf{r}_j,\varepsilon) \times G^A(\mathbf{r}_k,\mathbf{r}_1,\varepsilon) \Sigma^K(\mathbf{r}_j,\mathbf{r}_k,\varepsilon) ,$$

in which all the functions are evaluated at the same energy.

D. Density of states and occupation

Before we proceed let us recall some properties of the Green's functions which are well represented in the Wigner coordinates. We assume that the phonon bath is held in equilibrium and hence their Green's functions do not depend on the absolute time. Therefore the electron and phonon spectral weight functions are written as

$$A(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)=i[G^R(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)-G^A(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)]$$
$$=i[G^>(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)-G^<(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)]\ , \tag{2.19a}$$

$$B(\mathbf{r}_2,\mathbf{r}_1,|\varepsilon|)=i[D^R(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)-D^A(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)]\mathrm{sgn}(\varepsilon)$$
$$=i[D^>(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)-D^<(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)]\mathrm{sgn}(\varepsilon) \tag{2.19b}$$

from which the electronic and phonon local densities of states are obtained as

$$N_0(\mathbf{r},\varepsilon,t)=\frac{1}{2\pi}A(\mathbf{r},\mathbf{r},\varepsilon,t) \tag{2.20a}$$

and

$$J_0(\mathbf{r},\varepsilon)=\frac{1}{2\pi}B(\mathbf{r},\mathbf{r},\varepsilon)\ . \tag{2.20b}$$

In a similar way, from the imaginary part of the electron self-energies, a rate for the interaction can be defined:

$$2\Gamma(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)=-2\,\mathrm{Im}\Sigma^R(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)$$
$$=i[\Sigma^>(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)-\Sigma^<(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)]\ . \tag{2.21}$$

The advantage of this rate, as well as of the density of states defined by (2.19a) and (2.20a) is that in many cases they are weakly dependent on the variation of the occupation with time. A relation between them can be obtained using Eq. (2.11) or (2.18) to evaluate $[G^<-G^>]$:

$$N_0(\mathbf{r},\varepsilon,t)=\frac{1}{2\pi}\int\int d\mathbf{r}_j d\mathbf{r}_k\int\int\frac{d\omega}{2\pi}\exp[-i\omega(t-t_i)]G^R(\mathbf{r}_2,\mathbf{r}_j,\varepsilon+\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i))$$
$$\times 2\Gamma(\mathbf{r}_j,\mathbf{r}_k,t_i,\varepsilon)G^A(\mathbf{r}_k,\mathbf{r}_1,\varepsilon-\tfrac{1}{2}\hbar\omega,\tfrac{1}{2}(t+t_i))|_{\mathbf{r}_2=\mathbf{r}_1=\mathbf{r}}dt_i\ . \tag{2.22}$$

The use of a consistent approximation as (2.22) and (2.18) is essential to obtain density conservation. These equations will be simplified even more in the following sections where, besides the steady-spectrum approximation, we will use self-energies which are diagonal in the real space.

While the retarded (and advanced) Green's functions contain information about the nature of the states (spectral densities and transition probabilities), the Keldysh function contains information on the occupations. This is expressed by

$$G^K(\mathbf{r},\mathbf{r},\varepsilon,t)=-i2\pi N_0(\mathbf{r},\varepsilon,t)[1-2f] \tag{2.23}$$

and

$$D^K(\mathbf{r},\mathbf{r},\varepsilon)=-i2\pi J_0(\mathbf{r},\varepsilon)[1+2n]\ , \tag{2.24}$$

where as the system approaches equilibrium

$$f(\mathbf{r},\varepsilon,t)\rightarrow 1/\{\exp[(\varepsilon-\mu^0)/k_BT]+1\} \tag{2.25}$$

and

$$n\rightarrow 1/[\exp(\varepsilon/k_BT)-1]\ , \tag{2.26}$$

become the Fermi-Dirac and the Bose-Einstein distribution functions, respectively. In a general nonequilibrium situation the full dependence of the Keldysh function on the variables $(\mathbf{r},\mathbf{p},\varepsilon,t)$ or $(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)$ should be determined from the equations of motion. However, this complicated problem will be simplified using a particular form of the self-energy (which allows the integration on the momentum coordinate) and a linear-response approximation for a degenerate Fermi gas (which allows the integration on the energy variable). Our main interest will be the description of an electron density at a localized position and defined time. Within the linear response, we first evaluate

$$\delta G^K(\mathbf{r},\mathbf{r},t,\varepsilon)=G^K(\mathbf{r},\mathbf{r},\varepsilon,t)-G^{0K}(\mathbf{r},\mathbf{r},\varepsilon,t)\ ,$$

taking the difference between Eq. (2.11) and the corresponding equation describing the equilibrium. Then we proceed to integrate it over energy. Since only low-energy excitations are allowed, the density fluctuations occur around the Fermi surface. In this case the Green's functions can be approximated by their value at the Fermi surface. Hence the integral over energy only involves the distribution function. Even when the nonequilibrium distribution function differs from a Fermi-Dirac distribution, it may be characterized by a chemical potential $\mu(\mathrm{r,t})=\mu^0+\delta\mu(\mathrm{r,t})$ which serves as a measure of the local density at a given time. Therefore we obtain

$$\frac{1}{i4\pi}\int d\varepsilon\,\delta G^K(\mathbf{r},\mathbf{r},\varepsilon,t)=\delta\rho(\mathbf{r},t)\approx N_0(\mathbf{r},\varepsilon_F)\delta\mu(\mathbf{r},t)\ . \tag{2.27}$$

Here we dropped the dependence of the density of states on t because it gives a higher order on δt not necessary for the linear response. Our goal will be to obtain an equation describing $\delta\rho(\mathbf{r},t)$, and therefore avoid dealing with the nonequilibrium distribution function f. Notice that being a displacement from the equilibrium state, $\delta\rho$ can take both positive and negative values.

III. THE SELF-ENERGIES AS BOUNDARY CONDITIONS

A. The escape to the leads

In this subsection we will seek an effective operator acting in the subspace spanned by the isolated sample eigenfunctions which nevertheless is able to represent the escape of particles to the leads. For simplicity let us consider a discrete basis for the space coordinate (tight-binding model). The connection to a lead S is represented by a single hopping element. The noninteracting Hamiltonian is the direct sum of two terms, one describing electrons in the points $\mathbf{r}_i$ inside the sample and the other describing electrons in the points $\mathbf{r}_{i'}$ on the lead. Primed indices will be used to identify points in the leads. The interaction is turned on at a very early time $t_0 \ll 0$ and can be represented by

$$H_{\text{esc}} = V_{S',S}\psi^{\dagger}(\mathbf{r}_{S'},t)\psi(\mathbf{r}_S,t) + \text{c.c.} \tag{3.1}$$

Here ψ is the destruction operator at site $\mathbf{r}_S$ in the sample. Similarly, $\mathbf{r}_{S'}$ is the site in the lead. The interaction lead sample will be given by the retarded and advanced self-energy components:

$$\begin{aligned} {}^{\text{hop}}\Sigma^{R}(\mathbf{r}_j,\mathbf{r}_k,t_j,t_k) &= {}^{\text{hop}}\Sigma^{A}(\mathbf{r}_j,\mathbf{r}_k,t_j,t_k) \\ &= V_{S,S'}\delta(\mathbf{r}_j-\mathbf{r}_S)\delta(\mathbf{r}_{S'}-\mathbf{r}_k) \\ &\quad \times\delta(t_j-t_k)\Theta(\tfrac{1}{2}(t_j+t_k)-t_0) , \end{aligned} \tag{3.2}$$

while the Keldysh part of the self-energy is

$${}^{\text{hop}}\Sigma^{k} \equiv 0 , \tag{3.3}$$

representing that no particle is lost or gained by cause of the interaction. In what follows we will forget the time variables and we will use a subindex representing the spatial variables. In absence of interaction with the sample, the lead is represented by the function in the Keldysh space $\hat{G}^{0}_{S',S'}$. Iterating once with Eq. (2.9), using ${}^{\text{hop}}\Sigma$ as an interaction, and selecting coordinates inside the sample in Eq. (2.9), the Keldysh function becomes

$$\begin{aligned} G^{K}_{2,1} = {}& G^{0K}_{2,1} + G^{0K}_{2,S}[{}^{\text{hop}}\Sigma^{A}_{S,S'}G^{0A}_{S',S'}\,{}^{\text{hop}}\Sigma^{A}_{S',S}]G^{A}_{S,1} + G^{0R}_{2,S}[{}^{\text{hop}}\Sigma^{K}_{S,S'}G^{0A}_{S',S'}\,{}^{\text{hop}}\Sigma^{A}_{S',S}]G^{A}_{S,1} \\ & + G^{0R}_{2,S}[{}^{\text{hop}}\Sigma^{R}_{S,S'}G^{0K}_{S',S'}\,{}^{\text{hop}}\Sigma^{A}_{S',S}]G^{A}_{S,1} + G^{0R}_{2,S}[{}^{\text{hop}}\Sigma^{R}_{S,S'}G^{0R}_{S',S'}\,{}^{\text{hop}}\Sigma^{K}_{S',S}]G^{A}_{S,1} + G^{0R}_{2,S}[{}^{\text{hop}}\Sigma^{R}_{S,S'}G^{0R}_{S',S'}\,{}^{\text{hop}}\Sigma^{R}_{S',S}]G^{K}_{S,1} . \end{aligned} \tag{3.4}$$

The second and fourth terms in square brackets are zero. Since the terms in square brackets have external indices denoting points on the sample, the first, third, and fifth brackets may be identified as the only nonzero elements of a new self-energy:

$${}^{S}\Sigma^{R}_{S,S} = V_{S,S'}G^{0R}_{S',S'}V_{S',S} , \tag{3.5a}$$

$${}^{S}\Sigma^{K}_{S,S} = V_{S,S'}G^{0K}_{S',S'}V_{S',S} , \tag{3.5b}$$

and

$${}^{S}\Sigma^{A}_{S,S} = V_{S,S'}G^{0A}_{S',S'}V_{S',S} , \tag{3.5c}$$

respectively. These account for the correction due to the escape toward the lead S which must occur through the site $\mathbf{r}_S$. The difference with the original self-energy which accounts for the hopping between the sample and the lead, is that the one just defined operates only on the sample subspace. All the degrees of freedom in the lead are traced out in the evaluation of the $G_{S',S'}$. Therefore, Eqs. (3.5) represent the process of decimation[11] of the lead. Besides, in the above expression there are two integrals over internal time variables. Since ${}^{\text{hop}}\Sigma(t_j,t_k)$ is a δ function in the time difference, both integrals are trivial. Consequently, the dependence of ${}^{\text{hop}}\Sigma$ on the time variables is just that of the function $G^{0}(t_j,t_k)$. Substituting in (2.25), one obtains

$${}^{S}\Gamma(\mathbf{r}_j,\mathbf{r}_k,\varepsilon,t) = \frac{\hbar}{2\tau_S}\delta(\mathbf{r}_j-\mathbf{r}_S)\delta(\mathbf{r}_S-\mathbf{r}_k)\Theta(t-t_0) \tag{3.6a}$$

and

$$\begin{aligned} {}^{S}\Sigma^{K}(\mathbf{r}_j,\mathbf{r}_k,\varepsilon,t) = {}& -i\frac{\hbar}{\tau_S}[1-2f(\mathbf{r}_{S'},\varepsilon,t)]\delta(\mathbf{r}_j-\mathbf{r}_S) \\ & \times\delta(\mathbf{r}_S-\mathbf{r}_k)\Theta(t-t_0) , \end{aligned} \tag{3.6b}$$

both with

$$\frac{1}{\tau_S} = \frac{2\pi}{\hbar}|V_{S,S'}|^2 N_0(\mathbf{r}_{S'},\varepsilon) . \tag{3.7}$$

An important observation is that the occupation function that enters in this Keldysh self-energy is the occupation in the lead, which does not need to be a Fermi-Dirac distribution. We also notice that the results of this section did not require any particular model for the electrons in the sample or the lead. The only simplifying consideration was the use of a discrete basis for the spatial variable. Besides, from Eq. (3.6) we see that *if* the steady-spectrum approximation is valid for electrons in the leads (we will assume that this is the case), this approximation is automatically valid in the description of the lead-sample interaction. A further simplification arises when one considers the linear-response regime. According to Eq. (2.27), one is interested in the integral over energy of the variation of Σ^{K} compared with its equilibrium value. We can call $\delta\mu_S(\mathbf{r}_S,t) = \delta\mu_S(t)$ and this gives

$$\int d\varepsilon\, \delta^{S}\Sigma^{K} = i\frac{\hbar}{\tau_S}2\delta\mu_S(\mathbf{r}_S,t) . \tag{3.8}$$

From (3.5a) we see that the validity of the steady-spectrum approximation to describe the sample will depend on its validity for the description of the lead. Finally, it is obvious that the presence of many leads or different propagating channels within a lead will simply add a summation index n taking the values $\{S,L,R,\ldots\}$, in self-energies of the form given above, that is,

$${}^{\text{esc}}\Sigma = \sum_{n} {}^{n}\Sigma . \tag{3.9}$$

Note that according to Eqs. (3.5) and (3.6) these self-energies may contribute in different regions of the real space.

B. The electron-phonon interaction

In this section we follow the results introduced by Caroli *et al.*[15] and we will transform them to our notation using approximations that reduce them to the simple self-energy forms used in Refs. 3, 4, and 6. The electron-phonon interaction can be described by the Hamiltonian

$$H_{e\text{-ph}}=g\int d\mathbf{r}\,\psi^{\dagger}(X)\psi(X)\phi(X)\ . \tag{3.10}$$

The electron-phonon contribution to the self-energy, in the Migdal approximation,[16] is given by

$$\begin{aligned}{}^{\phi}\Sigma^{<(>)}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)=g^2\int d\varepsilon_i D^{<(>)}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon_i,t)\\ \times G^{<(>)}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon-\varepsilon_i,t)\ .\end{aligned} \tag{3.11}$$

From these expressions we evaluate the Keldysh function and the corresponding energy broadening according to

$$\begin{aligned}{}^{\phi}\Sigma^{K}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)&=[{}^{\phi}\Sigma^{>}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)+{}^{\phi}\Sigma^{<}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)]\ ,\\ 2\,{}^{\phi}\Gamma(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)&=-2\,\mathrm{Im}{}^{\phi}\Sigma^{R}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)\\ &=i[{}^{\phi}\Sigma^{>}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)-{}^{\phi}\Sigma^{<}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)]\ .\end{aligned} \tag{3.12}$$

In order to get expressions that can be handled analytically we will need to perform some approximations in Eq. (3.11). A nice simplifying assumption introduced by Caroli *et al.*[15] is the local phonon model, which consists in approximating the phonon spectral weight by

$$B(\mathbf{r}_2,\mathbf{r}_1,\varepsilon)=2\pi J_0(\mathbf{r}_2,\varepsilon)\delta(\mathbf{r}_2-\mathbf{r}_1)\ . \tag{3.13}$$

This is justified[15] by the slowness of a phonon excitation as compared with the electron Fermi velocity. As a further simplification, in the evaluation[16] of Eq. (3.11) we take $n(\varepsilon)+1\approx n(\varepsilon)$. This is equivalent to assuming that the temperature is high enough for the phonon absorption and emission to be considered similar. In that case we can write

$$\begin{aligned}2\,{}^{\phi}\Gamma(\mathbf{r},\varepsilon)&\equiv\hbar/\tau_{\phi}\\ &=g^2\int J_0(\mathbf{r},|\varepsilon_i|)n(|\varepsilon_i|)\\ &\quad\times\tfrac{1}{2}[N_0(\mathbf{r},\varepsilon+\varepsilon_i)+N_0(\mathbf{r},\varepsilon-\varepsilon_i)]d\varepsilon_i\ .\end{aligned} \tag{3.14}$$

In this approximation the mean-life results independent of the electron occupation. This leads to the cancellation, in the kinetic equation, of the terms quadratic in the electron occupation. This, in turn, leads to a time-independent equation for the retarded Green's function consistent with the steady-spectrum approximation. Since the thermalization on the leads can be described by (3.10) this is consistent with the approximation adopted to get Eqs. (2.18) and (3.8). In order to decouple the equations for different energies, we can write

$$\begin{aligned}{}^{\phi}\Sigma^{K}(\mathbf{r}_j,\mathbf{r}_k,\varepsilon,t)=-\,i2\,{}^{\phi}\Gamma(\mathbf{r}_i,\varepsilon)[1-2f(\varepsilon,\mathbf{r}_i,t)]\\ \times\delta(\mathbf{r}_j-\mathbf{r}_i)\delta(\mathbf{r}_i-\mathbf{r}_k)\ ,\end{aligned} \tag{3.15}$$

This expresses that the scattered electrons are reinjected with the same energy. By doing this, we renounce the possibility of describing the energy dissipation. Instead, we get a much simpler equation in which the densities of electrons are balanced for each energy independently. Therefore the structure of the self-energy due to the electron-phonon interaction looks similar to that due to the leads. However, even when we will employ the usual assumption that the phonon bath is kept in thermal equilibrium, the electron distribution function should be evaluated self-consistently with the kinetic equation because it contains the nonequilibrium occupations within the sample. This is a substantial difference with the self-energy produced by a lead acting as a voltage source.

In the same spirit as Eq. (2.27), we can define the variation of the self-energy with respect to equilibrium, and evaluate its integral over energies in a linear-response approximation,

$$\int d\varepsilon\,\delta{}^{\phi}\Sigma^{K}(\mathbf{r}_i,\mathbf{r}_i,\varepsilon,t)=i\frac{\hbar}{\tau_{\phi}}2\delta\mu(\mathbf{r}_i,t)\ , \tag{3.16}$$

which here implies replacing the energy-dependent interaction rate by its value at the Fermi energy.

IV. THE KINETIC EQUATION

Until now we have developed the basic formalism. Let us apply it to the solution of the time-dependent transport, restricting ourselves to the cases in which the spectra are time independent (steady-spectrum approximation). We are interested in the evaluation of the occupation in a given point of the space $\mathbf{r}=[\mathbf{r}_2+\mathbf{r}_1]/2$ integrated over the momentum coordinate $\mathbf{p}$. Besides, in our model we have adopted a form for the self-energies which is a superposition of δ functions in the space. In this case the meaning of Eq. (2.18) will become more transparent if we write it as

$$G^{K}(\mathbf{r}_2,\mathbf{r}_1,\varepsilon,t)|_{\mathbf{r}_2=\mathbf{r}_1=\mathbf{r}}=\int dt_i\int d\mathbf{r}_i\frac{2\pi}{\hbar}P_{\varepsilon}(\mathbf{r},\mathbf{r}_i,t-t_i)N_0(\mathbf{r}_i,\varepsilon)\Sigma^{K}(\mathbf{r}_i,\mathbf{r}_i,\varepsilon,t_i)\ , \tag{4.1}$$

where we have defined

$$P_\varepsilon(\mathbf{r},\mathbf{r}_i,t-t_i)=\int\frac{d\omega}{2\pi}\exp[-i\omega(t-t_i)]P_\varepsilon(\mathbf{r},\mathbf{r}_i,\omega) \quad (4.2)$$

and

$$P_\varepsilon(\mathbf{r},\mathbf{r}_i,\omega)=\frac{\hbar}{2\pi}G^R(\mathbf{r}_2,\mathbf{r}_i,\varepsilon+\hbar\omega/2) \times G^A(\mathbf{r}_i,\mathbf{r}_1,\varepsilon-\hbar\omega/2)\frac{1}{N_0(\mathbf{r}_i,\varepsilon)}\Bigg|_{\mathbf{r}_2=\mathbf{r}_1=\mathbf{r}} . \quad (4.3)$$

Notice that from Eq. (4.3) we immediately verify that (a) $P(\mathbf{r},\mathbf{r}_i,\omega)$ is analytic in the upper complex ω plane, (b) its real part is even and its imaginary part is odd with respect to real ω, and (c) $P(\omega)\rightarrow 0$ uniformly as $|\omega|\rightarrow\infty$. Therefore P is a response function which should have a simple meaning in its hydrodynamic limit. These considerations suggest that for low frequencies we can perform an expansion of the form

$$P_\varepsilon(\mathbf{r},\mathbf{r}_i,\omega)\approx P_\varepsilon(\mathbf{r},\mathbf{r}_i,\omega)|_{\omega=0}\frac{1}{1-i\omega\tilde{\tau}_q} , \quad (4.4)$$

where

$$\tilde{\tau}_q=i\frac{\hbar}{2}\left\{G^R(\mathbf{r},\mathbf{r}_i,\varepsilon)\frac{\partial}{\partial\varepsilon}[1/G^R(\mathbf{r},\mathbf{r}_i,\varepsilon)] -G^A(\mathbf{r}_i,\mathbf{r},\varepsilon)\frac{\partial}{\partial\varepsilon}[1/G^A(\mathbf{r}_i,\mathbf{r},\varepsilon)]\right\} . \quad (4.5)$$

This is still too formal. In order to understand more deeply the meaning of P, let us consider a few limiting cases for which we know explicitly the behavior of the Green's functions. Notice that Eqs. (2.3)–(2.5) require the exact Green's functions of the many-body system renormalized by the inelastic processes. To get a simpler interpretation we consider the independent-particle Green's function and neglect the dephasing interactions. The latter can be included afterwards anyway.

In the case of *ballistic propagation* in a crystalline system the Green's function has the form[17]

$$G^{0R}(\mathbf{r},\mathbf{r}_i,\varepsilon)\propto\exp[ip_\varepsilon|\mathbf{r}-\mathbf{r}_i|/\hbar] . \quad (4.6)$$

Remembering that $v_\varepsilon=\partial E/\partial p_\varepsilon$, we can obtain an expression of the form of (4.4), being $\tau_q=|\mathbf{r}-\mathbf{r}_i|/v_\varepsilon$ the time of flight from the initial site to the final site of a wave packet with the Fermi energy.

The case of *resonant tunneling* is also an important one and will be analyzed more carefully in a later section. For now it is enough to notice that in this case the Green's function is dominated by a single eigenenergy[18] E_O and has the form

$$G^{0R}(\mathbf{r},\mathbf{r}_i,\varepsilon)\propto\frac{1}{\varepsilon-E_O-\Delta+i\Gamma} , \quad (4.7)$$

where Δ and Γ depend on ε, but at $\varepsilon\approx E_O-\Delta(\varepsilon)$ they can be taken as constant in a first approximation. Again, we obtain an expression of the form of (4.4), now with $\tau_q=\hbar/\Gamma$. That is, the resonance width determines the transit time through the resonance region.

Finally, we can consider a *diffusive* case. In this case, the electron collides elastically with impurities within a characteristic time τ_{el}. It might seem more difficult than the previous cases because we do not have an explicit expression for the Green's functions. However, we can evaluate P^o averaged over configurations of impurities in a ladder approximation. In fact, we know[19,6] that

$$P^o_\varepsilon(\mathbf{r},\mathbf{r}_i,t-t_i)=\int\int\int\frac{\hbar}{2\pi}\left\langle G^{0R}\left[\mathbf{p}+\frac{\hbar\mathbf{q}}{2},\varepsilon+\frac{\hbar\omega}{2}\right]G^{0A}\left[\mathbf{p}-\frac{\hbar\mathbf{q}}{2},\varepsilon-\frac{\hbar\omega}{2}\right]\right\rangle_{\mathrm{av}} \times\frac{1}{N_0(\varepsilon)}d\mathbf{p}\exp[-i\omega(t-t_i)]d\omega\exp[\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_i)]d\mathbf{q}$$

$$=\Theta(t-t_i)[4\pi D_\varepsilon(t-t_i)]^{d/2}\exp[-|\mathbf{r}-\mathbf{r}_i|^2/4D_\varepsilon(t-t_i)] , \quad (4.8)$$

where $D_\varepsilon=v_\varepsilon^2\tau_{\mathrm{el}}/d$. For a dimension $d\leq 2$, the integral in time diverges unless the exponential attenuation arising from the dephasing rate $1/\tau_\phi$ is taken into account explicitly, and the integral depends on τ_ϕ. However, for higher dimensions the time decay is fast enough and we an approximate the finite frequency result by the form of (4.4) with τ_{q} being replaced by $\tau_{\mathrm{q}}=|\mathbf{r}-\mathbf{r}_i|^2/(2D_\varepsilon)$, that is, the diffusion time.

Therefore, from the above examples we see that P^2 given by Eq. (4.9) is the density propagator in absence of dephasing processes. It gives the probability, that a particle placed in position $\mathbf{r}_i$ at time t_i, reach point $\mathbf{r}$ at time t,

$$P^o_\varepsilon(\mathbf{r},\mathbf{r}_i,t-t_i)\approx P^o_\varepsilon(\mathbf{r},\mathbf{r}_i)\Theta(t-t_i)\frac{1}{\tau_q} \times\exp[-(t-t_i)/\tau_q] . \quad (4.9)$$

The above approximation neglects the contribution of quantum beats. In the general case Eq. (4.2) can oscillate between positive and negative values, representing the energy-time uncertainty. The nice property of the low-frequency expansion is that it captures the essential features of the function (positive integral, characteristic decay) without introducing new parameters. This would not be the case in a calculation with actual wave packets.

Besides, the approximations (4.4) and (4.9), while simplifying the interpretation, are not a necessary assumption of our formalism.

All the above results are easily extended to include the presence of an homogeneous dephasing field. As seen in Sec. III B, the degradation of the coherent beam described by P^o appears automatically[6] in the Green's functions satisfying the Dyson equation (2.10). The imaginary part in the self-energies $E \rightarrow E - i\hbar/2\tau_\phi$ results in a change $\omega \rightarrow \omega + i/\tau_\phi$ in Eq. (4.5), that is, $P_\varepsilon(\omega) = P_\varepsilon^o(\omega + i/\tau_\phi)$. For very weak dephasing, the time-dependent probability is also obtained substituting τ_q by $\tilde{\tau}_q = \tau_q\tau_\phi/[\tau_q + \tau_\phi]$ in the coherent expression. Therefore, $P \approx (1 - \tau_q/\tau_\phi)P^o$ is the coherent part of a density propagator. P is reduced from P^o due to the leaks produced by the dephasing collisions along the pathways.

Now we are in a position to return and analyze the physics contained in Eq. (4.1) in the linear-response approximation. With this purpose we first evaluate $\delta G^K(\mathbf{r},\mathbf{r},t,\varepsilon)$ as defined in Eq. (2.27).

Let us now simplify Eq. (4.1) using a linear-response approximation which allows one to neglect the dependence of P_ε on energy and take it out of the integral. Using (2.27) and self-energies of the form (3.9) in the approximations (3.8) and (3.16), we obtain

$$\delta\rho(\mathbf{r},t) = \sum_\alpha \int\int d\mathbf{r}_i P_{\varepsilon_F}(\mathbf{r},\mathbf{r}_i,t-t_i)\frac{dt}{\tau_\alpha}\delta\rho_\alpha(\mathbf{r}_i,t_i) \; . \qquad (4.10)$$

The nature of this integral equation becomes more clear when the only process contributing to the self-energy is the electron-phonon interaction. Then, the only channels are those associated with the phonon field and $\delta\rho(\mathbf{r},t) = \delta\rho_\phi(\mathbf{r},t)$. Introducing an electron at point $\mathbf{r}_0$ at time t_0, the resulting variation in the density at a later time t will be

$$\begin{aligned}\tilde{P}_{\varepsilon_F}(\mathbf{r},t,\mathbf{r}_0,t_0) = {} & P_{\varepsilon_F}(\mathbf{r},\mathbf{r}_0,t-t_0) \\ & + \int\int d\mathbf{r}_i P_{\varepsilon_F}(\mathbf{r},\mathbf{r}_i,t-t_i)\frac{dt_i}{\tau_\phi} \\ & \times \tilde{P}_{\varepsilon_F}(\mathbf{r}_i,t_i,r_0,t_0) \; , \end{aligned} \qquad (4.11)$$

where now it is clear that with this special boundary condition $\delta\rho(\mathbf{r},t) = \tilde{P}_{\varepsilon_F}(\mathbf{r},t,\mathbf{r}_0,t_0)$ can be interpreted as a density propagator[20] in presence of dephasing interactions. This equation also makes explicit an important feature of our model for dephasing: a δ function in space coordinates relaxes both phase and momentum. That is, after the interaction there is no memory on what the momentum was. This fact is essential to simplify the original Eq. (2.18), because in the nonequilibrium situation the distribution function is momentum dependent, representing the finite currents present in the system. However, it is clear from Eq. (4.11) that the number of dephased electrons at any time t_i is proportional to the total variation on the local density $\delta\rho(\mathbf{r}_i,t_i)$ and to the probability dt_i/τ_ϕ that a decoherence process takes place in the time interval dt_i.

For computational purposes, it is more practical to write Eq. (4.1) in the form of a generalized Landauer-Büttiker equation. We can write this equation in terms of the transmittances used in Eq. (1.1), by using a Fisher-Lee formula:[21]

$$\begin{aligned} T_{\beta,\alpha}(\mathbf{r}_m,\mathbf{r}_i,\omega) = {} & \frac{2\pi}{\hbar}[2\,{}^\beta\Gamma(\mathbf{r}_m,\varepsilon)]P_\varepsilon(\mathbf{r}_m,\mathbf{r}_i,\omega) \\ & \times[2\,{}^\alpha\Gamma(\mathbf{r}_i,\varepsilon)]N_0(\mathbf{r}_i,\varepsilon) \; , \end{aligned} \qquad (4.12)$$

which now is generalized to include time-dependence and dephasing processes. It reduces to the usual transmission probability $T_{\beta,\alpha}(\mathbf{r}_m,\mathbf{r}_i)$ by taking $\omega \rightarrow 0$. Here β and α label the different processes (channels) contributing to the self-energy at sites $\mathbf{r}_m$ and $\mathbf{r}_i$, respectively. With this notation the right-hand term in Eq. (2.18) can be reduced to the form of the out term in Eq. (1.1), by writing the self-energies in the linear-response approximation (3.8) and (3.16). The term on the left of (2.18) can be reduced to the in term in (1.1), using the linear-response approximation of Eq. (2.25) and writing the density of states using Eq. (2.22):

$$\begin{aligned} 2\pi N_0(\mathbf{r},\varepsilon)[2\,{}^\phi\Gamma(\mathbf{r},\varepsilon)] & = \sum_\beta \int\int dt_i d\mathbf{r}_i T_{\phi,\beta}(\mathbf{r},\mathbf{r}_i,t-t_i) \\ & = \sum_\beta \int d\mathbf{r}_i T_{\phi,\beta}(\mathbf{r},\mathbf{r}_i) \\ & = [1 - R_\phi(\mathbf{r})] \equiv [g(\mathbf{r})]^{-1} \; . \end{aligned} \qquad (4.13)$$

Here $R_\phi(\mathbf{r})$ defines a reflection coefficient slightly different from the usual because we did not set the usual restriction $\beta \neq \phi$ in the sum. The "locator" g will be later used in the series expansion of the density propagator. Therefore, setting the term in Eq. (4.2) at the right and performing the substitutions of Eq. (2.27) and (4.12), we obtain

$$\begin{aligned} 0 = \frac{2e}{h}\Bigg[& \sum_\beta \int\int d\mathbf{r}_i dt_i T_{\phi,\beta}(\mathbf{r},\mathbf{r}_i,t-t_i)\delta\mu_\beta(\mathbf{r}_i,t_i) \\ & - [1 - R_\phi(\mathbf{r})]\delta\mu_\phi(\mathbf{r},t) \Bigg] \; , \end{aligned} \qquad (4.14)$$

which is the generalized Landauer-Büttiker equation (GLBE). Here we have multiplied by a factor 2, representing the spin degeneracy, and by the electron charge so the equation has the units of an electric current. The greek subscripts label the processes contributing to the self-energy associated with each point in the real space. By relabeling the sum over space and channels over a single summation index, say β', the above equation is reduced to the form given by Eq. (1.1). Equation (4.14) establishes that no electron is lost due to scattering with the phonon field. We will analyze the actual current in the next section.

V. EVALUATION OF THE CURRENTS

Once we have obtained the self-consistent Σ^K, either exactly or using the linear-response approximation of Eq. (4.15), we can evaluate the Keldysh function using Eq. (4.1) with $\mathbf{r}_2 \neq \mathbf{r}_1$ and from this evaluate the current through any surface. However, in order to obtain a simpler expression for the current in the spirit of the Landauer-Büttiker equations, let us consider again the discrete lattice with a lead attached as introduced in Sec. III B. The current leaving the site S and entering the site S',

$$\begin{aligned} j_{S',S} &= \frac{i}{\hbar}(V_{S,S'}\psi_S^\dagger\psi_{S'} - V_{S',S}\psi_{S'}^\dagger\psi_S) \\ &= V_{S,S'}G^<_{S',S} - V_{S',S}G^<_{S,S'} \ . \end{aligned} \tag{5.1}$$

That is, the current is simply expressed in terms of the nondiagonal elements of $G^<$, which are related to G^K by Eq. (2.5c) or equivalently

$$G^< = \tfrac{1}{2}G^K + \frac{i}{2}A \tag{5.2}$$

and

$$\Sigma^< = \tfrac{1}{2}\Sigma^K + i\Gamma \ . \tag{5.3}$$

Using Eq. (2.9) and its transpose, we write:

$$\begin{aligned} G^<_{S,S'}V_{S',S} &= (G^R_{S,S}V_{S,S'}G^{0<}_{S',S'} + G^<_{S,S}V_{S,S'}G^{0A}_{S',S'})V_{S',S} \\ &= G^R_{S,S}\,{}^S\Sigma^<_{S,S} + G^<_{S,S}\,{}^S\Sigma^A_{S,S} \end{aligned} \tag{5.4}$$

and

$$\begin{aligned} V_{S,S'}G^<_{S',S} &= V_{S,S'}(G^{0<}_{S',S'}V_{S',S}G^A_{S,S} + G^{0R}_{S',S'}V_{S',S}G^<_{S,S}) \\ &= {}^S\Sigma^<_{S,S}G^A_{S,S} + {}^S\Sigma^R_{S,S}G^<_{S,S} \ . \end{aligned} \tag{5.5}$$

The above quantities are evaluated at $t_2 = t_1 = t$. It remains an integral over internal time which can be evaluated by expanding in series and dropping the gradient term. In that case all factors in the products on the right-hand side (rhs) result evaluated at the same (final) time and the integral on internal times becomes an integral in energy. With the use of (5.2) and (5.3), Eq. (5.1) can be written in terms of G^K and Σ^K. The electric current leaving the sample becomes

$$\begin{aligned} I_S(t) = \frac{2e}{hi}\int \{ & {}^S\Gamma(\mathbf{r}_S,\varepsilon,t)G^K(\mathbf{r}_S,\mathbf{r}_S,\varepsilon,t) \\ & -\tfrac{1}{2}A(\mathbf{r}_S,\mathbf{r}_S,\varepsilon,t)\,{}^S\Sigma^K(\mathbf{r}_S,\mathbf{r}_S,\varepsilon,t)\}d\varepsilon \ . \end{aligned} \tag{5.6}$$

Equation (5.6) is very useful because it describes a general nonlinear regime (provided that one has the Keldysh function). The first term on the rhs is an out contribution. It accounts for electrons leaving the sample and entering the current lead at time t, having had their last interaction at some previous time. Reciprocally, the second term represents the electrons which at time t are leaving the lead toward the sample. It is the in term. This is interpreted more clearly in the linear-response regime. Since the corresponding current in the equilibrium case vanishes, it is convenient to subtract it from Eq. (5.6) as we did in Eq. (2.27). We replace δG^K and N_0 using the expressions (2.18) and (2.22) evaluated in the steady-spectrum approximation. We obtain (5.6) with the substitutions $G^K \rightarrow \delta G^K$ and $\Sigma^K \rightarrow \delta\Sigma^K$. Then we perform the energy integration according to Eqs. (2.27) and (3.8). Using the notation of Eqs. (4.12) and (4.13), we can write

$$\begin{aligned} I_S(t) = \frac{2e}{h}\Bigg\{ & \sum_\beta \int\int d\mathbf{r}_i dt_i T_{S,\beta}(\mathbf{r}_S,\mathbf{r}_i,t-t_i)\delta\mu_\beta(\mathbf{r}_i,t_i) \\ & -[1-R_S(\mathbf{r}_S)]\delta\mu_S(\mathbf{r}_S,t)\Bigg\} \ , \end{aligned} \tag{5.7}$$

which has an obvious interpretation in the Landauer-Büttiker picture.

It is worthwhile to consider the case in which the external lead is itself a finite system (e.g., a dangling wire), so that the exchange of electrons is only possible through the contact described by Eq.(3.1). This situation is relevant for the experiments because it can be used to model a *voltage probe.* In that case the net current produces a change in the total charge Q_S in the lead:

$$\begin{aligned} I_S(t) = \frac{d}{dt}Q_S(t) &= \frac{2e}{h}\frac{d}{dt}\int_{\Omega_S}\frac{1}{i4\pi}G^K(\mathbf{r}_{S'},\mathbf{r}_{S'},t,t)d\mathbf{r}_{S'} \\ &= 2e\bar{N}_S\frac{d}{dt}\overline{\delta\mu}_S(t) \ , \end{aligned} \tag{5.8}$$

where $\bar{N}_S \approx \underline{N}_S\Omega_S$ is the total density of states in the volume Ω_S. $\delta\mu_S(t)$ is a mean shift in the chemical potential which, in general, is different from the chemical potential at the contact site defined in Eq. (3.8). However, they are equal under certain conditions, as will be discussed in Sec. VI C. If that is the case, equating (5.7) and (5.8), we obtain a generalized master equation for the chemical potentials.

Another usual situation is that of a dissipative sample connected, at points $\mathbf{r}_L$ and $\mathbf{r}_R$, to two leads (left and right) which act as *voltage sources.* Assume $\delta\mu_L > \delta\mu_R$ so they act, respectively, as current source and sink. With the use of a decimation procedure,[3,11] it is possible to express all the internal chemical potentials associated with the electron-phonon interaction in terms of the external voltage V determined by the difference $\delta\mu_{\text{ext}}(t) = \mu_L - \mu_R \equiv eV(t)$. Using Eq. (4.13), we get

$$I_R(t) = \frac{2e}{h}\int dt_i \tilde{T}_{R,L}(t-t_i)\delta\mu^{\text{ext}}(t_i) \tag{5.9}$$

with

$$\begin{aligned} \tilde{T}_{R,L}(t-t_i) = {} & T(\mathbf{r}_R,\mathbf{r}_L,t-t_i) + \int\int dt_j d\mathbf{r}_j T(\mathbf{r}_R,\mathbf{r}_j,t-t_j)g(\mathbf{r}_j)T(\mathbf{r}_j,\mathbf{r}_L,t_j-t_i) \\ & + \int\int\int\int dt_j d\mathbf{r}_j dt_k d\mathbf{r}_k T(\mathbf{r}_R,\mathbf{r}_j,t-t_j) \\ & \times g(\mathbf{r}_j)T(\mathbf{r}_j,\mathbf{r}_k,t_j-t_k)g(\mathbf{r}_k)T(\mathbf{r}_k,\mathbf{r}_L,t_k-t_i) + \cdots \ , \end{aligned} \tag{5.10}$$

which is a generalization of Eq. (2.3b) of the work from D'Amato and Pastawski.[3] Here it was extended to consider problems with time dependence. The locator g is defined by Eq. (4.13) and is a manifestation of the local model adopted for the self-energies.

VI. TIME-DEPENDENT RESONANT TUNNELING

A. General features

We apply the formalism introduced to the problem of resonant tunneling with different dephasing processes under time-dependent boundary conditions. For concreteness we can think of the situation schematized in Fig. 1(a). There, a quantum dot, O, is in contact with two electron reservoirs L (left) and R (right) through some weak connections. Since their chemical potentials will be given as boundary conditions, they play the role of voltage sources. Besides, the electrons in the dot can interact with some generic source of decoherence, S, characterized by a time τ_S (or τ_ϕ). We consider two different decoherence processes, a dephasing field and a side probe, as schematized in Figs. 1(b) and 1(c) respectively. In both cases we neglect the dynamics of the electrons while they are tunneling through the barrier. This approximation is correct provided that the energy height $[\propto(\kappa)^{1/2}]$ and length L_x of the barrier are optimized so that traversal time,[22] ($\tau_q \propto L_x/\kappa$), is minimized while the tunneling amplitude, proportional to $\exp(-\kappa L_x)$, is maintained constant. As an idealization we assume that the electron-electron interaction has been turned off. The electron-phonon interaction inside the reservoir is implicitly taken into account by allowing the relaxation rate inside the reservoirs to be instantaneous. This is justified because the number of quasidegenerate degrees of freedom within the range $\hbar/\tau_\phi$ allows any dephasing process to be very effective there. These assumptions will allow us to concentrate on the physics of the decoherence processes during the tunneling through the dot and the time-dependent problem.

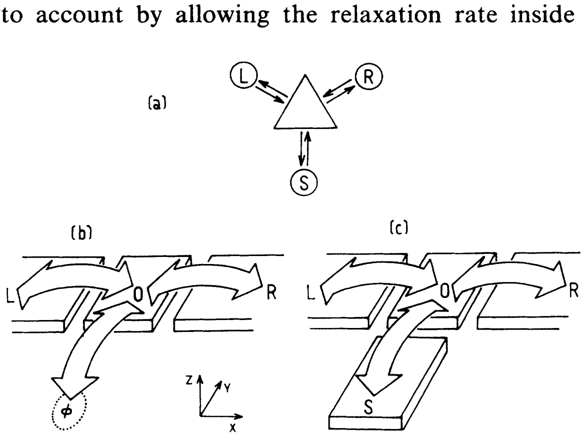

FIG. 1. (a) Scheme for the steady-state dissipative tunneling. The triangle is a scattering center and the circles represent reservoirs. The left (L) and right (R) channels are connected to voltage sources (external reservoirs). The channel S is connected to a voltage probe or an inelastic process, also represented as a reservoir. (b) Quantum dot with dissipation. The boxes represent the confining region for the electron gas. The channel ϕ represents a dephasing field (e.g., phonon bath), the dotted circle indicates that interacting electron remains in the central dot O. If the confinements along the y and z axes are removed we get a double-barrier resonant tunnel diode. (c) Quantum dot coupled to a dephasing side dot. The side dot is assumed to have fast phase relaxation. If the confinement along z is removed a quantum wire configuration is obtained.

In case (b) the electrons can interact with some dephasing field while they pass through the dot. Therefore, during the interaction they find themselves localized inside the dot and this becomes the initial condition for a new evolution. Examples of this are a capacitive contact with an external lead, in which the photons play the role of a dephasing field, and the phonon field already discussed. The later is considered here by using the approximated self-energies given in Sec. III B. These cannot account for the effects related to energy transfer (vertical processes). Therefore, we will refer to them as dephasing processes instead of inelastic. This restriction does not affect the main features of transport.

In case (c), there is no dephasing interaction inside the dot but the electrons can tunnel toward a side dot S. No particle can escape from this dot except through the SO connection. However, S will be considered to have a good coupling rate $1/\tau_{\phi'}$ with the external world through some dephasing processes.[23] We can assume that it has magnetic impurities, a better coupling with the phonon bath, or simply a quantum nature which allows any of these couplings to be more effective. In the last case, the side dot may be disordered or chaotic so that the degeneracies are broken, giving a typical energy spacing $\delta E \ll \hbar/\tau_{\phi'}$. This would make the dephasing very efficient in scrambling the incident state into a wide region of the phase space. Under any of these situations, we will not need to know the exact nonequilibrium distribution function since it will be a smooth function of the energy. In the linear-response regime, upon integration over energy and space, a chemical potential shift $\delta\mu_S$ is enough to characterize the state of the side dot.

Both cases, (b) and (c), appear as equivalent in the steady-state transport but will show up their differences in the time-dependent problem. In case (b) when an electron is lost from the coherent beam, it remains in the central dot. In contrast, in case (c) the electrons actually leave the dot and are eventually reinjected at a later time. A steady-state problem which can be assimilable to the above cases was already addressed in the literature.[24,25] Büttiker noticed that a voltage probe S, represented by an additional electron reservoir adjusted to provide zero net current, can be interpreted as a decoherence process. By using a scattering matrix to represent the interactions between those three reservoirs, he got the transmission probabilities $T_{R,L}$, $T_{R,S}$, and $T_{S,L}$, and found that the effective transmittance (or conductance G) between the reservoirs L and R is

$$\tilde{T}_{R,L}=\tilde{T}_{R,L}(\omega)\big|_{\omega=0}=\frac{h}{2e}G(\omega)\Big|_{\omega=0}=T_{R,L}+\frac{T_{R,S}T_{S,L}}{T_{R,S}+T_{S,L}}\ . \qquad (6.1)$$

This has an obvious interpretation in terms of a circuit analogy in which the T's are conductances. However, the T's are not independent because they are obtained from a unitary scattering matrix. This property makes evident the fundamental feature that distinguishes the Landauer-Büttiker description from a classical one. The equations *look* like a classical master equation with independent transition probabilities; however, these probabilities should be chosen so that they satisfy the precise features of the quantum interference. This interdependence is best accounted by the use of a Hamiltonian model. Büttiker also noticed[25] that the first term of (6.1) represents a coherent tunneling while the second accounts for incoherent processes originated in the presence of the voltage probe S.

In what follows we show that the above picture of the steady state is right and we solve the time-dependent situation. For this we use a simple Hamiltonian which can model various different physical situations depending on the values adopted for the parameters. Let us assume that there is a single resonant state at the dot with characteristic energy E_O and whose occupation may fluctuate to allow the transport in the linear-response regime.

The unperturbed Hamiltonian which describes the isolated dot O of volume Ω_O is

$$H^{o}=E_O c_O^{\dagger} c_O \ . \tag{6.2}$$

The left lead L and the hopping interaction can be represented by the Hamiltonians:

$$H^{L}=\bar{E}_{L'} c_{L'}^{\dagger} c_{L'} \equiv \int dk_L E_{k_L} c_{k_L}^{\dagger} c_{k_L} \ , \tag{6.3}$$

$$H^{OL}=V_{L'L} c_{L'}^{\dagger} c_L + \text{c.c.} \tag{6.4}$$

Here $\bar{E}_{L'}(\varepsilon)=E_{L'}+\Delta_{L'}(\varepsilon)-i\Gamma_{L'}(\varepsilon)$ and the equivalence between the localized and the extended description is given by the fact that

$$[\varepsilon-\bar{E}_{L'}(\varepsilon)]^{-1}=\int \frac{|\langle L|k_L\rangle|^2}{(\varepsilon-E_{k_L})} dk_L \ . \tag{6.5}$$

For the particular case in which the lateral lead is a periodic linear chain, expression (6.4) becomes simple because we know that

$$\Delta_{L'}(\varepsilon)=(\varepsilon-E_{L'})/2 \ , \tag{6.6a}$$

while

$$\Gamma_{L'}(\varepsilon)=\{V^2-[(\varepsilon-E_{L'})/2]^2\}^{1/2} \ , \tag{6.6b}$$

and from these we evaluate

$${}^{L}\Delta(\varepsilon)-i\,{}^{L}\Gamma(\varepsilon)=\frac{|V_{L,L'}|^2}{\varepsilon-E_{L'}-\Delta_{L'}(\varepsilon)+i\Gamma_{L'}(\varepsilon)} \ . \tag{6.7}$$

In the notation used $\Sigma_{L'}$ is the self-energy correction to the site *of the lead* in contact with the dot, due to the rest of the lead. ${}^{L}\Sigma$ is the self-energy correction to the dot state due to the presence of the lead.

To obtain the energy shift from an expression such as (3.6) or its equivalent in the momentum space, we exploit the analytic properties of Σ^R using

$${}^{L}\Delta(\varepsilon)=\frac{1}{\pi}\mathrm{P}\int \frac{{}^{L}\Gamma(\varepsilon')}{\varepsilon-\varepsilon'} d\varepsilon' \ . \tag{6.8}$$

A similar description will be adopted for the right-hand side lead and the side dot S (or phonon field ϕ). We can replace the label L by R or S (or ϕ). In the resonant case, in which there is no need for a spatial argument inside the dot, we obtain as the total self-energy:

$$\Gamma(\varepsilon)={}^{L}\Gamma(\varepsilon)+{}^{R}\Gamma(\varepsilon)+{}^{S}\Gamma(\varepsilon) \ , \tag{6.9}$$

with the individual contributions given by expressions of the form of Eq. (3.7) [or (3.15) for ${}^{\phi}\Gamma$]. From (6.8) we also obtain

$$\Delta(\varepsilon)={}^{L}\Delta(\varepsilon)+{}^{R}\Delta(\varepsilon)+{}^{S}\Delta(\varepsilon) \ . \tag{6.10}$$

The central dot plays a decisive role in the kinetics because it determines the transmission probabilities. These are evaluated in terms of the Green's function at the central dot,

$$G_{O,O}^{R}(\varepsilon)=\frac{1}{\varepsilon-E_O-\Delta(\varepsilon)+i\Gamma(\varepsilon)} \ , \tag{6.11}$$

where the real and imaginary contributions to the self-energy are given above. If we consider the limit in which $|V_{L,L'}|/V \ll 1$ we can evaluate

$$G_{O,O}^{R}(\varepsilon+\hbar\omega/2)G_{O,O}^{A}(\varepsilon-\hbar\omega/2) \approx G_{O,O}^{R}(\varepsilon)G_{O,O}^{A}(\varepsilon)\frac{1}{1-i\omega\tilde{\tau}_q} \ , \tag{6.12}$$

where

$$\tilde{\tau}_q(\varepsilon)=\frac{\hbar}{\Gamma(\varepsilon)} wm \tag{6.13}$$

with

$$w(\varepsilon)=\frac{\Gamma(\varepsilon)^2}{[\varepsilon-E_O-\Delta(\varepsilon)]^2+\Gamma(\varepsilon)^2}$$

and

$$m(\varepsilon)=\left|1-\frac{\partial}{\partial\varepsilon}\Delta(\varepsilon)+\frac{[\varepsilon-E_O-\Delta(\varepsilon)]}{\Gamma(\varepsilon)}\frac{\partial}{\partial\varepsilon}\Gamma(\varepsilon)\right| .$$

At resonance, the term in square brackets cancels out. Γ is very weakly dependent on ε. Since $|V_{L,L'}|/V \ll 1$, the last two terms contributing to m are small and we can take $m \approx 1$. Hence the transport time has a Lorentzian shape described by w. Therefore the relevant independent parameters in the transport equation are the escape rates to the left, $\tau_L=\hbar/(2\,{}^{L}\Gamma)$, to the right $\tau_R=\hbar/(2\,{}^{R}\Gamma)$, and to the side $\tau_S=\hbar/(2\,{}^{S}\Gamma)$ (or dephasing time τ_ϕ). The reciprocal of the natural lifetime in the absence of dephasing is defined as $1/\tau_1=1/\tau_L+1/\tau_R \equiv 2w/\tau_q$ and the total decay rate from the coherent resonant state is $1/\tau_O=1/\tau_1+1/\tau_S \equiv 2w/\tilde{\tau}_q$.

We can obtain an alternative way to write the transmission coefficients using Eqs. (4.13) and (4.14) and taking $\omega \rightarrow 0$ and $m=1$:

$$T_{R,L}=4\frac{(\tau_O)^2}{\tau_L\tau_R}w \tag{6.14}$$

and

$$\frac{T_{R,S}T_{S,L}}{T_{R,S}+T_{S,L}}=4\frac{(\tau_O)^2}{(\tau_L+\tau_R)\tau_S}w \ . \tag{6.15}$$

These equations are useful because they are written in terms of parameters which can be controlled independently [e.g., the width of the channels separating the dot of Fig. 1(b) from the external world]. We will consider only the resonant situation ($w=1$), which simplifies the analysis of the main physical processes involved in dissipative tunneling. To study other energies we can rewrite the Lorentzian factor $w(\varepsilon)$ in the expressions for T's and $\tilde{\tau}_q$.

We will use $\mu_L(t)$ and $\mu_R(t)$ as boundary conditions, in particular we will take

$$\mu_L(t)-\mu^0=\delta\mu_L(t)=\delta\mu^{\text{ext}}\cos[\omega t] \ , \tag{6.16}$$

while

$$\mu_R(t)-\mu^0=\delta\mu_R\equiv 0 \ . \tag{6.17}$$

That is, the leads are *voltage sources* because the values of their chemical potentials are not affected by the transport through the dot. We obtain the current entering the right-side lead

$$I_R(t)=\text{Re}[I_R(\omega)\exp(-i\omega t)] \ , \tag{6.18}$$

by evaluating $I_R(\omega)=(2e^2/h)\tilde{T}(\omega)\delta\mu^{\text{ext}}$.

We have already identified the main parameters of the transport equation and we can discuss the conditions of applicability of the model. The study of the interacting dot has been an object of great interest because it is related to devices which operate through the Coulomb blockade phenomena. The main physics on that phenomenon[26] lies in the fluctuation on the energy spectrum in a Hubbard energy U greater than the single-particle energy splitting. The linear-response regime can be studied with the use of the steady-spectrum approximation, but it still requires a self-consistent Green's function. Since this involves the specific state of occupation of the dot states, the Green's function is less simple than (6.11). However, this is not required if we consider systems with less-localized states because U is smaller. This is the case of a double-barrier resonant tunneling device (DBRTD) at finite temperature.[27] This corresponds to a dot whose confinement lengths in the directions y and z in Fig. 1(b) have become infinite. Provided that the appropriate integrations over the transverse degrees[28] of freedom are performed, the results of the next section will be valid in this case.

We may also conceive alternative configurations governed by independent electron physics. We search for a device that, while resembling closely a tunnel-diode, also includes the possibility of a side reservoir coupled to the resonant state. For example, if the confinement length in direction y in Fig. 1(c) becomes infinite, what we call a dot is actually a quantum wire, being the reservoirs L and R both two-dimensional semiplanes, and the side reservoir a second wire layered below (or above) the first. Hamiltonians of the form (6.2)–(6.4) remain valid for each transverse quantum number. For simplicity we keep referring to our model system as "quantum dot."

B. Resonant tunneling with decoherence

First, we consider a resonant structure, in which the electrons can lose coherence while they are inside the structure [Fig. 1(b)], for example, due to collision with phonons. The distribution function of the dot appears explicitly in the kinetic equation (4.14), which becomes

$$[1-R_\phi]\delta\mu_\phi(t)=\int[T_{\phi,L}(t-t_i)\delta\mu_L(t_i)+T_{\phi,R}(t-t_i)\delta\mu_R(t_i)+T_{\phi,\phi}(t-t_i)\delta\mu_\phi(t_i)]dt_i \ . \tag{6.19}$$

We proceed through similar considerations to that leading to Eq. (6.12) and show that the Fourier transform of the time-dependent transmission probability has the form

$$T_{\phi,L}(\omega)=\frac{T_{\phi,L}}{1-i\omega\tilde{\tau}_q} \tag{6.20a}$$

with

$$\frac{\hbar}{\tau_q}={}^L\Gamma+{}^R\Gamma+{}^\phi\Gamma=\frac{\hbar}{2\tau_1}+\frac{\hbar}{2\tau_\phi} \ . \tag{6.20b}$$

Notice that we set $m=1$ and take ε giving $w(\varepsilon)=1$. Here τ_1 is the mean life of an electron in the dot in the absence on electron-phonon interaction. Let us consider the boundary conditions represented by Eqs. (6.16) and (6.17). The local chemical potential becomes

$$\left[1-\frac{i\omega\tilde{\tau}_q}{1-i\omega\tilde{\tau}_q}\frac{T_{\phi,\phi}}{T_{L,\phi}+T_{R,\phi}}\right]\delta\mu_\phi(\omega) =\frac{T_{\phi,L}}{T_{L,\phi}+T_{R,\phi}}\frac{1}{1-i\omega\tilde{\tau}_q}\delta\mu^{\text{ext}} \ . \tag{6.21}$$

Notice that the term which contains ω on the left-hand side arises from the failure of the term

$$\int[T_{\phi,\phi}(t-t_i)\delta\mu_\phi(t_i)-\delta\mu_\phi(t)T_{\phi,\phi}(t-t_i)]dt_i \tag{6.22a}$$

to cancel exactly as occurs in the steady state. This term represents the fluctuation in time of the number of electrons which suffer reiterated inelastic collisions inside the dot. These electrons are lagged by a time

$$\tau_{\text{lag}}=\tilde{\tau}_q\frac{\tau_1}{\tau_\phi} \ . \tag{6.22b}$$

This is about $\tau_q = 2\tau_1 \gg \tilde{\tau}_q$ for very strong dephasing processes and becomes negligible when the dephasing process is weak. Dropping the term of order ω^2, we obtain

$$\delta\mu_\phi(\omega) = \frac{T_{\phi,L}}{T_{L,\phi}+T_{R,\phi}} \frac{1}{1-i\omega(\tilde{\tau}_q+\tau_{\text{lag}})} \delta\mu^{\text{ext}} . \tag{6.23}$$

This shows that the chemical potential is measuring the amount of electrons inside the well, no matter if they are coherent or not with the source. Besides, it is interesting to notice that the resulting time is not the tunneling time through the left barrier, τ_L, but a time which is essentially twice the minimum between τ_L, τ_R, and τ_ϕ. This is because the density of states on the well, which is essentially proportional to $\tilde{\tau}_q = 2\tau_O$, determines the dynamics.

The total current entering the right-hand-side reservoir can be evaluated using Eqs. (5.10) or (6.1), and we obtain

$$I_R(\omega) = {}^{\text{coh}}I_R(\omega) + {}^{\text{seq}}I_R(\omega) , \tag{6.24}$$

where the first term represents a coherent tunneling through the central dot:

$${}^{\text{coh}}I_R(\omega) = \frac{2e}{h} \frac{T_{R,L}}{1-i\omega\tilde{\tau}_q} \delta\mu^{\text{ext}} . \tag{6.25}$$

Its characteristic delay time is the mean life of the coherent electron in the well, which is shorter than that in absence of dephasing processes. The sequential part of the current is

$${}^{\text{seq}}I_R(\omega) = \frac{2e}{h} \frac{T_{R,\phi}T_{\phi,L}}{T_{R,\phi}+T_{\phi,L}} \frac{1}{1-i\omega(2\tilde{\tau}_q+\tau_{\text{lag}})} \delta\mu^{\text{ext}} , \tag{6.26}$$

which has the delay time showing two contributions, one is twice the time the electron would need to get into the well and the other is the contribution of the electrons lagged by subsequent dephasing collisions. The transmittances can be replaced using (6.17) and (6.18). Then, the sum is performed keeping terms up to order ω, and we get the tunneling impedance:

$$1/G(\omega) = 1/G(0) - i\omega L , \tag{6.27}$$

where $G(0)$ is the dc conductance given by (6.1). The inductance is

$$L = \tau_0 / G(0) . \tag{6.28}$$

This is a very remarkable result because it shows that the characteristic delay in the response of the device is independent of the presence of decoherence processes inside the dot. That is, even when the tunneling resistance becomes the classical addition of the resistances associated with the barriers, the delay is still determined by the quantum regime. Equation (6.28) is also valid out of resonance. In this case, since both the time and the conductance contain the shape factor $w(\varepsilon)$, the inductance results energy independent.

These results are consistent with the experiments[29] on frequency dependence of the differential conductance in a DBRTD at room temperature. Our model is particularly applicable to that system because, having the state of a two-dimensional degeneration, the problem of differential charging effects is negligible, and hence the drop of the time dependence in the Green's functions [Eq. (2.18)] is a good approximation. Since the static field (V_{dc}) polarizes the device ($eV_{\text{dc}} > \varepsilon_F$) completely, the current is carried out by the states of each transversal mode with energy close to the corresponding resonance. Besides, the differential conductance can be considered a linear response relative to the oscillating field ($eV_{\text{ac}} \ll \Gamma$). The experiments show that a differential tunneling resistance has associated an inductance with a value such that the delay time associated is of the order of the inverse of the breath of the resonance as given by a quantum calculation (without dissipation). For coherent tunneling, theoretical results were obtained by Frensley[30] from numerical solutions of the density-matrix formalism. A similar regime corresponds to the analytical results obtained by Chen and Ting[31] using a path-integral method. Both show that at low temperatures the delay is determined by the natural width of the resonance. However, the appearance of this characteristic time in the room-temperature experiment remained puzzling. The fact that the electron-phonon interaction broadens the resonance might suggest that the response could be made arbitrarily faster by increasing the temperature. Our result above, obtained in the linear-response regime at zero bias, shows that this is not the case, since the response time is quite stable against modifications in τ_ϕ. This result holds also in the calculation of the linear response of a biased DBRTD, which includes the integration over energy and transversal momentum. A more complete discussion of this experimental situation will be presented elsewhere.

C. Resonant dot coupled to a dephasing side dot

This case requires a model for the lateral dot S of volume Ω_S. Since S is finite it should have a discrete spectrum. However, since we assume that S is well coupled to a dephasing process, its spectrum becomes continuum and S is well described by a Hamiltonian H^S of the same form as (6.3). Again, we neglect any effect of the dynamics of electrons inside S by assuming an instantaneous chemical potential $\mu_S(t) \approx \bar{\mu}_S(t)$. Then Eq. (5.8) becomes

$$I_S(t) = 2e\bar{N}_S \frac{d}{dt}\delta\mu_S(t) , \tag{6.29}$$

where $\bar{N}_S \approx N_S \Omega_S$ is the density of states in the volume Ω_S.

Therefore, Eq. (5.7) gives the change in the number of particles in the lateral dot and becomes

$$2\pi\hbar\bar{N}_S \frac{\partial\delta\mu_S}{\partial t} = \int \{ T_{S,L}(t-t_i)\delta\mu_L(t_i) + T_{S,R}(t-t_i)\delta\mu_R(t_i) + T_{S,S}(t-t_i)\delta\mu_S(t_i) \} dt_i - [1-R_S]\delta\mu_S(t) . \tag{6.30}$$

Note that since we have not defined any dephasing process inside the central dot its occupation does not appear explicitly in the kinetic equation.

By using the Fourier transform of Eq. (6.30), we can obtain

$$\delta\mu_S(\omega)=\frac{T_{S,L}}{T_{L,S}+T_{R,S}}\frac{1}{(1-i\omega\tilde{\tau}_q)(1-i\omega\tau_{\mathrm{del}})}\delta\mu^{\mathrm{ext}}\ , \tag{6.31}$$

where we see that besides the time spent by the resonant electron in the central quantum dot, there is also an additional delay given by

$$\begin{aligned}\tau_{\mathrm{del}}&=\frac{2\pi\hbar N_S}{T_{L,S}+T_{R,S}}+\frac{T_{S,S}}{T_{L,S}+T_{R,S}}\frac{\tilde{\tau}_q}{1-i\omega\tilde{\tau}_q}\\&\approx(\overline{N}_S/\overline{N}_O)[\tau_1+\tau_S]+\tilde{\tau}_q\frac{\tau_1}{\tau_S}\ .\end{aligned} \tag{6.32}$$

Here the second term is a lagging analogous to Eq. (6.23), which now is produced by the side dot, and can be neglected for small interaction. The remaining term expresses the simple fact that an electron can enter the side dot *after* it was injected in the central dot *either* by the *L* *or* the *R* lead. We have written this time in a way which expresses the possibility of achieving its experimental control. In fact, the *total* density of states in the side dot is proportional to its size. On the other hand, the value of τ_S depends on the length of the barrier separating the central and the side dot, and some local density of states. Both can be eventually controlled by adequate gate voltages. The approximation above involves dropping a term of order ω^2.

The current entering the right lead is again a superposition of a coherent part and a sequential one. The coherent part is given by Eq. (6.25), now with the dephasing time τ_S of the form of Eq. (2.7) replacing τ_ϕ. The sequential part, however, now describes the electrons which are affected by dephasing processes in the side well. The sequential current is given by

$${}^{\mathrm{seq}}I_R(\omega)=\frac{2e}{h}\frac{T_{R,S}T_{S,L}}{T_{L,S}+T_{R,S}}\frac{1}{1-i\omega(2\tilde{\tau}_q+\tau_{\mathrm{del}})}\ , \tag{6.33}$$

showing a total delay time of about $2\tilde{\tau}_q+\tau_{\mathrm{del}}$ relative to the voltage. This is the time required by the device to reach the actual steady state after a dc voltage is applied. If the coupling is very weak $\tau_S \gg \tau_1$ this time is $(\overline{N}_S/\overline{N}_O)[\tau_1+\tau_S]$. Since it is dominated by τ_S it can become very large. However, since the actual importance of the process is determined by the sequential transmission factor (6.15) which becomes of order τ_1/τ_S, the transport through the device is not modified by the presence of the side dot. This situation represents a "noninvasive" voltage probe which cannot follow the fast changes of the system.

Equation (6.30) contains two other important physical limits. First, let us consider that the lateral dot is very large. This is represented by the condition $\overline{N}_S \rightarrow \infty$. In that case there is not sufficient current to shift the chemical potential, and this is manifested by the fact that $d\delta\mu_S/dt \rightarrow 0$. Therefore the lateral dot behaves as a *voltage source* like the current leads *L* and *R*.

Now consider the limit in which $\overline{N}_S \rightarrow 0$. This means that the side dot is not able to support any additional charge and its occupation factor would follow instantaneously that of the central dot to which it is connected. Its chemical potential coincides with that characterizing the nonequilibrium distribution in the central dot. The side dot is then an *ideal voltage probe.* We see that the resulting kinetic equation is just (1.1) and (6.19). Of course, for an actual side lead this is an ideal limit. In practice, any attempt to reduce the density of states while keeping constant the interaction rate should consider their relation, expressed by Eq.(3.7), and the changes on $|V_{S,S'}|^2$. Therefore, an ideal voltage probe can be better achieved by a dephasing field. A capacitive contact is suitable in this category.

VII. FINAL REMARKS

In the present paper we have obtained a generalized Landauer-Büttiker equation [Eq. (1.1)] that deals with irreversible time-dependent transport in the presence of dephasing processes. This equation required the introduction of time-dependent transmission probabilities and chemical potentials at interior points of the sample. A conceptually striking feature is that this equation was deduced from the reversible Schrödinger equation, expressed within the Keldysh formalism, by applying the appropriate boundary conditions and some suitable approximations. In order to simplify the structure of the exact Keldysh kinetic equation, we introduced an adiabatic-spectrum approximation, which considers that both spectral densities and occupations change in time but neglects some interferences in the time domain. A further simplification is the steady-spectrum approximation, in which the spectrum is steady in time and transport occurs because occupations are allowed to change. This approximation applies to transport in the linear-response regime which is the condition to obtain the GLBE. When the steady state is reached, the traditional Landauer-Büttiker equation is obtained. This connection between the GLBE and the Keldysh formalism gives a procedure to evaluate the transport parameters from a model Hamiltonian. In particular, we give an explicit expression for the time-dependent transmission probability in terms of the one-particle Green's functions. The resulting equations are simple enough to be computed numerically and even analytically in many cases. Besides this practical value, the above relations give a deep insight on the different quantities involved in the Keldysh formalism, and how irreversibility appears in quantum mechanics. The Keldysh self-energies represent the boundary condition of injection of incoherent electrons, associated with the "measurement" of the electron densities by the phonon bath or any dephasing process. The electronic state at any time is the sum of all the alternative histories originated on those previous dephasing events (or "measurements"). The propagation of each of those alternative histories is performed by the product between the retarded and advanced Green's functions which have the meaning of a density propagator. In these functions the degradation of the coherent beam is described by the imaginary part of the retarded and advanced self-energies, respectively. While the procedure we devised [Eq. (2.18)] is quite general and does not have particular restrictions about the type of interactions or transport regime, we find that in order to obtain the simple expression of the form of (1.1), it is convenient to use self-energies diagonal in the spatial coordinates representation and to apply the linear-response approximation which considers only small excitations.

We have applied our formalism to the case of a DBRTD in the presence of dephasing processes. We found that even with strongly dephasing collisions, the response of the device is characterized by τ_q, which at resonance is twice the natural mean life of the resonant state τ_1. That is, the speed of the device has a natural limit on this quantum time. This prediction is in agreement with the room-temperature experiment on differential conductance in a DBRTD.

We also considered a quantum dot with a dephasing dot connected to its side. In this case, it appears a further delay which is the time needed by the density in the side dot to equilibrate the density in the central dot. This delay is proportional to $\tau_1+\tau_S$, the sum of the escape to the leads and escape to the side (dephasing) times, showing that the process is sequential. Besides, it is also proportional to the ratio $\bar{N}_S/\bar{N}_O$ between the densities of states in the side dot and in the central dot. If the first becomes zero, the response of the dot is instantaneous, becoming an ideal voltage probe, satisfying Eq. (1.1). By contrast, if this ratio is too big, the side dot behaves as a voltage source. These examples clarify the concepts of ideal voltage probe and voltage source in a time-dependent problem. The first one is able to follow instantaneously the electronic density in a given point of the sample. A voltage source is able to provide a constant chemical potential independently of the current generated.

We should make some remarks on the use of the kinetic equation in more general cases. The effect of the external fields is considered exactly in the unperturbed Hamiltonian and in the Green's functions used to propagate electrons and holes. This does not require any additional effort in an actual computational algorithm to solve the kinetic equation. The energies used also contain the effect of self-consistent fields. The importance of the self-consistent fields originated in changes of the electronic density, was addressed by Landauer,[2] and considered by Datta and collaborators in the steady-state case. In a general time-dependent problem it might be solved in the adiabatic-spectrum approximation. In the simulation of a realistic device it is difficult to select the correct boundary condition. However, this is not a limitation. We have seen that boundary conditions are easily described using one-dimensional leads. We can always make a realistic model of the sample and the leads and impose voltage or currents as boundary conditions deep inside (at least $L_\phi=v_F\tau_\phi$) the real leads using the one-dimensional model presented in Sec. III A. The kinetic equations by themselves transform these artificial boundary conditions in a length L_ϕ and produce the realistic boundary conditions at the sample-lead interface. The value of τ_ϕ can be decreased locally to facilitate the achievement of this objective.

Once again, the picture of transport pioneered by Landauer and Büttiker has proved to be a powerful conceptual tool toward the description of irreversible processes in open systems. The formalism presented above, inspired in this picture, is open to a broad range of applications. It can be instrumented numerically without major difficulties and, in some simple situations, it even allows an analytical solution. Since the basis of the computation rests on the evaluation of the Green's function in a discrete system a complete treatment of the dynamics in the linear-response regime can be devised with an extension of the currently existing methods for steady-state transport.[3-5,32] While some analytical work is still needed to treat the far from equilibrium regimes and the strongly interacting systems, the conceptual structure to deal with these situations is already laid down in the present work. Without a doubt, further analytical and numerical works will suggest new experimental setups to test and exploit the quantum dynamics that we are just beginning to understand.

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