Adiabatic transport in nanostructures

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A confined system of noninteracting electrons, subject to the combined effect of a time-dependent potential and different external chemical potentials, is considered. The current flowing through such a system is obtained by using the adiabatic approximation in an iterative manner. A formula is derived for the charge pumped through an unbiased system (all external chemical potentials are kept at the same value); it reproduces the Brouwer formula for a two-terminal nanostructure. The formalism presented yields the effect of the chemical-potential bias on the pumped charge on one hand, and the modification of the Landauer formula (which gives the current in response to a constant chemical-potential difference) brought about by the modulating potential on the other. Corrections to the adiabatic approximation are derived and discussed.

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I. INTRODUCTION AND SUMMARY

The flow of a dc current in response to a slowly varying time-dependent potential operating on an *unbiased* system is termed ''adiabatic charge pumping.''[1] This phenomenon, considered in Ref. 2, has attracted recently much theoretical[3–14] and experimental[15–17] interest. In general, ''adiabatic pumping'' occurs when the charge transferred across a boundary during a single period of a certain modulating potential is independent of the modulation frequency. The periodic potential should vary very slowly in time, such that its frequency ω is smaller than any characteristic energy scale of the electrons.[15] The process is adiabatic when the frequency is much smaller than the Wigner delay time,[18] as long as the the modulating potential is very weak. For larger strengths of this potential, the criterion for the adiabaticity becomes more delicate (see below).

Eighteen years ago, Thouless[19] had shown, using the adiabatic approximation, that the ground state of an infinite one-dimensional (1D) system of noninteracting electrons subject to a slowly moving periodic potential can support a dc current. Later theoretical investigations of quantum pumping in confined nanostructures employed the result derived by Brouwer,[3] which gives the pumped charge in terms of the time-dependent scattering matrix related to the modulating potential. The derivation presented by Brouwer is based on the analysis of Ref. 20, which, in turn, utilizes an expansion in the amplitude of the modulating potential in the context of time-dependent scattering theory. Nevertheless, it is generally accepted that the formalism of Büttiker *et al.*[20] and the resulting Brouwer formula are valid[21] even for large amplitudes, as long as the adiabatic approximation holds.

This paper is devoted, among other issues, to the exploration of this point. We consider a spatially confined system of noninteracting electrons, connected by leads (denoted by α) to electronic reservoirs which are kept at various chemical potentials, μ_α. The system is also subject to a slowly varying periodic potential. We derive an expression for the instantaneous current flowing in this system, using time-dependent scattering states. The formalism is based on an iterative solution of those states, in the adiabatic approximation, in which the temporal derivative of the scattering potential (and the scattering states) is the small parameter. The formal derivation is summarized in Sec. II, where we obtain the instantaneous current in the lowest-order adiabatic approximation. This current is averaged over a single period of the modulating potential. In this way we obtain the effect of the chemical-potential bias on the pumped charge on one hand, and the modification of the Landauer formula caused by the modulating potential on the other. We find an expression for the charge pumped through an unbiased system [see Eq. (1) below], which is particularly useful in cases where the modulating potential operates on the entire nanostructure,[22] and is spatially dependent. The Appendix includes the derivation of the next order correction to the current.

We investigate the lowest-order expression for the current in Sec. III, confining ourselves for simplicity to a system connected to two reservoirs. Our results there can be summarized as follows. In a two-terminal structure, the current averaged over a single period, τ, consists of two parts. The first, denoted by $I_{\rm pump}$, flows even when the system is unbiased (but is modified by the presence of the chemical-potential difference). To the lowest order in the adiabatic approximation, that current reads

$$I_{\rm pump}=\frac{e}{4\pi}\oint\frac{dt}{\tau}\int dE\left(-\frac{\partial}{\partial E}[f_l(E)+f_r(E)]\right)\times\sum_m[\langle rm|\dot{V}|rm\rangle-\langle lm|\dot{V}|lm\rangle], \tag{1}$$

where l and r denote the left and the right leads, respectively, and $f_{l,r}(E)\equiv(e^{(E-\mu_{l,r})/k_{\rm B}T}+1)^{-1}$ are the Fermi distributions in the reservoirs connected to the left and right leads. In Eq. (1), $|\beta m\rangle\equiv\chi^t_{\beta m}$ is the instantaneous scattering state at time t, excited by an incoming wave in channel m of lead β, and $\dot{V}$ is the temporal derivative of the time-dependent scattering

potential. Interestingly enough, the matrix element appearing in Eq. (1) can be written in terms of the instantaneous scattering matrix, reproducing the Brouwer formula.[3]

The second part of the current, denoted by $I_{\rm bias}$, flows only when the system is biased, i.e., $\mu_l \neq \mu_r$. When this current is integrated over a single period, τ, of the modulating potential, one obtains the Landauer formula, modified by the modulated potential in two ways: (i) The transmission coefficient is the instantaneous one, T^t, averaged over a single period of the time-dependent potential; (ii) there appears a correction to the Landauer expression, which is related to the temporal derivative of the modulating potential and the ensuing instantaneous scattering matrix. In the simplest case in which the two leads are single-channel ones, $I_{\rm bias}$ takes a particularly simple form,

$$I_{\rm bias}=\frac{e}{\tau\pi}\oint dt\int dE\left[T^t+\frac{1}{2}T^t\frac{d\psi^t}{dt}\frac{\partial}{\partial E}\right](f_l(E)-f_r(E)), \tag{2}$$

in which ψ^t is the instantaneous Friedel phase (i.e., the transmission phase) of the nanostructure. The first term in Eq. (2) yields the Landauer formula for the present case. The second term is a correction, being of higher order in the adiabatic approximation. The corrections to the adiabatic approximation are derived in the Appendix, and discussed in Sec. III, using a simple example. In particular we find that the validity regime of the adiabatic approximation is restricted by the strength of the modulating potential: The ratio of the second-order contribution to the first-order one involves the temporal derivative of the instantaneous Green function, which in turn, is proportional to the temporal derivative of the modulating potential. (See also Ref. 23.)

II. TIME-DEPENDENT SCATTERING THEORY IN THE ADIABATIC APPROXIMATION

In the first part of this section we solve for the time-dependent scattering states iteratively, using the adiabatic approximation. We then use those scattering states in the second part, to obtain the current. The formalism presented below borrows from the derivations in Refs. 24 and 25, extended to include the effect of a time-dependent scattering potential.

A. Time-dependent scattering states

We consider a ballistic nanostructure of arbitrary geometry, which consists of a nanostructure connected to several electronic reservoirs. This system is described by the Hamiltonian

$$\mathcal{H}(\mathbf{r},t)=\mathcal{H}_0(\mathbf{r})+V(\mathbf{r},t), \tag{3}$$

where the scattering potential $V(\mathbf{r},t)$ is assumed to be confined in space, so that asymptotic behaviors of the scattering solutions can be defined unambiguously. This confined region is attached to leads, numbered by the index α, and each lead is connected to a reservoir having the chemical potential μ_α. The Hamiltonian $\mathcal{H}_0$ consists of the kinetic energy. We use the adiabatic approximation, expanding the time-dependent states in terms of the temporal derivatives of the instantaneous solutions. This necessitates that the characteristic inverse time constant, $1/\tau$, which describes the time dependence of V, will be smaller than any characteristic energy scale of the electrons. For a simple oscillatory potential, $\tau=2\pi/\omega$. As is shown in the Appendix, this expansion also requires that the amplitude of the modulating potential V will be small.

As in the usual scattering treatment, we denote the incoming wave with energy E in lead α by $w^-_{\alpha n}$, where n is the transverse mode number. This wave is a solution of the free Hamiltonian

$$[\mathcal{H}_0(\mathbf{r})-E]w^-_{\alpha n}(\mathbf{r})=0, \tag{4}$$

and is normalized such that it carries a unit flux. The scattering solution of the full Hamiltonian, excited by this incoming wave, can be written in the form

$$\Psi_{\alpha n}(\mathbf{r},t)=e^{-iEt}\chi_{\alpha n}(\mathbf{r},t),$$

$$\chi_{\alpha n}(\mathbf{r},t)=w^-_{\alpha n}(\mathbf{r})+\tilde{\chi}_{\alpha n}(\mathbf{r},t). \tag{5}$$

The time dependence of the scattered wave function, $\tilde{\chi}_{\alpha n}(\mathbf{r},t)$, is expected to have the same characteristic time scale as V. For example, when the modulating potential is oscillating in time, $\tilde{\chi}$ contains all harmonics of the frequency ω.

The scattering solution $\Psi_{\alpha n}$ should satisfy the time-dependent Schrödinger equation

$$i\frac{\partial\Psi_{\alpha n}(\mathbf{r},t)}{\partial t}=\mathcal{H}(\mathbf{r},t)\Psi_{\alpha n}(\mathbf{r},t). \tag{6}$$

Inserting Eqs. (5) into (6), using Eq. (4), we find

$$(G^t(E))^{-1}\tilde{\chi}_{\alpha n}(\mathbf{r},t)=V(\mathbf{r},t)w^-_{\alpha n}(\mathbf{r})-i\frac{\partial\tilde{\chi}_{\alpha n}(\mathbf{r},t)}{\partial t}, \tag{7}$$

where G^t is the instantaneous Green function of the full Hamiltonian, such that

$$(E-\mathcal{H}(\mathbf{r},t))G^t(E;\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}'-\mathbf{r}). \tag{8}$$

We now solve Eq. (7), using the adiabatic approximation: The temporal derivative appearing on the right-hand side of that equation is regarded as a small correction (of order $1/\tau$), and the equation is solved iteratively. The zeroth order is just the instantaneous scattering solution, which we denote by $\chi^t_{\alpha n}$,

$$\chi^t_{\alpha n}(\mathbf{r})=w^-_{\alpha n}(\mathbf{r})+\int d\mathbf{r}'G^t(E;\mathbf{r},\mathbf{r}')V(\mathbf{r}',t)w^-_{\alpha n}(\mathbf{r}'). \tag{9}$$

The instantaneous scattering state $\chi^t_{\alpha n}$ is the solution of the instantaneous Schrödinger equation, with energy E,

$$(E-\mathcal{H}(\mathbf{r},t))\chi^t_{\alpha n}(\mathbf{r})=0. \tag{10}$$

Turning back to Eq. (7), we replace the derivative term on the right-hand side by the temporal derivative of the instan-

taneous scattering state, χ^t, and multiply both sides of the equation by the instantaneous Green function. Then [using Eqs. (5) and (9)], one finds that to first order in the time derivative the scattering solution reads

$$\chi_{\alpha n}(\mathbf{r},t)=\chi^t_{\alpha n}(\mathbf{r})-i\int d\mathbf{r}'\,G^t(E;\mathbf{r},\mathbf{r}')\dot{\chi}^t_{\alpha n}(\mathbf{r}'), \quad (11)$$

in which $\dot{\chi}^t_{\alpha n}$ is the time derivative of the instantaneous scattering state. Hence, to first order in the adiabatic approximation the time-dependent scattering states are given entirely in terms of the *instantaneous* solutions [namely, $\chi^t_{\alpha m}$ and $G^t(E;\mathbf{r},\mathbf{r}')$] of the problem at hand. One notes that the adiabatic solution (11) of the scattering state is analogous to the Thouless[19] solution for the ground-state wave function in his model. In the Appendix, we discuss the corrections to the lowest-order adiabatic approximation.

B. The current

Here we outline the derivation of the current in the scattering states formalism, as developed, e.g., in Refs. 24–26. One writes the field operator of the electron, $\hat{\Psi}(\mathbf{r},t)$, in terms of the scattering states as

$$\hat{\Psi}(\mathbf{r},t)=\int\frac{dE}{2\pi}\sum_{\alpha}\,\hat{a}_{\alpha n}(E)e^{-iEt}\chi_{\alpha n}(\mathbf{r},t), \quad (12)$$

in which $\hat{a}_{\alpha n}$ destroys an electron incoming in channel n of lead α. The thermal average of the latter operators is given by the Fermi distributions of the various reservoirs, such that

$$\langle\hat{a}^\dagger_{\alpha n}(E)\hat{a}_{\alpha' n'}(E')\rangle=2\pi\delta(E-E')\,\delta_{\alpha n,\alpha' n'}f_\alpha(E), \quad (13)$$

where $f_\alpha(E)$ is the Fermi distribution in the reservoir connected to the α lead. With these definitions, the thermal average of the current-density operator becomes

$$\langle\mathbf{j}(\mathbf{r},t)\rangle=\frac{e}{m}\Im\int\frac{dE}{2\pi}\sum_{\alpha}\,f_\alpha(E)\chi^*_{\alpha n}(\mathbf{r},t)\frac{\partial\chi_{\alpha n}(\mathbf{r},t)}{\partial\mathbf{r}}, \quad (14)$$

where e stands for the negative electron charge.

It is convenient to evaluate this quantity when $\mathbf{r}$ approaches ∞ in lead β (which will be denoted by $\mathbf{r}\to\infty\beta$), and then to integrate the current density over the cross section of that lead (noting that the incoming and outgoing waves are normalized to carry a unit flux). In so doing, we may take advantage of the asymptotic properties of the instantaneous quantities $\chi^t_{\alpha n}$ and $G^t(E)$, as documented in Refs. 24 and 26,

$$G^t(E;\mathbf{r},\mathbf{r}')|_{\mathbf{r}\to\infty\beta}=-i\sum_m\,w^+_{\beta m}(\mathbf{r})\chi^t_{\beta m}(\mathbf{r}'),$$

$$\chi^t_{\alpha n}(\mathbf{r})|_{\mathbf{r}\to\infty\beta}=\delta_{\alpha\beta}w^-_{\alpha n}(\mathbf{r})+\sum_m\,w^+_{\beta m}(\mathbf{r})S^t_{\beta m,\alpha n}. \quad (15)$$

Here, $w^+_{\beta m}$ is the outgoing wave in channel m of lead β and $S^t_{\beta m,\alpha n}$ is the matrix element of the instantaneous scattering matrix. As a result, the current flowing into lead β is given by

$$I_\beta(t)=e\int\frac{dE}{2\pi}\sum_{\alpha n}\,f_\alpha(E)\Big(\delta_{\alpha\beta}-\sum_m\,[|S^t_{\beta m,\alpha n}|^2-2\,\Re(S^t_{\beta m,\alpha n}U^*_{\beta m,\alpha n})]\Big), \quad (16)$$

with

$$U_{\beta m,\alpha n}=\int d\mathbf{r}\chi^t_{\beta m}(\mathbf{r})\dot{\chi}^t_{\alpha n}(\mathbf{r}). \quad (17)$$

The result (16) for the time-dependent current entering into lead β of the nanostructure holds for a general biased system, whose various terminals have different chemical potentials (as long as the time dependence of the periodic potential is slow enough). It is therefore interesting to consider charge conservation, using that result. Indeed, summing Eq. (16) over all leads, we obtain

$$\sum_\beta\,I_\beta(t)=e\int\frac{dE}{2\pi}\sum_{\alpha n}\,f_\alpha(E)\frac{d}{dt}\int d\mathbf{r}|\chi^t_{\alpha n}(\mathbf{r})|^2, \quad (18)$$

which shows that when the total current entering the system, $\Sigma_\beta I_\beta(t)$, is integrated over a single period of the modulating potential, the result is zero, i.e., the charge per period is conserved. In deriving the result (18) we have employed (i) the unitarity of the instantaneous scattering matrix, $\Sigma_{\beta m}S^{t*}_{\beta m,\alpha n}S^t_{\beta m,\alpha' n'}=\delta_{\alpha n,\alpha' n'}$, and (ii) the following property of the scattering matrix:[24,26]

$$\sum_{\beta m}\,S^{t*}_{\beta m,\alpha n}\chi^t_{\beta m}(\mathbf{r})=\chi^{t*}_{\alpha n}(\mathbf{r}). \quad (19)$$

Equation (16) can be considered as a generalization of the Landauer formula, extended to include the effect of a time-dependent potential, in the adiabatic approximation. The new ingredient is the quantity $U_{\alpha n,\beta m}$, Eq. (17). This quantity can be expressed in terms of the temporal derivative of the scattering potential,

$$U_{\beta m,\alpha n}=\int d\mathbf{r}\Big(-\frac{\partial\chi^t_{\beta m}(\mathbf{r})}{\partial E}\Big)\dot{V}(\mathbf{r},t)\chi^t_{\alpha n}(\mathbf{r}). \quad (20)$$

To prove this, we take the temporal derivative of Eq. (10), and use Eq. (8), to obtain

$$\dot{\chi}^t_{\alpha n}(\mathbf{r})=\int d\mathbf{r}'\,G^t(E;\mathbf{r},\mathbf{r}')\dot{V}(\mathbf{r}',t)\chi^t_{\alpha n}(\mathbf{r}'). \quad (21)$$

We insert this expression into Eq. (17), and carry out one of the spatial integrations using

$$\int d\mathbf{r}'\,G^t(E;\mathbf{r},\mathbf{r}')\chi^t_{\alpha n}(\mathbf{r}')=-\frac{\partial\chi^t_{\alpha n}(\mathbf{r})}{\partial E}, \quad (22)$$

which follows directly by differentiating Eq. (10) with respect to the energy, and using Eq. (8) and the symmetry of the Green function $G^t(E;\mathbf{r},\mathbf{r}')=G^t(E;\mathbf{r}',\mathbf{r})$. This produces the result (20).

III. THE TWO-TERMINAL SYSTEM

Let us now confine ourselves to a nanostructure connected to two terminals, with left (l) and right (r) leads. Then we can use Eq. (16) to write the current entering the system from the left terminal in the form

$$I_l(t)=e\int\frac{dE}{2\pi}\sum_{nm}[(f_l(E)-f_r(E))[|S^t_{rm,ln}|^2 +\Re(S^t_{lm,ln}U^*_{lm,ln}-S^t_{lm,rn}U^*_{lm,rn})]+(f_l(E)+f_r(E)) \times\Re(S^t_{lm,ln}U^*_{lm,ln}+S^t_{lm,rn}U^*_{lm,rn})]. \tag{23}$$

An analogous expression holds for $I_r(t)$. The net, average current flowing in the system during a single period of the modulating potential then consists of two parts,

$$I=\oint\frac{dt}{\tau}(I_l(t)-I_r(t))=I_{\rm bias}+I_{\rm pump}, \tag{24}$$

where the first, $I_{\rm bias}$, flows only when the system is biased, whereas the second, $I_{\rm pump}$, is established by the time-dependent potential (though it is affected by the chemical-potential difference, when the latter is applied). Using Eqs. (19) and (20), the pumped current, $I_{\rm pump}$, takes the form

$$I_{\rm pump}=e\oint\frac{dt}{\tau}\int\frac{dE}{2\pi}(f_l(E)+f_r(E)) \times\frac{1}{2}\sum_m\left[-\frac{\partial}{\partial E}(\langle\chi^t_{lm}|\dot V|\chi^t_{lm}\rangle-\langle\chi^t_{rm}|\dot V|\chi^t_{rm}\rangle)\right]. \tag{25}$$

For the biased current we find

$$I_{\rm bias}=e\oint\frac{dt}{\tau}\int\frac{dE}{2\pi}(f_l(E)-f_r(E))\sum_{nm}[2|S^t_{rm,ln}|^2 +\Re(S^t_{lm,ln}U^*_{lm,ln}-S^t_{lm,rn}U^*_{lm,rn}-S^t_{rm,ln}U^*_{rm,ln} +S^t_{rm,rn}U^*_{rm,rn})]. \tag{26}$$

The pumped part of the current, $I_{\rm pump}$, can be written in terms of the temporal derivatives of the instantaneous scattering matrix. In order to vindicate this statement, we start from the asymptotic form for $\chi^t_{\alpha n}$, Eq. (15), for the wave going from lead α into lead β. Noting that

$$w^-_{\alpha n}(\mathbf{r}\to\infty,\beta)=w^-_{\alpha n}\delta_{\alpha\beta}+(1-\delta_{\alpha\beta})\sum_m w^+_{\beta m}, \tag{27}$$

we conclude that

$$S^t_{\beta m,\alpha n}=1-\delta_{\alpha\beta}-i\int d\mathbf{r}\chi^t_{\beta m}(\mathbf{r})V(\mathbf{r},t)w^-_{\alpha n}(\mathbf{r}). \tag{28}$$

Differentiating this expression with respect to time and using Eqs. (9) and (21) yields

$$i\dot S^t_{\beta m,\alpha n}=\int d\mathbf{r}\chi^t_{\beta m}(\mathbf{r})\dot V(\mathbf{r},t)\chi^t_{\alpha n}(\mathbf{r}). \tag{29}$$

Note that this expression is *not* a matrix element. To turn it into an expression involving matrix elements, we use Eq. (19), by which

$$i\dot S^t_{\beta m,\alpha n}=\int d\mathbf{r}\dot V(\mathbf{r},t)\chi^t_{\beta m}(\mathbf{r})\sum_{\beta' m'}S^t_{\beta' m',\alpha n}\chi^{t*}_{\beta' m'}(\mathbf{r}). \tag{30}$$

Then, multiplying by $S^{t*}_{\beta m,\alpha n}$ and summing over α and n yields

$$\sum_{\alpha n}\dot S^t_{\beta m,\alpha n}S^{t*}_{\beta m,\alpha n}=-i\int d\mathbf{r}\chi^{t*}_{\beta m}(\mathbf{r})\dot V(\mathbf{r},t)\chi^t_{\beta m}(\mathbf{r}). \tag{31}$$

One notes that this identity makes the expression for $I_{\rm pump}$, Eq. (25) above, to be identical with the Brouwer[3] formula, in the case where the system is unbiased.

In the simplest case where each of the leads is a single-channel one, the expression for the current takes a particularly simple form. In this situation, the instantaneous scattering matrix becomes a 2×2 matrix, which can be parametrized (in the absence of a magnetic field) as

$$S^t=e^{i\psi^t}\begin{bmatrix}\sqrt{R^t}e^{i\alpha^t} & i\sqrt{T^t}\\ i\sqrt{T^t} & \sqrt{R^t}e^{-i\alpha^t}\end{bmatrix}. \tag{32}$$

Here, T^t and R^t are the instantaneous transmission and reflection, respectively. The reflection phase α^t describes the asymmetry of the nanostructure. A finite time-dependent reflection phase is a necessary ingredient to obtain the pumped current. Finally, ψ^t is the transmission (Friedel) phase. With the parametrization, Eq. (32), one finds, using Eqs. (29) and (31),

$$I=\frac{e}{2\pi}\oint\frac{dt}{\tau}\int dE\Bigg\{(f_l(E)-f_r(E))\Bigg[2T^t -\frac{1}{2}\left(\frac{\partial}{\partial E}\left((R^t-T^t)\frac{d\psi^t}{dt}\right)+\frac{d}{dt}\left((R^t-T^t)\frac{\partial\psi^t}{\partial E}\right)\right)\Bigg] +(f_l(E)+f_r(E))\frac{\partial}{\partial E}\left(R^t\frac{d\alpha^t}{dt}\right)\Bigg\}. \tag{33}$$

The charge passing through the nanostructure during a single period of the potential, Q, is then

$$Q=Q_{\rm bias}+Q_{\rm pump}. \tag{34}$$

Here,

$$Q_{\rm bias}=\frac{e}{2\pi}\oint dt\int dE\Bigg[(f_l(E)-f_r(E))2T^t +\frac{\partial}{\partial E}(f_l(E)-f_r(E))T^t\frac{d\psi^t}{dt}\Bigg]. \tag{35}$$

It is seen that the first term here is just the Landauer formula, with the transmission coefficient averaged over the temporal period. The second term forms a correction to this result, brought about by the modulating potential. The pumped charge is given by

$$Q_{\mathrm{pump}}=-\frac{e}{2\pi}\oint dt\int dE\,\frac{\partial}{\partial E}(f_l(E)+f_r(E))R^t\frac{d\alpha^t}{dt} \tag{36}$$

(see Ref. 6), and it vanishes unless α^t is time dependent.

A. Example—the single-level quantum dot

It is seen that both Q_{pump} and the second term of Q_{bias} are determined by the temporal dependence of the phases, α^t and ψ^t, of the scattering matrix. Clearly, a comparison between these two quantities is called for. Consider for simplicity zero temperature. Then, Q_{pump} is given by the values of $R^t d\alpha^t/dt$ at $E=E_F\pm\delta\mu/e$, where $\delta\mu$ is the chemical-potential difference, and E_F denotes the Fermi level. On the other hand, the second term in Q_{bias} is given by $\sim\int dE[-(\delta\mu/e)(\partial^2 f/\partial E^2)T^t(d\psi^t/dt)]$, and hence should be much smaller than the Landauer contribution. Nevertheless, it may be of interest to explore this term experimentally, as it is related to the Friedel phase of the nanostructure.

To further explore this point, we consider the following simple example: a quantum dot, with a single localized level, coupled to two ideal 1D leads.[27] Adopting the tight-binding description, we model the two leads connecting the quantum dot to the electronic reservoirs by a 1D chains of sites, whose on-site energies are assumed to vanish, and whose nearest-neighbor transfer amplitudes are denoted by $-J$. Thus the energy of an electron of wave vector k moving on such a chain is

$$E_k=-2J\cos ka, \tag{37}$$

where a is the lattice constant. The localized level, of energy ϵ_0, is attached to the left-hand-side lead with matrix element $-J_l$, and to the right-hand-side lead with matrix element $-J_r$. The latter two quantities are assumed to vary slowly in time, in a periodic way. Our formalism requires just the knowledge of the instantaneous scattering matrix of the system. For the case at hand,

$$S^t=\begin{bmatrix} -1+\left(\frac{J_l}{J}\right)^2 M_k & \frac{J_lJ_r}{J}M_k \\ \frac{J_lJ_r}{J}M_k & -1+\left(\frac{J_r}{J}\right)^2 M_k \end{bmatrix}, \tag{38}$$

with

$$M_k=\frac{2iJ\sin ka}{E_k-\epsilon_0+e^{ika}(J_l^2+J_r^2)/J}. \tag{39}$$

Let us consider first the pumped charge. At zero temperature, it is given by

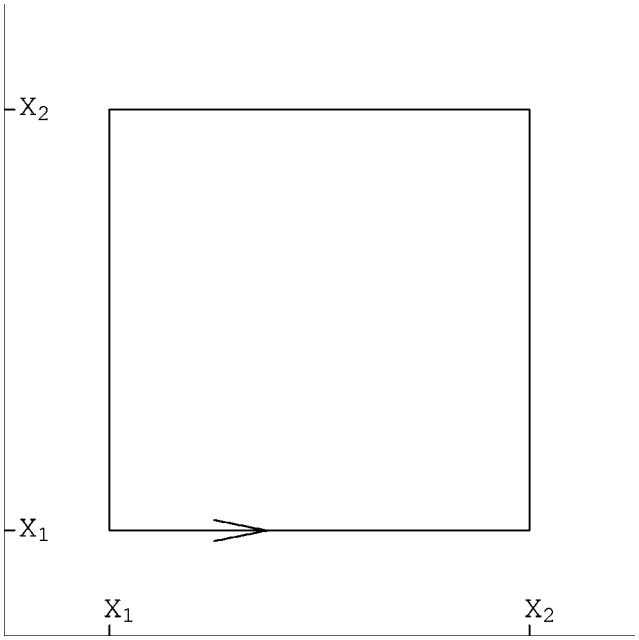

FIG. 1. The periodic temporal evolution of the parameters X_l and X_r in the parameter plane.

$$\begin{aligned} Q_{\mathrm{pump}}&=\frac{e}{2\pi}\oint dtR^t\frac{d\alpha^t}{dt} \\ &=\frac{e}{2\pi}\oint dt\frac{\sin ka}{|E_k-\epsilon_0+e^{ika}(X_l+X_r)|^2} \\ &\quad\times[(\dot X_l-\dot X_r)(\epsilon_0-E_k)+E_k(X_r\dot X_l-X_l\dot X_r)], \end{aligned} \tag{40}$$

in which energies are measure in units of J, and

$$X_l\equiv\left(\frac{J_l}{J}\right)^2,\quad X_r\equiv\left(\frac{J_r}{J}\right)^2 \tag{41}$$

are the time-dependent parameters of the system. Note that these two parameters can be thought of as the ''contact conductances'' of the quantum dot. Now imagine those to vary in time as follows: Initially, both are equal to X_1. Then X_l is increased linearly in time until it reaches the value X_2, while X_r is being held fixed at the value X_1. From that point, X_l is held fixed, while X_r increases linearly to the value X_2, and so on, see Fig. 1.

It is quite straightforward to find Q_{pump} for such a cycle. One obtains

$$Q_{\mathrm{pump}}=\frac{e}{\pi}\int_{X_1}^{X_2}dX(F(X;X_1)-F(X;X_2)), \tag{42}$$

with

$$F(X;Z)=\frac{\sin ka(\epsilon_0-E_k+E_kZ)}{|E_k-\epsilon_0+e^{ika}(X+Z)|^2}. \tag{43}$$

The resulting charge differs significantly from zero, and approaches unity (in units of e) as long as the line of maximal

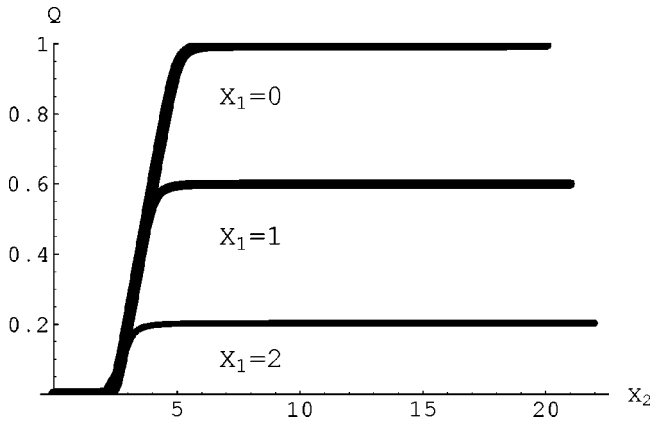

FIG. 2. The pumped charge (in units of e) as function of X_2, for several values of X_1, indicated on the figure. Here $ka=\pi-0.1$, and $\epsilon_0=-3J$.

transmission in the X_l-X_r plane is well within the closed orbit forming the period.[9] In the present model, that line is given by

$$X_l+X_r=2\frac{E_k-\epsilon_0}{E_k}. \tag{44}$$

We will elaborate on this point, which is exemplified in Fig. 2, in a future publication.[28] For the parameters used to produce the results shown in Fig. 2, the maximal transmission line is contained within the pumping contour when $X_1=0$ (see Fig. 1), while for higher X_1 values the pumping contour shifts away from the maximal transmission line.

Let us next consider the time average that appears in the second term of the biased current, i.e., $\oint T^t d\psi^t/dt$. In our example, this quantity becomes

$$\oint dt T^t \frac{d\psi^t}{dt} = -\oint dt \frac{4\sin^3 ka(E_k-\epsilon_0)X_lX_r(\dot{X}_l+\dot{X}_r)}{|E_k-\epsilon_0+e^{ika}(X_l+X_r)|^4}. \tag{45}$$

On a symmetric periodic curve like that presented in Fig. 1 this integral vanishes. Hence, in such a symmetric configuration, there will be no deviation from the Landauer formula due to the temporal variation of the Friedel phase. One may conclude from this example that when the pumping orbit in the plane of the time-dependent parameters is not as simple as the one considered above, there might be a small correction, related to the asymmetry of the orbit.

IV. CONCLUDING REMARKS

The motivation for this work is mainly to examine the validity of the adiabatic approximation in calculating the charge pumped quantum mechanically through a confined system of noninteracting electrons, and to study the effects of a constant bias. To this end, we have derived the time-dependent current generated when the system is subject to a slowly changing modulating potential, in addition to being connected to reservoirs of different chemical potentials. Our result is obtained as an expansion in the temporal derivatives of the modulating potential (and the ensuing temporal derivatives of the instantaneous scattering solutions). In the process, we have obtained an alternative expression for the pumped charge, Eq. (1), which gives it in terms of matrix elements of the temporal derivative of the potential between the instantaneous scattering states. It reproduces the widely used Brouwer formula which gives the pumped charge in terms of the instantaneous scattering matrix in the lowest order of the adiabatic approximation. We have derived and analyzed the effects of the modulating potential on the biased current, and showed them to be quite small.

Our formalism allows for the possibility to systematically obtain the corrections to the lowest-order adiabatic approximation. The result, Eq. (A12), shows that the strength of the modulating potential V cannot be arbitrarily strong: The second-order contribution to the current contains an ''extra'' factor of $\dot{V}$ [as can be seen by using Eq. (A10) in Eq. (A12)] as compared to the first-order contribution. The exact validity of the adiabatic approximation thus depends in a delicate way on, e.g., the value of $\dot{G}^t$, or $\ddot{V}G^t/\dot{V}$. We hope to pursue this point quantitatively in a future publication.

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APPENDIX: CORRECTIONS TO THE ADIABATIC APPROXIMATION

The results presented above have been obtained in the adiabatic approximation, in which only first derivatives with respect to time are kept. As stated above, this means that in the iterative solution of Eq. (7) only the first iteration has been maintained. Here we discuss the contribution of the next iteration. For the sake of simplicity, we carry out this calculation for an unbiased system with two single-channel leads.

To second order in the temporal derivative, the scattering solution can be presented in the form

$$\chi(\mathbf{r},t)=\chi^t(\mathbf{r})-i\int d\mathbf{r}' G^t(E;\mathbf{r},\mathbf{r}')(\dot{\chi}^t_\alpha(\mathbf{r}')+\Delta\dot{\chi}^t_\alpha(\mathbf{r}')), \tag{A1}$$

with

$$\Delta\dot{\chi}^t_\alpha(\mathbf{r}')=-i\int d\mathbf{r}''\frac{d}{dt}(G^t(E;\mathbf{r}',\mathbf{r}'')\dot{\chi}^t_\alpha(\mathbf{r}'')). \tag{A2}$$

It follows that the quantity U, Eq. (17), is now modified into

$$\tilde{U}_{\beta\alpha}=U_{\beta\alpha}+\Delta U_{\beta\alpha},$$

$$U_{\beta\alpha}=\int d\mathbf{r}\chi^t_\beta(\mathbf{r})\dot{\chi}^t_\alpha(\mathbf{r}),$$

$$\Delta U_{\beta\alpha}=\int d\mathbf{r}\chi^t_\beta(\mathbf{r})\Delta\dot{\chi}^t_\alpha(\mathbf{r}). \tag{A3}$$

As a result, we find that the current entering lead β consists of two parts, the leading order in the adiabatic approximation, I_β, which has been discussed above, and a correction, ΔI_β. Explicitly,

$$\tilde{I}_\beta(t)=I_\beta(t)+\Delta I_\beta(t),$$

$$I_\beta(t)=e\int\frac{dE}{2\pi}\sum_\alpha f_\alpha(E)[\delta_{\alpha\beta}-|S^t_{\beta\alpha}|^2+2\,\Re(S^{t*}_{\beta\alpha}U_{\beta\alpha})],$$

$$\Delta I_\beta(t)=e\int\frac{dE}{2\pi}\sum_\alpha f_\alpha(E)[-|U_{\beta\alpha}|^2+2\,\Re(S^{t*}_{\beta\alpha}\Delta U_{\beta\alpha})]. \tag{A4}$$

Let us first verify that the correction ΔI_β obeys charge conservation over the entire period. To this end, we sum ΔI_β over β. Using Eq. (19), we have

$$\sum_\beta[|U_{\beta\alpha}|^2-2\,\Re(S^{t*}_{\beta\alpha}\Delta U_{\beta\alpha})]$$
$$=\int d\mathbf{r}\int d\mathbf{r}'\Bigg[\sum_\beta\chi^t_\beta(\mathbf{r})\dot{\chi}^t_\alpha(\mathbf{r})\chi^{t*}_\beta(\mathbf{r}')\dot{\chi}^{t*}_\alpha(\mathbf{r}')$$
$$-2\,\Im\left(\chi^{t*}_\alpha(\mathbf{r})\frac{d}{dt}G^t(E;\mathbf{r},\mathbf{r}')\dot{\chi}^t_\alpha(\mathbf{r}')\right)\Bigg]. \tag{A5}$$

We can now employ the fact that the current should be conserved upon integrating over the entire period, that is, when expression (A5) is inserted into $\oint dt$. Then we may integrate the second term by parts. Consequently, using the relation[24]

$$\sum_\alpha\chi^t_\alpha(\mathbf{r})\chi^{t*}_\alpha(\mathbf{r}')=-2\,\Im\,G^t(E;\mathbf{r},\mathbf{r}'), \tag{A6}$$

the two terms in Eq. (A5) exactly cancel one another.

Let us now turn to the expression for the correction ΔI_β, Eq. (A4), and insert the condition in which the system is unbiased, i.e., $f_\alpha(E)=f(E)$. Then, using Eqs. (19), (21), (22), and (A6), we find

$$\sum_\alpha|U_{\beta\alpha}|^2=-2\int d\mathbf{r}\int d\mathbf{r}'\left(\frac{\partial\chi^t_\beta(\mathbf{r})}{\partial E}\right)\dot{V}(\mathbf{r},t)$$
$$\times\Im(G^t(E;\mathbf{r},\mathbf{r}'))\dot{V}(\mathbf{r}',t)\left(\frac{\partial\chi^{t*}_\beta(\mathbf{r}')}{\partial E}\right), \tag{A7}$$

and

$$2\,\Re\sum_\alpha S^{t*}_{\beta\alpha}\Delta U_{\beta\alpha}=2\,\Im\int d\mathbf{r}\int d\mathbf{r}'\Bigg[\left(\frac{\partial\chi^t_\beta(\mathbf{r})}{\partial E}\right)\dot{V}(\mathbf{r},t)$$
$$\times\left(\frac{\partial G^t(E;\mathbf{r},\mathbf{r}')}{\partial E}\right)\dot{V}(\mathbf{r}',t)\chi^{t*}_\beta(\mathbf{r}')$$
$$+\left(\frac{\partial^2\chi^t_\beta(\mathbf{r})}{\partial E^2}\right)\dot{V}(\mathbf{r},t)G^t(E;\mathbf{r},\mathbf{r}')$$
$$\times\dot{V}(\mathbf{r}',t)\chi^{t*}_\beta(\mathbf{r}')\Bigg]$$
$$+\Im\int d\mathbf{r}\left(\frac{\partial^2\chi^t_\beta(\mathbf{r})}{\partial E^2}\right)\ddot{V}(\mathbf{r},t)\chi^{t*}_\beta(\mathbf{r}). \tag{A8}$$

To obtain the last equality, we have made use of the relations

$$\frac{\partial^2\chi^t_\beta(\mathbf{r})}{\partial E^2}=-2\int d\mathbf{r}'\left(\frac{\partial\chi^t_\beta(\mathbf{r}')}{\partial E}\right)G^t(E;\mathbf{r}',\mathbf{r}), \tag{A9}$$

and

$$\dot{G}^t(E;\mathbf{r},\mathbf{r}')=\int d\mathbf{r}_1G^t(E;\mathbf{r},\mathbf{r}_1)\dot{V}(\mathbf{r}_1,t)G^t(E;\mathbf{r}_1,\mathbf{r}'). \tag{A10}$$

Both relations are obtained by taking derivatives of Eqs. (8) and (10) with respect to the energy and the time.

Collecting all these terms, we obtain

$$\Delta I_\beta(t)=\frac{-e}{\pi}\int dEf(E)\Im\frac{\partial}{\partial E}\langle\chi^t_\beta|\dot{V}(t)\dot{G}^t(E)$$
$$+\tfrac{1}{2}\ddot{V}(t)G^t(E)|\chi^t_\beta\rangle. \tag{A11}$$

It is satisfactory to note that, again (upon integrating by parts with respect to the energy), the energy integral includes the derivative of the Fermi function. Hence, up to the second order in the adiabatic approximation, we find

$$\tilde{I}_\beta(t)=\frac{e}{2\pi}\int dE\left(\frac{\partial f(E)}{\partial eE}\right)[\langle\chi^t_\beta|\dot{V}|\chi^t_\beta\rangle+\Im(\langle\chi^t_\beta|2\dot{V}(t)\dot{G}^t(E)$$
$$+\ddot{V}(t)G^t(E)|\chi^t_\beta\rangle)]. \tag{A12}$$

To estimate the relative magnitude of the correction (the second term above) compared to the leading-order one (the first term there), consider first the part including the second derivative of the potential. Using Eq. (22), this part becomes

$$\int d\mathbf{r}\chi^{t*}_\beta(\mathbf{r})\ddot{V}(\mathbf{r},t)\left(-\frac{\partial\chi^t_\beta(\mathbf{r})}{\partial E}\right). \tag{A13}$$

It follows that this correction will be smaller than the leading-order term by a factor proportional to $1/\tau$, due to the extra temporal derivative, multiplied by the energy derivative

of the instantaneous scattering state. The latter will include the energy derivatives of the instantaneous transmission and reflection amplitudes (which appear in χ^t), and possibly a term proportional to the 1D density of states, i.e., the velocity (coming, e.g., from the factors e^{ika} which appear in χ^t of our simple example discussed in Sec. III). We may conclude that as long as the energy derivative of the instantaneous scattering solution is small on the scale of $\omega \propto 1/\tau$, this correction will be small. The other second-order correction term in Eq. (A12) has the factor $\dot{G}^t$ as compared to the leading first order. This term [cf. Eq. (A10)] has an extra factor of $\dot{V}$, and hence its smallness hinges on the smallness of the potential amplitude. Thus, the validity regime of the expression (1) is restricted for small enough potential amplitudes.

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