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Steady-state transport in mesoscopic systems illuminated by alternating fields

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In this paper we present a Landauer-type expression for the time-averaged dc current in a mesoscopic device illuminated by a coherent ac field, assuming phase-breaking processes to be restricted to the contacts. This expression is derived starting from the nonequilibrium Green-function formalism which rigorously accounts for the exclusion principle. However, the $(1-f)$ factors that are often assumed do not appear in our expression. This does not affect the result if the transmission is reciprocal. But for traveling-wave fields the transmission is nonreciprocal even in zero magnetic fields and the magnitude of the resulting current is affected by the presence or absence of the $(1-f)$ factor.

We consider a two-terminal device illuminated by an arbitrary time-varying potential $V(\mathbf{r},t)$ (Fig. 1). The two terminals are connected to large contacts that are assumed to remain in local equilibrium with electrochemical potentials μ_1 and μ_2, respectively. The time-varying potential is assumed to be zero in the contacts. The subject of this paper is the dc current that flows (not the time-varying current) in the external circuit in response to the potential $V(\mathbf{r},t)$. We wish to find an expression for this *time-averaged dc current* I in terms of μ_1 and μ_2. This problem is relevant to a number of interesting experiments such as the mesoscopic photovoltaic effect,[1,2,3(a)] photocurrent in scanning tunnel microscope,[4] optical rectification,[5] and the proposed "Pauli pump."[3(b),6]

We assume that phase-breaking processes occur only in the contacts and not within the device, as is commonly assumed in the Landauer-Büttiker formalism. Indeed, if the potential V were independent of time, then the current-voltage relation is well known:[7–9]

$$I=\frac{e}{h}\int dE\,T(E)[f_1(E)-f_2(E)]\,. \qquad (1)$$

Here $f_1(E)$ and $f_2(E)$ represent the Fermi-Dirac functions with potentials μ_1 and μ_2, respectively. $T(E)$ is the total transmission at energy E summed over all possible input and output modes. In the linear-response regime, Eq. (1) reduces to the well-known Landauer formula.

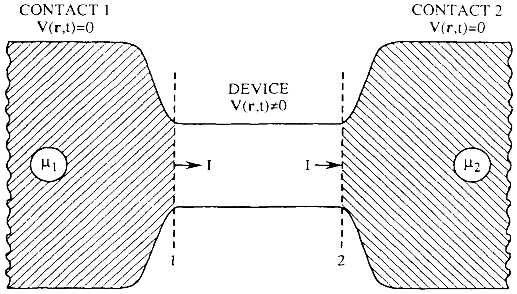

FIG. 1. Schematic representation of a two-terminal mesoscopic device with an arbitrary potential $V(\mathbf{r},t)$. Phase-breaking processes are assumed to occur only in the contacts.

If we generalize Eq. (1) to include time-varying potentials $V(\mathbf{r},t)$, we are faced with two choices for the time-averaged dc current:

$$I=\frac{e}{h}\int dE\int dE'\{t_{21}(E,E')f_1(E')[1-f_2(E)] - t_{12}(E',E)f_2(E)[1-f_1(E')]\}\,, \qquad (2)$$

$$I=\frac{e}{h}\int dE\int dE'[t_{21}(E,E')f_1(E')-t_{12}(E',E)f_2(E)]\,. \qquad (3)$$

Here $t_{21}(E,E')$ represents the total transmission summed over all input modes at energy E' (in terminal 1) and all output modes at energy E (in terminal 2). If $t_{21}(E,E')$ is equal to $t_{12}(E',E)$ then the two possibilities [Eqs. (2) and (3)] are equivalent. But this is not true in general.

Equation (2), which is used in Ref. 3(b), is based on the view that an electron makes transitions from an occupied state in one reservoir into an empty state in the other reservoir. But if only coherent processes (elastic or inelastic) occur within the device, then one can define orthogonal "scattering states"[10] for the entire structure composed of incident, reflected, and transmitted waves. Each such scattering state is populated according to the distribution function f at the incident port. From this point of view coherent inelastic processes are much like elastic processes and there is no reason to include factors of the form $(1-f)$.[11] This argument cannot be used for incoherent inelastic processes,[12–14] since one cannot define a wave function over the entire structure.

Starting from the nonequilibrium Green-function formalism,[15,16] which rigorously accounts for the exclusion principle, we obtain *Eq. (3) rather than Eq. (2).* The derivation is outlined at the end of this paper. (For simplicity we neglect magnetic fields in this paper though the approach can be extended to nonzero fields as well.) We obtain the following expression for transmission:

$$t_{21}(E,E')=\Delta E\int_{\mathbf{r}\in\text{contact "2"}} d\mathbf{r}\int_{\mathbf{r}'\in\text{contact "1"}} d\mathbf{r}'\,\frac{|G^R(\mathbf{r},E;\mathbf{r}',E')|^2}{4\pi^2\tau_\phi(\mathbf{r},E)\tau_\phi(\mathbf{r}',E')} \qquad (4)$$

where $\tau_\phi(\mathbf{r},E)$ is the phase-breaking time which is infinite everywhere except in the contacts. ΔE can be interpreted as the energy spread of individual wave packets or as $\hbar/T$ where T is the time window over which the current is averaged. It cancels out the δ functions in energy that arise in actual calculations. The Green function G^R is computed from a Schrödinger-like equation

$$\left[E+\frac{\hbar^2\nabla^2}{2m}-V_S(\mathbf{r})+\frac{i\hbar}{2\tau_\phi(\mathbf{r},E)}\right]G^R(\mathbf{r},E;\mathbf{r}',E') =\delta(\mathbf{r}-\mathbf{r}')\delta(E-E')+\sum_\omega V(\mathbf{r},\hbar\omega)G^R(\mathbf{r},E-\hbar\omega;\mathbf{r}',E') \quad (5)$$

where $V_S(\mathbf{r})$ is the static potential in the device and

$$V(\mathbf{r},t)=\sum_\omega V(\mathbf{r},\hbar\omega)e^{-i\omega t}. \quad (6)$$

Note that ω runs over both positive and negative values —positive components cause absorption while negative components cause emission. Since the potential $V(\mathbf{r},t)$ is real, $V(\mathbf{r},\hbar\omega)=V(\mathbf{r},-\hbar\omega)^*$.

The above result is an extension of our earlier work[14] to include coherent ac fields (dephasing processes inside the device, however, are neglected in this paper). It may seem surprising that the phase-breaking time τ_ϕ in the contacts enters the expression [Eq. (4)] for the transmission. However, as discussed in Ref. 14 the imaginary potential $i\hbar/2\tau_\phi$ in Eq. (5) causes the Green function G^R to damp out exponentially inside the contacts. Neglecting any reflection at the device-contact interfaces we can write in one dimension

$$|G^R(z,E;z',E')|^2\simeq|G^R(z_2,E;z_1,E')|^2\exp[-|z-z_2|/v_2(E)\tau_\phi(E)]\exp[-|z'-z_1|/v_1(E')\tau_\phi(E')] \quad (7)$$

where $v(E)$ is the velocity, $z\in$ contact "2," $z'\in$ contact "1," and z_1,z_2 are located right at the device-contact (1,2) interfaces. Using Eq. (7) we can simplify Eq. (4) to a form similar to the formula due to Fisher and Lee,[17]

$$t_{21}(E,E')=\frac{\hbar^2v_2(E)v_1(E')}{4\pi^2}|G^R(z_2,E;z_1,E')|^2\Delta E. \quad (8)$$

Thus, the transmission $t_{21}(E,E')$ is nearly independent of the phase-breaking time τ_ϕ inside the contacts. This result can easily be extended to include multiple modes.

RECIPROCITY

We can solve Eq. (5) iteratively to express G^R in the form of a Born series:

$$G^R(\mathbf{r},E,\mathbf{r}',E')=G_0^R(\mathbf{r},\mathbf{r}';E)\delta(E-E')+\sum_\omega\int d\mathbf{r}_1\,G_0^R(\mathbf{r},\mathbf{r}_1;E)V(\mathbf{r}_1,\hbar\omega)G_0^R(\mathbf{r}_1,\mathbf{r}';E')\delta(E-\hbar\omega-E')+\cdots \quad (9)$$

where G_0^R is the unperturbed Green function obtained by solving Eq. (5) with $V(\mathbf{r},\hbar\omega)$ set equal to zero. The unperturbed Green function G_0^R obeys reciprocity. From Eq. (9) it can be shown that the perturbed Green function G^R also obeys reciprocity $G^R(\mathbf{r},E;\mathbf{r}',E')=G^R(\mathbf{r}',E';\mathbf{r},E)$ *provided* $V(\mathbf{r},\hbar\omega)=V(\mathbf{r},-\hbar\omega)$. This condition is satisfied by standing-wave potentials of form $V(\mathbf{r},t)=v(\mathbf{r})\cos\omega t$ but not by traveling-wave potentials of the form $V(\mathbf{r},t)=\cos(\omega t-\mathbf{q}\cdot\mathbf{r})$.[18] We can thus distinguish between two categories of ac fields. For the *standing-wave–type*, transmission is reciprocal: $t_{21}(E,E')=t_{12}(E',E)$, while the *traveling-wave–type* transmission is nonreciprocal: $t_{21}(E,E')\neq t_{12}(E',E)$. In the former case the presence or absence of the factor $(1-f)$ makes no difference, so that our results are in complete agreement with Ref. 3(a). But in the latter case the magnitude of the current can be very different if we use Eq. (3) [rather than Eq. (2) which is used in Ref. 3(b)].

SHORT-CIRCUIT (ZERO-BIAS) CURRENT

Using Eq. (3) we write the short-circuit current as $(f_1(E)=f_2(E)\equiv f_0(E))$,

$$I_{sc}=\int dE'f_0(E')\int dE[t_{21}(E,E')-t_{12}(E,E')]. \quad (10)$$

We will now discuss a few simple examples illustrating the conditions that lead to a nonzero short-circuit current. For simplicity, we restrict our attention to low temperatures such that only energies $E'<E_F$ contribute to the current in Eq. (10). For a perfectly symmetric device with uniform illumination $[V(z,t)\sim V_0\cos\omega t]$, we expect that $t_{21}(E,E')=t_{12}(E,E')$, since there is no way to distinguish between terminals 1 and 2. Consequently, $I_{sc}=0$. But the zero-bias current can be nonzero if (a) the device is asymmetric and/or (b) the illumination is asymmetric. This is illustrated by the two examples in Fig. 2. In both examples, $t_{12}(E,E')=0$ for $E'<E_F$. In Fig. 2(a) this is because there are no states below E_F near contact 2 while in Fig. 2(b) the reason is that there is no illumination near contact 2. In either case electrons flow from contact 1 to contact 2.

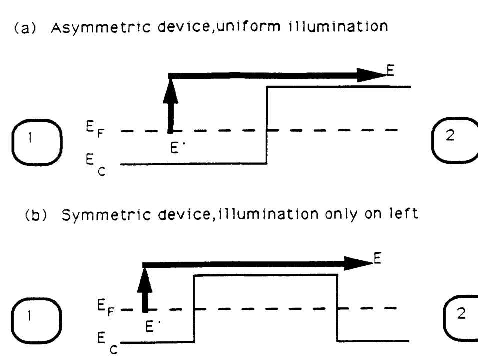

FIG. 2. Two simple examples where a nonzero short-circuit current flows from contact 1 to contact 2.

Finally, we consider a uniform quantum wire with a traveling-wave illumination $[V=V_0\cos(\omega t-qz)]$. In this case also there will be a short-circuit current which will normally be small if $\hbar\omega, V_0 \ll E'$. But with strong illumination significant acoustoelectric current could arise in the direction of the traveling wave.[19]

DERIVATION OF EQS. (3) AND (4)

Finally, we will outline the derivation of Eqs. (3) and (4) from the nonequilibrium Green-function formalism. Our starting point is the Keldysh equation[14,20]

$$G^<(1,2)=\int d1'\,d2'\,G^R(1,1')\Sigma^<(1',2')G^A(2',2) \qquad (11)$$

where $1\equiv(\mathbf{r}_1,t_1)$, $1'\equiv(\mathbf{r}_1',t_1')$, $2\equiv(\mathbf{r}_2,t_2)$, $2'\equiv(\mathbf{r}_2',t_2')$. The retarded Green function is obtained from $[H_0\equiv-\hbar^2\nabla^2/2m+V_S(\mathbf{r})+V(\mathbf{r},t)]$

$$\left[i\hbar\frac{\partial}{\partial t_1}-H_0(1)\right]G^R(1,2)-\int d3\,\Sigma^R(1,3)G^R(3,2)=\delta(1-2)\,. \qquad (12)$$

The current density is given by

$$\mathbf{J}(\mathbf{r}_1,t_1)=-\frac{e\hbar^2}{2m}(\nabla_1-\nabla_2)G^<(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)\Big|_{(r_2,t_2)\to(r_1,t_1)}\,. \qquad (13)$$

Equation (13) contains both the ac and dc components of the current density. By time averaging we can remove the ac component of current which is, in general, nonzero in the presence of a time-dependent field. The dc current flowing at the terminals is obtained by time averaging the net current from contact 1 (see Fig. 1) over a long time T and can be written as

$$I=\int_{-T/2}^{+T/2}\frac{dt_1}{T}\int \mathbf{J}\cdot d\mathbf{S}_1\,,$$

where $\mathbf{S}_1\in$ device-contact 1 interface. Using Eqs. (11) and (13) and the divergence theorem,[21]

$$I=\int_{-T/2}^{+T/2}\frac{dt_1}{T}\int d1'\int d2'\,\Sigma^<(1',2')\int_{\mathbf{r}_1\in\,\text{contact 1}} d\mathbf{r}_1\;\nabla_1\cdot\mathbf{J}_G \qquad (14)$$

where

$$\mathbf{J}_G=-\frac{e\hbar^2}{2m}\{[\nabla_1G^R(1,1')]G^A(2',1)-G^R(1,1')\times[\nabla_1G^A(2',1)]\}\,.$$

From Eqs. (12) and (14) we can write

$$I=-e\int_{-T/2}^{+T/2}\frac{dt_1}{T}\int_{\mathbf{r}_1\in\,\text{contact 1}} d\mathbf{r}_1\;Q(\mathbf{r}_1,t_1;\mathbf{r}_1,t_1) \qquad (15a)$$

where

$$Q=\Sigma^<G^A-G^R\Sigma^<+\Sigma^RG^R\Sigma^<G^A-G^R\Sigma^<G^A\Sigma^A \qquad (15b)$$

using matrix notation for compactness.[22]

We now make the assumption that incoherent processes are caused by point (local) inelastic scatterers. Defining

$$A(r_1,E_1;r_2,E_2)=\int dt_1\int dt_2\exp(iE_1t_1/\hbar)\exp(-iE_2t_2/\hbar)A(r_1,t_1;r_2,t_2)\,,$$

where A could be any of the G's or Σ's, Eq. (15a) can be rewritten as

$$I=\frac{-e}{T}\int_{r_1\in\,\text{contact 1}} d\mathbf{r}_1\int\frac{dE}{2\pi\hbar}\int\frac{dE'}{2\pi\hbar}\Big[(-2i)\Sigma^<(\mathbf{r}_1,E,E')\,\mathrm{Im}\,G^R(\mathbf{r}_1,E';\mathbf{r}_1,E)$$
$$+2i\,\mathrm{Im}\,\Sigma^R(\mathbf{r}_1,E,E')\int_{\mathbf{r}\in\,\text{all space}} d\mathbf{r}\int\frac{dE_1}{2\pi\hbar}\int\frac{dE_2}{2\pi\hbar}G^R(\mathbf{r}_1,E';\mathbf{r},E_1)\Sigma^<(\mathbf{r},E_1,E_2)G^A(\mathbf{r},E_2;\mathbf{r}_1,E)\Big]\,. \qquad (16)$$

Equation (16) is valid with point scatterers in both the device and contacts. We can simplify it further by assuming that phase-breaking processes occur only in the contacts. The contracts are assumed to be large reservoirs that remain in local equilibrium at all times despite the time-varying fields in the device. We can then write ($\mathbf{r}_1\in$ contact 1)

$$\mathrm{Im}\,\Sigma^R(\mathbf{r}_1,E,E')=\frac{-\hbar}{2\tau_\phi(\mathbf{r}_1E)}\delta(E-E')\,, \qquad (17a)$$

$$\Sigma^<(\mathbf{r}_1,E,E')=-2if_1(E)\,\mathrm{Im}\,\Sigma^R(\mathbf{r}_1,E,E')\,. \qquad (17b)$$

Equation (17a) follows from the assumption that $\Sigma^R(\mathbf{r}_1,t_1,t_2)$ depends only on (t_1-t_2) and not on (t_1+t_2) while Eq. (17b) follows from the assumption of local equilibrium. Then from Eqs. (16) and (17) we obtain

$$I=\frac{e}{T}\int_{\mathbf{r}_1\in\,\text{contact 1}} d\mathbf{r}_1\,\frac{dE_1}{2\pi}\,\frac{\hbar}{\tau_\phi(\mathbf{r}_1,E_1)}\left[(-2)f(\mathbf{r}_1,E_1)\,\mathrm{Im}\,G^R(\mathbf{r}_1,E_1;\mathbf{r}_1,E_1)-\int d\mathbf{r}\frac{dE}{2\pi}\frac{\hbar|G^R(\mathbf{r}_1,E_1;\mathbf{r},E)|^2}{\tau_\phi(\mathbf{r},E)}f(\mathbf{r},E)\right]. \qquad (18)$$

Equation (18) can be rewritten in the form

$$I=\frac{e}{T}\int_{\substack{\mathbf{r}_1\in\,\text{contact 1}\\ \mathbf{r}_2\in\,\text{contact 2}}} d\mathbf{r}_1\int dE_1\int d\mathbf{r}_2\int dE_2\left[\frac{\hbar^2|G^R(\mathbf{r}_2,E_2;\mathbf{r}_1,E_1)|^2}{4\pi^2\tau_\phi(\mathbf{r}_2,E_2)\tau_\phi(\mathbf{r}_1,E_1)}f_1(E_1)-\frac{\hbar^2|G^R(\mathbf{r}_1,E_1;\mathbf{r}_2,E_2)|^2}{4\pi^2\tau_\phi(\mathbf{r}_2,E_2)\tau_\phi(\mathbf{r}_1,E_1)}f_2(E_2)\right] \qquad (19)$$

making use of the following identity which can be proved using Eq. (5) [obtained from Eq. (12) by Fourier transformation and using Eq. (17)]

$$-\mathrm{Im}[G^R(\mathbf{r}_1,E_1;\mathbf{r}_1,E_1)] = \int d\mathbf{r}\int \frac{dE}{2\pi}\frac{\hbar|G^R(\mathbf{r},E;\mathbf{r}_1,E_1)|^2}{2\tau_\phi(\mathbf{r},E)} . \quad (20)$$

Equations (3) and (4) follow readily from Eq. (19) noting that $\Delta E = 2\pi\hbar/T$.

CONCLUDING REMARKS

Starting from the nonequilibrium Green-function formalism we have derived an expression for the time-averaged dc current through a mesoscopic device illuminated by ac fields, neglecting dephasing processes within the device. The $(1-f)$ factors that are often assumed do not appear in our result. This makes no difference for standing-wave fields (in zero magnetic field) since the transmission is reciprocal. But it can make a significant difference with traveling-wave fields when the transmission is nonreciprocal.

ACKNOWLEDGMENTS

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[21]Since the contact is assumed to be in equilibrium the current density is zero at any surface far from the device. Thus we can replace the integral over the surface S_1 by an integral over a closed surface enclosing contact 1.

[22]Note that we do not use Eq. (11) to replace $G^R\Sigma^< G^A$ by $G^<$ in Eq. (15b). The reason is that (Ref. 14) inside the contacts we impose a boundary condition on $G^<$ instead of solving Eq. (11) for it; consequently, Eq. (11) cannot be used inside the contact regions.