PHYSICAL REVIEW B VOLUME 58, NUMBER 16 15 OCTOBER 1998-II

Scattering approach to parametric pumping

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(Received 18 June 1998)

A dc current can be pumped through a quantum dot by periodically varying two independent parameters X_1 and X_2, like a gate voltage or magnetic field. We present a formula that relates the pumped current to the parametric derivatives of the scattering matrix $S(X_1,X_2)$ of the system. As an application we compute the statistical distribution of the pumped current in the case of a chaotic quantum dot. [S0163-1829(98)52240-0]

An electron pump is a device that generates a d.c. current between two electrodes that are kept at the same bias. In recent years, electron pumps consisting of small semiconductor quantum dots have received considerable experimental and theoretical attention.[1–11] A quantum dot is a small metal or semiconductor island, confined by gates, and connected to the outside world via point contacts. Several different mechanisms have been proposed to pump charge through such systems, ranging from a low-frequency modulation of gate voltages in combination with the Coulomb blockade[1,2,11] to photon-assisted transport at or near a resonance frequency of the dot.[5–8] Their applicability depends on the characteristic size of the system and the operation frequency.

Most experimental realizations of electron pumps in semiconductor quantum dots made use of the principle of Coulomb blockade. If the dot is coupled to the outside world via tunneling point contacts, the charge on the dot is quantized, and (apart from degeneracy points) transport is inhibited as a result of the high energy cost of adding an extra electron to the dot. Pothier *et al.* constructed an electron pump that operates at arbitrarily low frequency and with a reversible pumping direction.[2] The pump consists of two weakly coupled quantum dots in the Coulomb blockade regime and operates via a mechanism that closely resembles a peristaltic pump: Charge is pumped through the double dot array from the left to the right and electron-by-electron as the voltage $U_1 \propto \sin(\omega t)$ of the left dot reaches its minima and maxima before the voltage $U_2 \propto \sin(\omega t - \phi)$ of the right one.[2] The pumping direction can be reversed by reversing the phase difference ϕ of the two gate voltages.

A similar mechanism was proposed by Spivak, Zhou, and Beal Monod for an electron pump consisting of single quantum dot only.[4] In this case a d.c. current is generated by adiabatic variation of two different gate voltages that determine the shape of the nanostructure, or any other pair of parameters X_1 and X_2, like magnetic field or Fermi energy, that modify the (quantum mechanical) properties of the system, see Fig. 1(a). The magnitude of the current is proportional to the frequency ω with which X_1 and X_2 are varied and (for small variations) to the product of the amplitudes δX_1 and δX_2. The direction of the current depends on microscopic (quantum) properties of the system, and need not be known *a priori* from its macroscopic properties. As in the case of the double-dot Coulomb blockade electron pump of Ref. 2, the direction of the current in the single-dot parametric pump of Spivak *et al.*[4] can be reversed by reversing the phases of the parameters X_1 and X_2. An important difference between the two mechanisms is that a parametric electron pump like the one in Ref. 4 does not require that the quantum dot is in the regime of Coulomb blockade; it operates if the dot is open, i.e., well coupled to the leads by means of ballistic point contacts. Experimentally, an electron pump in an open quantum dot has been realized only very recently.[12] A measurement of the pumped current provides a promising tool to study properties of open mesoscopic systems at zero bias or at zero current.

In this paper we consider a parametric electron pump through an open system in a scattering approach. Our main result is a formula for the pumped current in terms of the scattering matrix $S(X_1,X_2)$. Such a formula is the analogue of the Landauer formula, which relates the conductance $G = \delta I/\delta V$ of a mesoscopic system with two contacts to a sum over the (squares of) matrix elements $S_{\alpha\beta}$,

$$\delta I = G\,\delta V = \frac{2e^2}{h}\,\delta V \sum_{\alpha\in 1}\sum_{\beta\in 2} |S_{\alpha\beta}|^2. \tag{1}$$

The indices α and β are summed over all channels in the left and right contacts, respectively, and δV is the applied voltage. For the case of the parametric electron pump, where two parameters X_1 and X_2 are varied periodically, $\delta X_1(t) = \delta X_1 \sin(\omega t)$ and $\delta X_2(t) = \delta X_2 \sin(\omega t - \phi)$, we find that the d.c. component of the current I depends on the *derivatives* $\partial S_{\alpha\beta}/\partial X$,

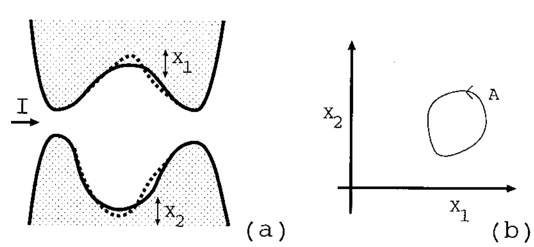

FIG. 1. (a) A quantum dot with two parameters X_1 and X_2 that describe a deformation of the shape of the quantum dot. As X_1 and X_2 are varied periodically, a dc current I is generated. (b) In one period, the parameters $X_1(t)$ and $X_2(t)$ follow a closed path in parameter space. The pumped current depends on the enclosed area A in (X_1,X_2) parameter space.

$$\delta I = \frac{\omega e \sin\phi\, \delta X_1 \delta X_2}{2\pi} \sum_{\alpha \in 1} \sum_{\beta} \mathrm{Im} \frac{\partial S^*_{\alpha\beta}}{\partial X_1} \frac{\partial S_{\alpha\beta}}{\partial X_2}. \qquad (2)$$

Like the Landauer formula, Eq. (2) is valid for a phase coherent system at zero temperature and to (bi)linear response in the amplitudes δX_1 and δX_2. [The nonlinear response is given by Eq. (8) below.] It captures both a classical contribution to the current and the quantum interference corrections. Quantum corrections can be important in the mesoscopic regime, especially if there is no ''classical'' mechanism that dominates the pumping process.[4,12] Equation (2) is valid to first order in the frequency ω. This is sufficient if the period $\tau = 2\pi/\omega$ is much larger than the time particles spend inside the quantum dot. For such low frequencies, we can assume that equilibrium is maintained throughout the pumping process. The scattering matrix formula does not capture effects of order ω^2 (or higher) that rely on the existence of a nonequilibrium distribution inside the quantum dot.[4] The existence of a scattering approach to parametric pumping allows us to borrow from the vast literature dealing with scattering matrices of disordered and chaotic microstructures and their parameter dependence,[13] and to directly relate the pumped current to other transport properties like, e.g., the conductance.

The system under consideration is shown schematically in Fig. 1(a). It consists of a quantum dot, coupled to two electron reservoirs by ballistic point contacts. The two electron reservoirs are held at the same voltage. Two external parameters $X_1(t)$ and $X_2(t)$ of the dot are varied periodically, see Fig. 1(a). They can be, e.g., the voltage of a plunger gate, parameters that characterize the shape, or a magnetic field. The two point contacts, which have N channels at the Fermi level E_F, are labeled 1 and 2. The scattering matrix S of the system has dimension $2N \times 2N$ and is a function of the parameters X_1 and X_2. Since the system is well coupled to the leads, the charge is no longer quantized, the Coulomb blockade is lifted, and to a first approximation, we can use a picture of noninteracting electrons.[14]

The starting point of our theory is a formula due to Büttiker, Thomas, and Prêtre[15] for the current in the contacts 1 and 2 that results from an infinitesimal change of a parameter X: For a small and slow harmonic variation $X(t) = X_0 + \delta X_\omega e^{i\omega t}$, the charge $\delta Q(m)$ entering the cavity through contact m ($m = 1,2$) reads as

$$\delta Q(m,\omega) = e \frac{dn(m)}{dX} \delta X_\omega, \qquad (3a)$$

$$\frac{dn(m)}{dX} = \frac{1}{2\pi} \sum_{\beta} \sum_{\alpha \in m} \mathrm{Im} \frac{\partial S_{\alpha\beta}}{\partial X} S^*_{\alpha\beta}. \qquad (3b)$$

The index α is summed from 1 to N for contact 1 and from $N+1$ to $2N$ for contact 2. The quantity $dn(m)/dX$ is the *emissivity* into contact m.[15] Equation (3) is valid to first order in the frequency ω and assumes that the scattering properties follow the time-dependent potentials instantaneously. After Fourier transformation one obtains

$$\delta Q(m,t) = e \frac{dn(m)}{dX} \delta X(t). \qquad (4)$$

Similarly, for a simultaneous infinitesimal variation of two parameters X_1 and X_2, the emitted charge $\delta Q(m,t)$ through contact m is ($m = 1,2$)

$$\delta Q(m,t) = e \frac{dn(m)}{dX_1} \delta X_1(t) + e \frac{dn(m)}{dX_2} \delta X_2(t). \qquad (5)$$

Next, we consider a *finite* variation of both parameters X_1 and X_2. The total charge emitted through contact m in one period $\tau = 2\pi/\omega$ is found from integration of Eq. (5) to X_1 and X_2, bearing in mind that the scattering matrix S and hence the emissivities $dn(m)/dX_1$ and $dn(m)/dX_2$ are functions of X_1 and X_2,

$$Q(m,\tau) = e \int_0^\tau dt \left(\frac{dn(m)}{dX_1} \frac{dX_1}{dt} + \frac{dn(m)}{dX_2} \frac{dX_2}{dt} \right). \qquad (6)$$

In one period, the pair of parameters $X_1(t)$ and $X_2(t)$ follows a closed path in the (X_1, X_2) parameter space, see Fig. 1(b). The total charge expelled from the dot through contact m can be rewritten as a surface integral over the area A enclosed by the path in parameter space using Green's theorem,

$$Q(m,\tau) = e \int_A dX_1 dX_2 \left(\frac{\partial}{\partial X_1} \frac{dn(m)}{dX_2} - \frac{\partial}{\partial X_2} \frac{dn(m)}{dX_1} \right).$$

Note that the surface area A, and hence the transported charge, vanish, if the parameters X_1 and X_2 vary in phase, or with a phase difference π. The surface area is maximal if their phases differ by $\pi/2$. Substitution of Eq. (3b) for the emissivities yields

$$Q(m,\tau) = \frac{e}{\pi} \int_A dX_1 dX_2 \sum_{\beta} \sum_{\alpha \in m} \mathrm{Im} \frac{\partial S^*_{\alpha\beta}}{\partial X_1} \frac{\partial S_{\alpha\beta}}{\partial X_2}. \qquad (7)$$

Hence the d.c. current I_m through contact m is given by

$$I_m = \frac{i\omega e}{4\pi^2} \sum_{\alpha \in m} \int_A dX_1 dX_2 [R_{X_1}, R_{X_2}]_{\alpha\alpha}, \qquad (8a)$$

$$R_X = -i \frac{\partial S}{\partial X} S^\dagger. \qquad (8b)$$

One verifies that $I_1 = -I_2$, indicating that no charge is accumulated. The response matrices R_{X_1} and R_{X_2} are hermitian $2N \times 2N$ matrices. For the (bi)linear response to the variations of the parameters X_1 and X_2, Eq. (8) simplifies to the result (2) above. Note that, since the parameters X_1 and X_2 are dimensionless, the current formula contains no factor h, unlike the Landauer formula (1). Planck's constant may however appear in the typical scales for the parameter dependence of the scattering matrix $S(X_1, X_2)$.

Equation (8) is the main result of this paper. It establishes the link between the pumped current I and the parametric derivatives of the scattering matrix S. Several qualitative observations can already be reached on the basis of Eq. (8). First, for a phase coherent quantum system, the out-of-phase variation of *any* pair of independent parameters will give rise to a dc current to order ω. Second, I is not quantized, unlike in the case of the electron pumps that operate in the regime of Coulomb blockade.[2] Third, if the size of the variations $\delta X_1(t) = \delta X_1 \sin(\omega t)$ and $\delta X_2(t) = \delta X_2 \sin(\omega t - \phi)$ is small

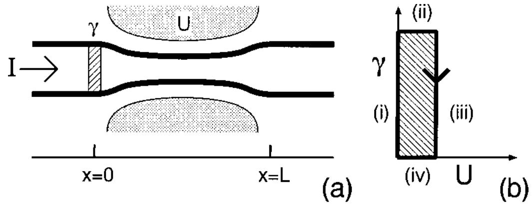

FIG. 2. (a) An electron pump, consisting of a one-dimensional wire with a tunnel barrier at $x=0$ and an adjustable electrostatic potential U for $0<x<L$. (b) Charge is pumped through the wire by varying the height γ of the tunnel barrier and the potential U in the following order: (i) $\gamma\to\infty$ (close barrier), (ii) $U\to\delta U$ (raise potential), (iii) $\gamma\to 0$ (open barrier), (iv) $U\to 0$ (lower potential).

compared to the characteristic correlation scales X_{1c} and X_{2c} needed to change the scattering properties of the sample, we may neglect the X_1 and X_2 dependence of the integrand in Eq. (8), and recover the (bi)linear response formula (2). On the other hand, for $\delta X_j \gg X_{jc}$ $(j=1,2)$, the integrand in Eq. (8) may have multiple sign changes within the integration area A, and the typical value of I is proportional to $(\delta X_1 \delta X_2 X_{1c} X_{2c} \sin\phi)^{1/2}$. [Although the typical value of the current scales as $(\sin\phi)^{1/2}$, the ϕ dependence of the sample-specific current may be quite random.]

Like the Landauer formula, the scattering matrix formula (8) describes both a classical contribution to the current and the quantummechanical corrections. Their roles are illustrated below in two examples. First, we consider a simple pump in a one dimensional wire. The wire contains a tunnel barrier at $x=0$ and for $0<x<L$ a region where the electrostatic potential U can be varied, e.g. by varying the voltage of a nearby gate, see Fig. 2(a). The Schrödinger equation for this system reads as

$$k^2\psi(x)=\left(-\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x),$$
$$V(x)=\gamma\delta(x)+U\theta[x(L-x)], \tag{9}$$

where $\theta(z)=1$ if $z>0$ and 0 otherwise. We pump electrons through the system by opening and closing the tunnel barrier and raising and lowering the potential U as indicated in Fig. 2(b). This system operates as a classical ''peristaltic'' electron pump. To find the dc current I, we compute the scattering matrix S and apply the scattering matrix formula (8),

$$I=\frac{eL\omega}{8\pi^2 k}\delta U+\frac{e\omega\delta U}{16\pi^2 k^2}(\pi\sin^2 kL-\sin 2kL). \tag{10}$$

The first term is the classical contribution to the pumped current. [Note that the local density of states for this one-dimensional system is $1/(2\pi k)$.] The second term is the correction due to quantum interference.

As a second example, we consider the case where electrons are pumped through a disordered or chaotic quantum dot. This application is relevant for the experiments of Ref. 12. The two (dimensionless) parameters X_1 and X_2 characterize two different deformations of the shape of the dot, see Fig. 1(a). Unlike in the previous example, where the pumping mechanism was of a mainly classical origin, for a chaotic quantum dot, there is no ''classical'' contribution to the pumped current. The current results from quantum interference and its size and direction depend on microscopic details of the system. Pumping occurs because the wave functions near the two point contacts are different and strongly parameter dependent, so that different amounts of current flow through the two contacts if the parameters X_1 and X_2 are varied.

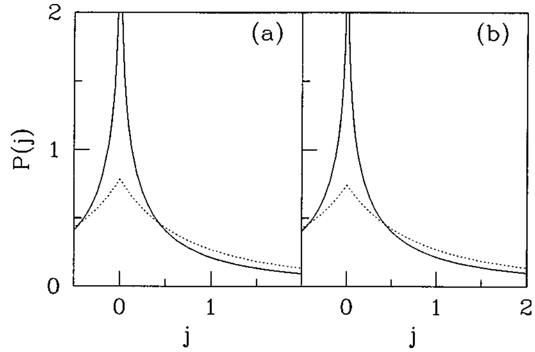

FIG. 3. (a) Distribution of current $I=\omega j\sin\phi\delta X_1\delta X_2$ for single-channel point contacts. The case of presence (absence) of time-reversal symmetry is shown as a solid (dashed) line. (b) The same, but with capacitive interactions taken into account by a self-consistent Hartree approach, in the limit $C\ll\rho e^2$.

For a disordered or chaotic quantum dot, the statistical distribution of the scattering matrix $S(X_1,X_2)$ and its dependence on X_1 and X_2 are given by the random matrix theory.[13] Within random matrix theory, the parameter-dependent Hamiltonian $\mathcal{H}(X_1,X_2)$ of the quantum dot is replaced by a large $M\times M$ hermitian matrix $H(X_1,X_2)$

$$H(X_1,X_2)=H+M^{-1/2}X_1H_1+M^{-1/2}X_2H_2, \tag{11}$$

where the matrix elements of H, H_1, and H_2 are independently and identically distributed Gaussian random numbers. A distinction is made between the cases that time-reversal symmetry (TRS) is present [$H(X_1,X_2)$ is real] or absent [$H(X_1,X_2)$ is complex]. We now compute the distribution of the pumped current I in the regime of small parametric variations $\delta X_j \ll X_{jc}$ $(m=1,2)$.[16] Using the distribution of the matrices R_{X_1} and R_{X_2} from Ref. 17, we find that for many-channel leads $(N\gg 1)$, the current I is Gaussian distributed with $\langle I\rangle=0$ and r.m.s. $I=e\omega\sin\phi\delta X_1\delta X_2/2\pi N$, both with and without TRS. In the opposite case of single-channel leads $(N=1)$, the distribution is highly non-Gaussian, see Fig. 3. It has a logarithmic singularity (cusp) at zero current in the presence (absence) of time-reversal symmetry. The asymptotics for large $|I|$ are given by

$$P(I)\propto\begin{cases}|I|^{-9/4}, & \text{TRS},\\ |I|^{-3}, & \text{no TRS}.\end{cases} \tag{12}$$

The scattering matrix formula (8) allows us not only to find the statistical distribution of the pumped current I, but also the statistical correlation between I and the conductance G of a chaotic quantum dot. The correlation between I and G shows a remarkable dependence on the presence or absence of time-reversal symmetry: In Ref. 17, it was shown that the statistical distribution of R_{X_1} and R_{X_2} is correlated with that of the conductance in the presence of TRS only. Therefore, without TRS, I and G are statistically uncorrelated for a chaotic quantum dot, while they are correlated in the presence of TRS. In the latter case, we find that the width of the current distribution at a fixed conductance G is proportional to $G^{1/2}$ for single-channel leads.[18]

Our main result, Eq. (8), is readily extended to include the effect of a capacitive interaction in the quantum dot within a self-consistent Hartree treatment.[14,19] Following Ref. 19, the effect of the capacitive interaction is described by a self-consistent electric potential U. The potential U is related to the (kinetic) energy E and the Fermi energy E_F via $E_F = E + U$. Variation of X_1 and X_2 will cause a change of U and hence of $E = E_F - U$. (The Fermi energy E_F is kept constant.) Hence we have to deal with a simultaneous variation of E, X_1, and X_2. These simultaneous variations can still be described by the scattering matrix formula (8) provided we replace the response matrices R_{X_j} ($j=1,2$) by

$$R_{X_j} \to R_{X_j} + R_E \frac{\partial E}{\partial X_j}, \quad R_E = -i \frac{\partial S}{\partial E} S^\dagger. \tag{13}$$

The derivative $\partial E / \partial X_j$ reads[19]

$$\frac{\partial E}{\partial X_j} = - \frac{\mathrm{tr}\, R_{X_j}}{\pi C/e^2 + \mathrm{tr}\, R_E}, \quad j=1,2 \tag{14}$$

where C is the geometrical capacitance of the dot. For many-channel contacts, inclusion of the interactions has no effect on the current distribution. For single-channel leads, we have computed the current distribution for the experimentally relevant case $C \ll e^2 \rho$, where ρ is the (average) density of states in the dot, using the distribution of the matrices R_{X_j} and R_E in the presence of capacitive interactions.[20] The result, which is not much different from the non-interacting case, is shown in Fig. 3(b).

It is a pleasure to acknowledge discussions with I. L. Aleiner, M. Büttiker, B. I. Halperin, C. M. Marcus, and Y. Oreg. This work was supported by the NSF under Grant Nos. DMR 94-16910, DMR 96-30064, and DMR 97-14725.

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