PHYSICAL REVIEW E **71**, 035202(R) (2005)

Quantum pumping: The charge transported due to a translation of a scatterer

Doron Cohen,[1] Tsampikos Kottos,[2] and Holger Schanz[2]
[1]*Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel*
[2]*Max-Planck-Institut für Dynamik und Selbstorganisation, Universität Göttingen, Bunsenstraße 10, D-37073 Göttingen, Germany*
(Received 3 July 2004; published 15 March 2005)

The amount of charge that is pushed by a moving scatterer is $dQ=-GdX$, where dX is the displacement of the scatterer. The question is: what is G?. Does it depend on the transmission g_0 of the scatterer? Does the answer depend on whether the system is open (with leads attached to reservoirs) or closed? In the latter case what are the implications of having "quantum chaos" and/or coupling to the environment? The answers to these questions illuminate some fundamental aspects of the theory of quantum pumping. For the analysis we take a network (graph) as a model system, and use the Kubo formula approach.

DOI: 10.1103/PhysRevE.71.035202 PACS number(s): 05.45.Mt, 73.23.−b, 03.65.Vf

Consider an Aharonov-Bohm ring with a Fermi sea of noninteracting spinless electrons as in Fig. 1(b). Assume that the ring is either disordered or chaotic, and that the temperature is known. In such a case the ring has a well-defined Ohmic conductance $G^{\rm ohm}$. This means that if we change the magnetic flux Φ through the ring, then we have the electromotive force $-\dot{\Phi}$ and the current is $\mathcal{I}=G^{\rm ohm}\times(-\dot{\Phi})$. Therefore the charge that is transported is $dQ=-G^{\rm ohm}d\Phi$. Next we can ask what is the charge that is transported if we vary some other parameter (X) that controls the potential in which the electrons are held (in practice it may be a gate voltage). Then, in complete analogy with Ohm's law, we expect to get $dQ=-GdX$, where G is a *generalized conductance*. The calculation of G is the so-called problem of "quantum pumping."

Most of the studies of quantum pumping were (so far) about open systems [Fig. 1(e)]. Inspired by Landauer who pointed out that $G^{\rm ohm}$ is essentially the transmission of the device, Büttiker, Pretre, and Thomas (BPT) have developed a formula that allows the calculation of G using the S matrix of the scattering region [1,2]. It turns out that the nontrivial extension of this approach to closed systems involves quite restrictive assumptions [5]. Thus the case of pumping in closed systems has been left unexplored, except to some past works on adiabatic transport [3,4]. Yet another approach to quantum pumping is to use the powerful *Kubo formalism* [6,7]. In this paper we report on a nontrivial demonstration of this formalism. Namely, we illuminate the interplay of "quantum chaos" with nonadiabaticity and environmental effects, and in particular we derive specific results for the (generalized) conductance in closed (chaotic) system.

To be specific we ask what is the amount of charge that is transported if we make a displacement dX of some scatterer or of some wall element ("piston"). The answer to this question in case of the one-dimensional (1D) system of Fig. 1(e) is well known. Using the BPT formula one gets

$$G=-(1-g_0)\times\frac{e}{\pi}k_{\rm F}, \tag{1}$$

where $k_F=\mathbf{m}v_F/\hbar$ is the Fermi wave number, and g_0 is the transmission of the scatterer. This result is analogous to the Landauer formula $G^{\rm ohm}=(e^2/\hbar)g_0$. The charge transport mechanism that is represented by Eq. (1) has a very simple heuristic explanation, which is reflected in the term "snow plow dynamics" [2]. On the other hand, in the case of Figs. 1(a) or 1(c), if we translate the scatterer at some constant velocity $\dot{X}$, it is clear that

$$G=-1\times\frac{e}{\pi}k_{\rm F}. \tag{2}$$

In Eq. (2) the transmission of the scatterer is assumed to be $g_0<1$ [in Fig. 1(a) the role of g_0 is played by the relative size of the scatterer]. Irrespective of g_0 the steady state is a distribution that moves with the same velocity as the scatterer. (In the moving frame of the scatterer the steady state is a standing wave.) Though g_0 does not influence the value of G, it should be remembered that in the limit $g_0\to 1$, it takes an infinite time to get into the steady state.

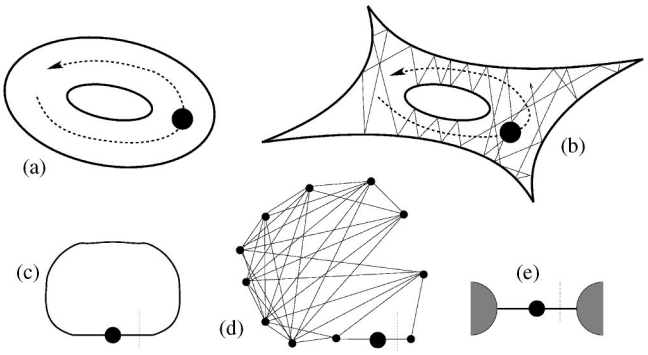

FIG. 1. A scatterer (represented by a black circle) is translated through a systems that has a Fermi occupation of spineless noninteracting electrons. In (a) the system is a simple ring. In (b) it is a chaotic ring (Sinai billiard). In (c) and in (d) we have network systems that are of the same type of (a) and (b), respectively. In the network, the scatterer ("piston") is a delta function (represented as a big circle) located at $x=X$. The current is measure at a section (represented by a dotted vertical line) through $x=x_1$. In (e) we have an open geometry with left and right leads that are attached to reservoirs that have the same chemical potential.

 ©2005 The American Physical Society

What about Fig. 1(b)? Here the system has an inherent time scale $\tau_{\rm cl}$ that governs the relaxation to an ergodic distribution in the laboratory frame irrespective of the driving. The scatterer should push its way through the ergodizing distribution, and therefore its relative size (or its transmission) matters. Thus we expect to find $G \propto (1-g_0)$ in the analogous network model of Fig. 1(d). Moreover, we expect to have a dependence of G on the overall transmission g_T of the ring. Using the Kubo formalism we are going to derive

$$G = -\frac{e}{\pi} k_{\rm F} \left[\frac{1-g_0}{g_0}\right]\left[\frac{g_T}{1-g_T}\right] \tag{3}$$

and discuss the conditions for its validity. In particular we are going to discuss whether the effect of nonadiabaticity is to induce a crossover from Eq. (3) to Eq. (1). We are going to present both semiclassical and quantum mechanical derivations, and to consider the generalization of "universal conductance fluctuations."

Our model system [8] is the network of Fig. 1(d). It is composed of one-dimensional (1D) wires ("bonds"). The scatterer is represented by a delta function that is located on some selected bond. Thus the Hamiltonian $\mathcal{H}$ incorporates a potential $U(x)=\lambda(\hbar^2/2\mathbf{m})\delta(x-X)$, where X is the location of the scatterer along the bond. The parameter λ determines the transmission of the scatterer $g_0=[1+(\lambda/2k_F)^2]^{-1}$.

The generalized conductance G is, in fact, an element of the generalized conductance matrix, that gives the response of the current $\mathcal{I}$ to the driving via X. With X we associate the operator $\mathcal{F}=-(\partial\mathcal{H}/\partial X)=\lambda(\hbar^2/2\mathbf{m})\delta'(x-X)$. Since dX is a displacement, it follows that $\mathcal{F}$ is a Newtonian force. We measure the current through another section $x=x_1$ along the same bond [see the dotted line in Fig. 1(d)]

$$\mathcal{I} = \frac{e}{2\mathbf{m}}[\delta(x-x_1)p + p\delta(x-x_1)]. \tag{4}$$

The Kubo expression for G can be expressed using a generalized fluctuation-dissipation (FD) relation [7]

$$G = g(E_F)\int_0^\infty C_{E_F}(\tau)d\tau, \tag{5}$$

where $C_E(\tau)$ is the cross-correlation function of $\mathcal{I}(\tau)$ and $\mathcal{F}(0)$, and $g(E)$ is the one-particle density of states at the Fermi energy. Equation (5) is the Kubo analog of the BPT formula. In fact, the latter can be obtained as a special limit of the former [7]. Equation (5) would become the standard FD relation if we were looking for $G^{\rm ohm}$. In such a case the symmetric current-current correlation function would be involved, and consequently one would obtain $G^{\rm ohm}=\frac{1}{2}g(E_F)\tilde{C}_{E_F}(\omega\sim 0)$. But in the case of our pumping calculation $C_E(\tau)$ is antisymmetric, and therefore such simplification is not possible.

Disregarding the assumption of having Fermi occupation, Eq. (5) has a classical derivation. In such a case, $C_E(\tau)$ is the classical cross-correlation function, and there is an implicit thermal averaging over E_F. The analogous quantum mechanical (QM) derivation is based on perturbation theory. Later we are going to discuss its limitations. In the QM context, $C_E(\tau)$ is the *symmetrized* correlation function. Furthermore, considerations that are based on a Markovian treatment of perturbation theory to infinite order, suggest the replacement

$$C_E(\tau) \mapsto C_E(\tau)e^{-(\Gamma/2\hbar)\tau}, \tag{6}$$

where $\Gamma \propto |\dot{X}|^{2/3}$ is related to the nonadiabaticity of the driving [6], or, more generally, it may incorporate also the influence of an external bath. Thus we get

$$G = \hbar g(E)\int_{-\infty}^{\infty} \frac{-i\tilde{C}_{E_F}(\omega)}{\hbar\omega - i(\Gamma/2)}\frac{d\omega}{2\pi}, \tag{7}$$

where

$$\tilde{C}_E(\omega) = \frac{\hbar}{2g(E)}[C(E+\hbar\omega,E) + C(E-\hbar\omega,E)] \tag{8}$$

and

$$C(E',E) = 2\pi\sum_{nm}\mathcal{I}_{nm}\delta(E'-E_m)\mathcal{F}_{mn}\delta(E-E_n)$$

$$= \frac{2}{\pi}\,\mathrm{trace}[\mathcal{I}\,\mathrm{Im}[\mathbf{G}(E')]\mathcal{F}\,\mathrm{Im}[\mathbf{G}(E)]]. \tag{9}$$

In the first equality $C(E',E)$ is expressed using the eigenenergies E_n and the matrix elements of $\mathcal{I}$ and $\mathcal{F}$. In the second equality it is expressed using $\mathrm{Im}[\mathbf{G}]=-i\frac{1}{2}(\mathbf{G}^+-\mathbf{G}^-)$, where $\mathbf{G}^\pm=1/(E-\mathcal{H}\pm i0)$ are the Green functions of the system.

Thus we have three options for calculation. In the classical treatment it is simplest to calculate directly the correlation function in the time domain. In the QM case we can use expressions for the Green function in order to make the calculation. Optionally we can express the conductance using the eigenenergies and the matrix elements of the associated operators

$$G = 2\hbar\sum_n f(E_n)\sum_{m(\neq n)}\frac{\mathrm{Im}[\mathcal{I}_{nm}\mathcal{F}_{mn}]}{(E_m-E_n)^2+(\Gamma/2)^2}, \tag{10}$$

where $f(E)$ is the Fermi occupation function. The latter expression is valid also in the strict adiabatic limit $\Gamma\to 0$, where it can be regarded as geometric magnetism [3].

We can get a semiclassical estimate for G by studying the classical correlation function $C(\tau)$. But first we should define what classical calculation means in the context of this network model. Recall that dX is displacement, so $\mathcal{F}$ has the meaning of Newtonian force. Therefore in the classical calculation $\mathcal{F}(t)$ consists of spikes whose *area* has the meaning of impact $(=2\mathbf{m}v_F)$. Possibly it is more intuitive to think of the scatterer as a rectangular barrier with two vertical walls. The vertical walls of the scatterer are regularized by giving them finite slops. In such case the spikes of $\mathcal{F}(t)$ become short rectangular pulses of some duration τ_0 and height $(2\mathbf{m}v_F)/\tau_0$. Obviously this regularization drops out from the final result, because the product $\mathcal{I}(t)\mathcal{F}(0)$ is weighted by the probability of having nonzero $\mathcal{F}(0)$, which is $(v_F\tau_0)/(2L)$. The possibility to tunnel through the scatterer is taken into account by adopting a stochastic point of view. Namely,

upon collision there is a probability g_0 to go through the scatterer (in such case there is no impact). Using the above stochastic picture one deduces that the short-time correlations are

$$C(\tau) = \frac{v_F}{2L} e(2\mathbf{m}v_F)\left[(1-g_0)\sum_{\pm} \pm \delta(\tau \pm \tau_1)\right], \qquad (11)$$

where $\tau_1 = (x_1 - X)/v_F$. However there are tails due to multiple reflections, leading (after geometric summation) to

$$\int_0^\infty C(\tau)d\tau = -e\frac{\mathbf{m}v_F^2}{L}\left[\frac{1-g_0}{g_0}\right]\left[\frac{g_T}{1-g_T}\right]. \qquad (12)$$

Substitution into Eq. (5) leads to Eq. (3). The validity of the final result can be double checked by solving the classical Master equation to find the (quasi) steady-state solutions of the problem. The current in the steady state, to linear order in the rate of the driving, leads to the same result [Eq. (3)] for the conductance.

We turn now to the proper quantum mechanical calculation. The matrix elements between eigenstates of the network are

$$\mathcal{I}_{nm} = -i\frac{e\hbar}{2\mathbf{m}}(\psi^n\partial\psi^m - \partial\psi^n\psi^m)_{x=x_1}, \qquad (13)$$

$$\mathcal{F}_{nm} = -\lambda\frac{\hbar^2}{2\mathbf{m}}(\psi^n\partial\psi^m + \partial\psi^n\psi^m)_{x=X}, \qquad (14)$$

where the gradient $\partial\psi$ should be interpreted as the average value of the left and right slopes. (To derive this result it is convenient to regard the delta function as a narrow rectangular barrier.) Without loss of generality we set from now on $X=0$. It is convenient to express $\mathcal{F}_{nm}$ using the wave function at $x=+0$. Thus we get

$$\mathcal{F}_{nm} = -\lambda\frac{\hbar^2}{2\mathbf{m}}(\psi^n\partial\psi^m + \partial\psi^n\psi^m - \lambda\psi^n\psi^m)_{x=+0}. \qquad (15)$$

Substitution of (13) and (15) into (10) leads to an expression that can be written in terms of the Green function $\mathbf{G}$. [An alternate procedure is to substitute in Eq. (9) the implied differential representation of the operators.]

$$G = -\frac{\lambda e}{\pi}\left(\frac{\hbar^2}{2\mathbf{m}}\right)^2\langle \mathbf{G}^R\mathbf{G}^I_{xx'} - \mathbf{G}^R_{xx'}\mathbf{G}^I + \mathbf{G}^R_x\mathbf{G}^I_{x'} - \mathbf{G}^R_{x'}\mathbf{G}^I_x + \lambda(\mathbf{G}^R_{x'}\mathbf{G}^I - \mathbf{G}^R\mathbf{G}^I_{x'})\rangle_E, \qquad (16)$$

where $\langle\cdot\rangle_E = -\int dE f'(E)$ implies thermal averaging and we have defined $G^R = \mathrm{Re}\,\mathbf{G}(x,x';E+i\Gamma/2)$, and $G^I = \mathrm{Im}\,\mathbf{G}(x,x';E+i0)$. The subscripts indicate derivatives with respect to x and x'. The expression is evaluated for $x=+0$ and $x'=x_1$.

In case of a network the Green function is given by [9]

$$\mathbf{G}(x,x';E) = -\frac{i}{\hbar v_F}\sum_p A_p e^{ik_E L_p}, \qquad (17)$$

where the sum extends over all the paths that start at x and end at x'. The A_p are the product of the associated transmission and reflection amplitudes (T_i or R_i for each encountered vertex (i), while L_p is the total length of the path. Upon substitution in (16) we get a double sum Σ_{pq} over paths with endpoints $x=+0$ and $x'=x_1$. In a term that involves derivatives the amplitude A_p (A_q) is multiplied by a sign factor s and/or s', which indicates, respectively, the initial and final sign of the velocity. Gathering all the contributions, one ends up with

$$G = -\frac{e}{\pi}k_F\sqrt{\frac{1-g_0}{g_0}}\sum_L\sum_{p,q\in L} s'_p s_q\,\mathrm{Im}\left[\frac{1}{\mathsf{T}_0}A_pA_q^*\right]e^{-L/L_\Gamma},$$

where $L_\Gamma = 2\hbar v_F/\Gamma$. Above we neglected off-diagonal terms that involve pairs of trajectories with different lengths L. This is justified if the energy averaging is over a sufficiently large range. It is also important to realize that any trajectory that starts at $x=+0$ and departs in the positive direction represents, in fact, the contribution of two degenerate *paths*: one starts with a positive velocity, while the other starts with a negative velocity but is immediately reflected. Assuming that this is the only significant length degeneracy we get

$$G = -\frac{e}{\pi}k_F\frac{1-g_0}{g_0}\sum_p s_p s'_p|A_p|^2 e^{-L_p/L_\Gamma}. \qquad (18)$$

The sum is over the same paths as in Eq. (17), and it can be verified that the above-mentioned degenerate paths adds correctly. The summation over p involves a geometric sum in $[g_T-(1-g_T)]$ and gives the factor $g_T/(1-g_T)$. Thus we see that a careful treatment within the framework of the diagonal approximation recovers the classical result.

We turn to discuss the validity of our result. The derivation of the Kubo formula Eq. (10) assumes $\Gamma \ll \Delta_b$. By definition the bandwidth $\Delta_b \approx \hbar/\tau_{cl}$ is the energy range $|E_n - E_m| < \Delta_b$ for which $\mathcal{I}_{nm}\mathcal{F}_{mn}$ are non-negligible. It is determined by the classical correlation time τ_{cl} that characterizes $C(\tau)$. For a generic chaotic system the mean level spacing is $\Delta \propto \hbar^d$, where d is the dimensionality of the system. Hence the bandwidth in dimensionless units is $b = \Delta_b/\Delta \propto \hbar^{1-d}$. It follows that $b \gg 1$ is the generic case for any quantized chaotic system. For a chaotic network $d=1$, and b is roughly equal to the number of bonds.

There is a practical implication of the above discussion to pumping in general. For some geometries we have $\tau_{cl} \ll \tau_1$. The notable example is the dot-wire geometry of Ref. [7] where τ_{cl} is related to the motion inside the dot, while the current is measured outside at a section on the (very long) wire. Thus we may have $\Gamma > \hbar/\tau_1$ in Eq. (6) without breaking the validity condition $\Gamma < \hbar/\tau_{cl}$. Consequently we stay only with the short-time correlations in Eq. (11), and we get Eq. (1) rather that Eq. (3).

An additional assumption enters into the derivation of the generalized FD relation and the associated Green function expression. Namely, it is assumed that $\Gamma \gg \Delta$. In order to test the significance of this assumption, we consider a generic network with $b=35$. In Fig. 2 we plot the exact result for G as a function of Γ. We also plot the dispersion of G. One may regard this dispersion as the analog of *universal conductance fluctuations*. As Γ becomes larger than Δ these fluctuations are smoothed away. We also see that the result is quite in-

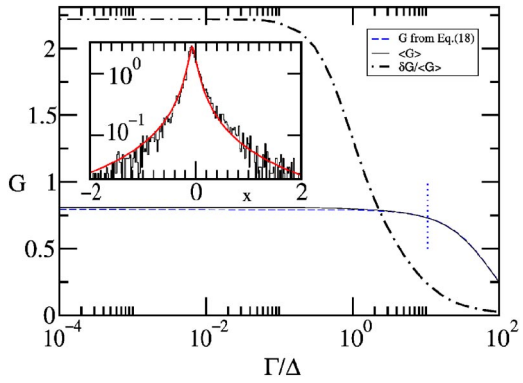

FIG. 2. Comparison of the exact quantum result Eq. (10) for $\langle G\rangle$ with the diagonal approximation Eq. (18) in case of the network of Fig. 1(d). The average is taken over more than 20 000 levels around E_F, while the calculation (for each Fermi level) was performed in an interval of 32 000 levels. The valency v of each vertex is picked up randomly. The transmission of the piston is $g_0 \approx 0.1$. The perpendicular dotted line indicates the border of the regime where the QM calculation is valid (see text). We also plot the standard deviation $\delta G/\langle G\rangle$, while the inset displays the distribution $P(G-\langle G\rangle)$ for $\Gamma=0.0001\Delta$. Notice the slight asymmetry. The smooth line is the best fit with $0.068/(0.024+|x+0.065|^{1.5})$. In these calculations the temperature is $T=0$.

sensitive to the exact value of Γ as long as $\Gamma \ll \Delta_b$, which is the regime where the quantum mechanical derivation of the Kubo formula makes sense. Throughout all regimes the diagonal approximation is very precise, as expected for quantities related to the statistics of matrix elements.

If the condition $\Gamma \ll \Delta_b$ breaks down we enter into a *nonperturbative regime* where the QM recipe Eq. (6) does not hold. However, if the system has a *classical limit*, then it can be argued (on semiclassical grounds) that in the nonperturbative regime the classical calculation can be trusted. Since the classical calculation gives the same estimate as the diagonal approximation, it follows that there should be no apparent breakdown of validity as we cross from the perturbative to the nonperturbative regime. We have studied this issue [10] in the context of energy absorption (the $G^{\rm ohm}$ conductance).

It is now interesting to discuss what happens in the nongeneric case $b \sim 1$. For this purpose we consider two specific examples: a scatterer on a closed ring [Fig. 1(c)]; and a scatterer on a disconnected bond [Fig. 1(e) but without the reservoirs]. In the first example the adiabatic result Eq. (2) can be recovered from Eq. (3) by substituting $g_T=g_0$, while in the second case $G=0$ because $g_T=0$. The latter result requires further discussion. Since $g_T=0$ the possibility of getting a steady-state circulating current is blocked. The zero-order adiabatic picture is as follows: At any moment the lowest energy levels are populated, hence at any moment the charge distribution is roughly uniform (ergodic). If we plot the current as a function of time, we find that the snow plow dynamics is counterbalanced by adiabatic passages of the particles through the moving barrier. The latter manifest themselves in the current as short spikes that compensate the otherwise steady (snow plow) flow of current. The statistical properties of the current should be regarded as the simplest example for the generalized universal conductance fluctuations that we have discussed previously. If the driving is nonadiabatic, then the particles do not have the time to make adiabatic passages through the scatterer, and then the snow plow dynamics becomes more effective. Thus the nonadiabatic translation of the scatterer induces a steady nonzero current in the bond, which is associated with accumulation of charge on the heading side of the scatterer and depletion in the trailing side. Hence the current within the bond becomes (during some transient period) of the same order of magnitude as in the case of an open system [Fig. 1(e)], where the reservoirs are assumed to be of an infinite size.

In summary, the Kubo approach to quantum pumping allows us to explore the crossover from the strictly adiabatic "geometric magnetism" regime to the nonadiabatic regime. In particular we were able to derive specific results for the generalized conductance, using either classical stochastic modeling or diagonal approximation, which are supported by numerical analysis.

D.C. has the pleasure to thank M. Büttiker for an instructive visit in Geneve. This research was supported by the Israel Science Foundation (Grant No. 11/02), and by a grant from the GIF, the German-Israeli Foundation for Scientific Research and Development.

[1] M. Büttiker *et al.*, Z. Phys. B: Condens. Matter **94**, 133 (1994); P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).
[2] J. E. Avron *et al.*, Phys. Rev. B **62**, R10618 (2000).
[3] M. V. Berry and J. M. Robbins, Proc. R. Soc. London **442**, 659 (1993).
[4] J. E. Avron *et al.*, Rev. Mod. Phys. **60**, 873 (1988).
[5] M. Moskalets and M. Büttiker, Phys. Rev. B **68**, 161311(R) (2003).
[6] D. Cohen, Phys. Rev. B **68**, 155303 (2003).
[7] D. Cohen, Phys. Rev. B **68**, 201303(R) (2003).
[8] T. Kottos and U. Smilansky, Phys. Rev. Lett. **79** 4794 (1997).
[9] A. G. M. Schmidt, B. K. Cheng, and M. G. E. da Luz, J. Phys. A **36**, L545 (2003).
[10] D. Cohen and T. Kottos, Phys. Rev. Lett. **85**, 4839 (2000); J. Phys. A **36**, 10151 (2003).