Energy averaging and the flux-periodic phenomena in small normal-metal rings

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The low-frequency ac conductivity, σ, is evaluated numerically with use of the Kubo formula with inelastic lifetimes for a small one-dimensional (1D) closed metallic ring with random potentials. The effects of thermal excitations at finite temperatures and of increasing inelastic scattering are considered. It is found that energy averaging over a range larger than the typical level spacing (in 1D) markedly reduces the fundamental (hc/e) and odd harmonic periodicities of σ as a function of the Aharonov-Bohm flux, ϕ, through the ring. Thus, energy averaging makes the lowest even harmonic ($hc/2e$) appear to be the fundamental period.

I. INTRODUCTION AND STATEMENT OF THE PROBLEM

There has recently been a great deal of interest in the question of the sensitivity of physical properties of a small normal-metal ring-type structure to an Aharonov-Bohm[1] magnetic flux, ϕ, normal to the ring. All energy levels, matrix elements, etc. (and, thus, all measurable properties), are guaranteed by exact and very general[2] theorems to be periodic in ϕ with a period

$$\phi_0 = hc/e \ , \tag{1}$$

where ϕ_0 is the single-electron flux quantum. The effect of ϕ is to change the phase relationships for the wave functions, thereby modifying their interference around the ring. For systems in which the electronic motion is effectively ballistic—i.e., the system's length, L, is less than an electron's scattering mean free path, $l_{\rm eff}$—the above oscillations as a function of ϕ have been expected[3-5] and observed.[6] The situation is more subtle when $l_{\rm eff} \ll L$. It has only recently been appreciated[7-9] that only effectively irreversible scattering processes, such as inelastic ones, really scramble the phase of the wave function to eliminate the interference effects and the ensuing ϕ dependence. Purely elastic scattering, as long as it is not strong enough to cause strong localization of the wave functions, does retain wave functions with definite phases that reach around the ring and, hence, allows a significant sensitivity to ϕ. The condition for this is, therefore, just that

$$L \lesssim L_\phi \ , \tag{2}$$

L_ϕ is the effective phase randomization length, usually controlled by inelastic scattering. $L \gg l$ is possible, l being the elastic mean free path. When $\tau_{\rm in}$ denotes the characteristic time between inelastic collisions that are strong enough to wash out the electron's phase, one has

$$L_\phi \sim \begin{cases} v_F \tau_{\rm in}, & \text{for } L_\phi \lesssim l \quad (3a) \\ (D\tau_{\rm in})^{1/2}, & \text{for } L_\phi \gtrsim l. \quad (3b) \end{cases}$$

v_F is the Fermi velocity, and D is the diffusion constant $D \sim v_F l$. According to Refs. 8–10, for $L \ll L_\phi$ the resistance of the ring, measured between two appropriate contacts made on its perimeter, should oscillate in ϕ with a basic period ϕ_0. While the relative size of these oscillations is inversely proportional to the cross section of the wires used (or to the number of channels,[10] $N_\perp$, involved in the transport), these oscillations should be observable in realistic systems with $N_\perp \lesssim 2 \times 10^4$. Prior to this, Altshuler, Aronov, and Spivak[11] (henceforth abbreviated as AAS) have predicted that the resistance of such a ring, as well as that of a long small-radius hollow cylinder, should oscillate with ϕ with a basic period $\phi_0/2$ ($=hc/2e$, the superconducting flux quantum). This was based on a perturbation-theory evaluation of the Kubo formula for the conductivity, using the weak-localization-type, maximally crossed diagrams. This correctly took into account the interference of the electrons in the weak-scattering limit $k_F l \gg 1$. Indeed, the predictions of AAS have received ample experimental confirmation on both long small-radius cylinders[12-16] and arrays of small rings.[17,18]

The oscillation with period $\phi_0/2$ is the second harmonic of the fundamental one, with period ϕ_0. It is, of course, not surprising that the second harmonic exists—since there is no reason that the conductance $G(\phi)$ be a purely sinusoidal function (see below). Calculations[19] on one-dimensional (1D) models indeed revealed that such a second harmonic exists but that it is usually much smaller than the fundamental ϕ_0 oscillation. It is thus important to understand why the fundamental ϕ_0 period is absent in the AAS theory and in the aforementioned experiments.

One might have thought that the ϕ_0 component could average out almost to zero in a more realistic $N_\perp \gg 1$ case, in contrast to the 1D models mentioned above. In

fact, it is[10] of relative size $O(N_\perp^{-1})$ compared with the average G. However, it turns out that the AAS contribution is also of this order, so that having $N_\perp \gg 1$ does *not* explain the absence of the ϕ_0 component. In analogy, Carini *et al.*[20] found that the periodicity with period $\phi_0/2$ is also valid to $O(1/L)$ where L is the system length. However, this follows from their averaging their calculated property, the "participation ratio," over a *whole band* of states. We believe that had they looked into the same quantity for one state, or for a small number of states, their $1/L$ result would not hold. It should also be kept in mind that there might be a difference between the conductance of the ring as measured between two contacts, as in the Landauer approach, and as measured via absorption of electromagnetic radiation with no contacts. In this work we are going to use the latter definition of the conductance—and still obtain a basic period of ϕ_0. We shall, however, present and demonstrate some of the physical ingredients needed to average out the ϕ_0 component.

The key observation in this respect has been made by Gefen.[21] Carini *et al.*[20] and Browne *et al.*[22] have also arrived at the same conclusions. The point is that when considering the properties of small systems that are much larger than microscopic (i.e., atomic size) but not yet in the "macroscopic" limit (it has been suggested to denote this novel size range as "mesoscopic") there is a significant difference between the specific behavior of a given system[23] and the ensemble average. The latter means a suitable average over a large number of such systems, produced under the same macroscopic conditions—for example, a given average impurity concentration—but with both the exact overall impurity number as well as the precise location of the impurities differing among ensemble members. In fact, ensemble averaging should eliminate the ϕ_0-periodic component in $G(\phi)$, but the $(\phi_0/2)$-periodic one might survive. A qualitative reason for this is that an important contribution to the latter component turns out in the weak-localization calculation to be always minimal at $\phi=0$ (for weak spin-orbit scattering) while the former one does not have such a definite phase of oscillation.[19] The reason for the definite behavior of this $(\phi_0/2)$-periodic contribution, the one obtained by AAS, is that it is due to coherent backscattering.[12,24,25] This means that the probability for a diffusing particle to come back to the origin is enhanced at $\phi=0$ by the constructive interference of each closed path with its time-reversed partner. Those paths that encircle the ring's opening to lead to the AAS $(\phi_0/2)$-periodic contribution. In fact, both the AAS calculations and the cylinder[12–16] and array[17,18] experiments involve ensemble averaging over many incoherent rings. This explains why the $\phi_0/2$ period becomes the fundamental one for these cases. A proof for the vanishing of the ϕ_0 component as well as numerical demonstrations for the two-terminal geometry utilized in the Landauer formula will be presented in Ref. 26. The calculations reported here show indeed that the $\phi_0/2$ component survives ensemble averaging; however, its phase of oscillations is different from the one mentioned above. The different mechanism for that behavior will be discussed below.

The above considerations suggest a fundamental difference between experiments that effectively ensemble average and those done on a specific ensemble member. In this paper we find a condition for this to happen. We remark that while earlier experiments[27–30] on single rings have not shown a clear ϕ_0 component, very recent experiments,[31–34] performed during the preparation of this paper, have in fact revealed a large, clear, ϕ_0-periodic component. The complicating aperiodic structure[28–30] is also understood as due to the non—Aharonov-Bohm flux inside the arms of the ring.[30,35]

Considering a single ring, one is led to the following observation: If an experiment is performed at a temperature T, then electrons within a "thermal band" of width k_BT around the Fermi energy participate in the conduction process. These electrons have different "optical path lengths" around the system, so that their interference patterns will shift relative to each other. Once k_BT is larger than some appropriate energy-correlation range ΔE_c, these phase differences will be large enough for the thermal band to mimic an ensemble averaging. Thus, we may say that for $k_BT \gg \Delta E_c$, the system should be "self-averaging" and, in particular, exhibit only the $(\phi_0/2)$-periodic component for $G(\phi)$. It is the purpose of this paper to demonstrate this idea by computations on a simple 1D model. This actually has an advantage, compared to real experiments, that we can, in principle, vary k_BT and L_ϕ independently. In a real system they will be related due to $\tau_{\rm in}$ being a definite function of T, so that it is more difficult to separate the effects of energy averaging from those of inelastic scattering. We shall find that in our 1D model ΔE_c is on the order of a typical level separation at E_F which we denote by w. This is apparently not a general result. In a higher dimension one may put forward arguments,[36,26,37,38] in the weakly localized regime, that ΔE_c is on the order of the "Thouless V"—the sensitivity of the energy levels to a change in boundary conditions. We also remark that the $1/N_\perp$ estimate for the relative size of the ϕ_0-periodic component has recently been sharpened to $l/N_\perp$ in Refs. 35–39.

In the next section we describe the model to be considered and methods used. Results will be presented and discussed in Sec. III.

II. THE MODEL AND EXPRESSIONS FOR THE CONDUCTIVITY

We consider a small closed 1D loop, with a potential modeling the disorder that leads to elastic scattering. We evaluate $\sigma(\omega)$, the real part of the frequency-dependent conductivity, by calculating the absorption of energy from an electromagnetic field, such as would be observed by placing the sample in a cavity. The sample, thus, has no contacts and it may turn out that even in the dc, $\omega \to 0$ limit, this conductivity will be different from the one between two contacts on the ring. We start with the usual Kubo formula, written here for a finite system, i.e., with sums instead of integrals over the initial and final states:

$$\sigma_{xx}(\omega)=\frac{2\pi e^2\hbar}{\mathscr{V}}\sum_{i,j}\frac{f_i-f_j}{E_j-E_i}\,|v_{ij}|^2\delta(E_j-E_i-\hbar\omega)\,, \qquad (4)$$

where E_i, E_j are the energies of the ith and jth states and

f_i their (Fermi) occupation numbers; i.e., we are working in the grand canonical ensemble.[40] $v_{ij}=\langle i \mid v \mid j \rangle$, and v should be thought of as an azimuthal velocity around the ring (we shall later omit the x subscripts). This formula is derived for an "infinite" system; the volume factor $\mathcal{V}$ in the denominator makes σ size independent in the macroscopic limit.

Since we have in mind a finite system, Eq. (4) is really inapplicable if the spectrum is truly discrete. Its derivation, in fact, assumes a continuous spectrum, in order to have real transitions. If one insists on using (4) for a finite system, and monochromatic radiation, the result is "zero" for almost all ω's. We are aware of two ways around this difficulty. For a large ensemble of such small systems, such as in the work of Gor'kov and Eliashberg[41] on small metallic particles, one may use the continuous averaged level distribution. However, since we are interested in the absorption by a single specific system, our physical considerations are different. In fact, the small system can absorb energy from the electromagnetic field only by virtue of its being (albeit perhaps weakly) coupled to a large bath of, for example, phonons. This coupling, resulting in an inelastic lifetime for the electrons, endows the levels with a finite width

$$\eta \sim \hbar/\tau_{\text{in}} , \tag{5}$$

which now allows finite absorption of energy via the irreversible processes in the bath.

An accepted procedure to take this into account first suggested, as far as we know, by Czycholl and Kramer[42] and used also by Thouless and Kirkpatrick,[43] is to add an imaginary part, $i\eta$, to the frequency, which will broaden the δ functions into Lorentzians. In the dc limit

$$\sigma(i\eta)=\frac{2e^2}{\mathcal{V}}\hbar\eta\sum_{i,j}\frac{f_i-f_j}{E_j-E_i}\mid v_{ij}\mid^2\frac{1}{(E_j-E_i)^2+(\eta)^2} , \tag{6}$$

which is in agreement with the absorption, as obtained by Van Vleck and Weisskopf[44] for collision-broadened lines (see the Appendix). We remark that if we evaluate the sums as if the system were infinite, we find, for $\eta \ll w$, where w is the level separation at E_F, that

$$\sigma(i\eta)\sim\sigma_{\text{KG}}\frac{\eta}{w} , \tag{7}$$

where σ_{KG} is the usual zero-temperature Kubo-Greenwood conductivity that one would obtain for this system, assuming that $\mid v_{ij} \mid^2$ does not depend strongly on i and j and replacing sums by integrals. Thus σ does vanish in the limit $\eta \to 0$, as expected.

The latter result is opposite to that of Landauer and Büttiker,[45] and Büttiker,[46,39] who obtained the response of a ring to a small emf around it, brought about by a time-dependent flux ϕ. In the limit that the frequency of this time-dependent flux goes to zero their conductance is *inversely* proportional to η.[47] They have not used the Kubo formula, and obtained a net energy absorption via the tendency of the inelastic scattering to bring the levels, which change with time due to the changing flux, into thermodynamic equilibrium.

We evaluate Eq. (6) for the following model: In polar coordinates (r,θ) the one-electron Hamiltonian for a ring of radius R in a magnetic field H, normal to the plane of the ring is[48]

$$\begin{aligned}&\mathcal{H}=\mathcal{H}_0+V(\theta) ,\\ &\mathcal{H}_0=-(\hbar^2/2mR^2)\left[\frac{\partial}{\partial\theta}-i\Phi\right]^2 ,\end{aligned} \tag{8}$$

where we have taken the vector potential to be $A_\theta=RH/2$. Φ is the flux through the ring in units of the flux quantum ϕ_0 and m is the effective mass. The potential $V(\theta)$ provides elastic scattering, and both $\mathcal{H}$ and V are periodic in θ. The wave functions and energies corresponding to $\mathcal{H}_0$ are $\mid n \rangle = 1/\sqrt{2\pi}e^{in\theta}$ and $E_n=(\hbar^2/2mR^2)(n-\Phi)^2$, $(n=0,\pm1,\pm2,\ldots)$. The velocity is diagonal $v_n=\hbar/mR\,(n-\Phi)$. It should be noted that these are not the only matrix elements of the velocity operator, $v(\theta)$. In general there are others corresponding to all terms in a Fourier expansion of the operator.[49,50] The diagonal elements, which we have used, are the appropriate ones for a θ-independent electric field, F, in the ring, such as that due to a time varying flux; i.e., $F_\theta=-c^{-1}\partial A_\theta/\partial t$. Our model, therefore, does *not* apply to a ring with current flowing between contacts. The latter case is briefly discussed in Sec. III.

We proceed by assuming a form for $V(\theta)=V_0 f(\theta)$ using a basis set of $\mid n \mid \leq N$ wave functions of $\mathcal{H}_0$ and numerically diagonalizing the $(2N+1)\times(2N+1)$ matrix of Eq. (7) with $N=16$. The initial values of the matrix $V_{n',n}$ were evaluated as the Fourier transform of $V(\theta)$:

$$\begin{aligned}&f(\theta)=\sum_{k=-2N}^{2N}G_k e^{ik\theta} ,\\ &V_{n',n}=V_0 G_k \delta_{k+n,n'} .\end{aligned} \tag{9}$$

Because the energies and velocities are periodic in Φ, we restricted the calculation to values of Φ between ± 0.5. We thus obtain the energies E_i and the transformation matrix, which diagonalizes $\mathcal{H}$. Utilizing the latter, we compute the velocity matrix v_{ij} in the new representation for insertion into Eq. (6). The density matrix ρ_{ij} is diagonal in this representation, and its values were calculated from the Fermi function f at the assumed temperature T, with the Fermi level determined by the number of electrons which we have usually taken equal to or less than N.

We have tried various forms for the function $f(\theta)$ including the following: (a) a single δ function, (b) several $(<N)\delta$ functions at random positions around the ring, (c) a normally distributed random function. We find that the qualitative character of our results in their dependences on T, η, and V_0 are only weakly influenced by the choices of N, $f(\theta)$, and the number of electrons; this holds even for the single δ function scatterer of case (a).

III. RESULTS

In Fig. 1 one of the random potentials used is shown (for $-\pi \leq \theta \leq \pi$) along with its energy levels as functions of ϕ/ϕ_0. (Note that in all figures energies are in units of $\hbar^2/2mR^2$; σ is in units of $2e^2R/\pi\hbar$; temperature T and

level width η are in units of the average level separation $\Delta E_{\rm AV}$.) A series of computed curves of $\sigma(\phi/\phi_0)$ for that potential at a number of increasing temperatures keeping η constant is given in Fig. 2. The crossover of the fundamental periodicity from ϕ_0 to effectively $\phi_0/2$ is clearly seen.

We note that the averaged $\sigma(\phi)$ is maximal at $\phi=0, \pm\phi_0/2$, which does not agree with the coherent backscattering picture, in which σ is minimal at those points.[11,24] The different behavior in our model results partly because the smallest energy denominators in Eq. (6) occur at the above points, especially for weak disorder. More importantly, however, the velocity matrix elements which we have used do not connect pure states, $|n\rangle$, and so are greatest where mixing of the states is greatest. Both these effects produce maximal ac absorption ($\propto[|v_{ij}|/(E_i-E_j)]^2$), and therefore maximal conductivity, at $\phi=0, \pm\phi_0/2$. In the purely 1D case considered here, this effect is stronger than the effect of coherent backscattering. We leave open the question of the relevance of this effect for finite cross section, not purely 1D, systems.

For this particular case, $\sigma(\phi/\phi_0)$ is very nonsinusoidal and has many higher harmonics. Figure 3 shows the strengths of the successive (nth) harmonics as functions of n for different temperatures. At low temperatures this strength varies monotonically with n, while at higher temperatures the odd harmonics ($\phi_0,\phi_0/3,\ldots$) are considerably averaged out and the even harmonics ($\phi_0/2,\phi_0/4,\ldots$) are much stronger. Figure 4 depicts the strengths of the ϕ-independent part, fundamental, and second-harmonic components as functions of temperature. It is clearly seen that the fundamental decreases sharply at higher temperatures while the constant and second harmonic have similar temperature dependences and seem to

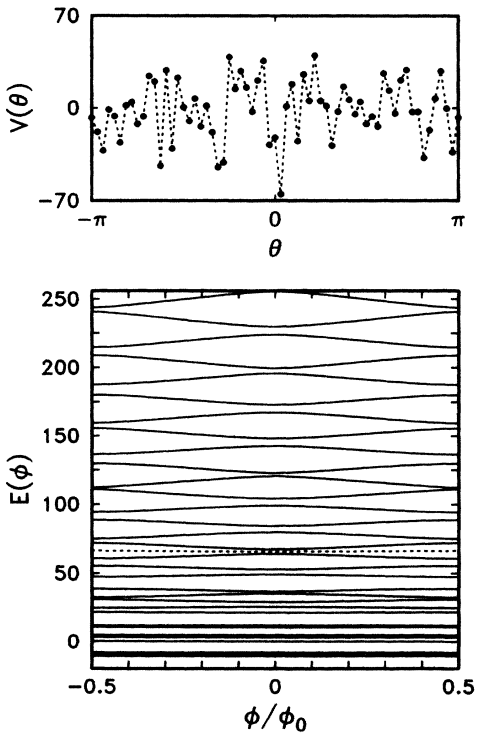

FIG. 1. Top: a "random" scattering potential $V(\theta)$ computed at 64 values of θ. (Dashed lines for visualization only.) This particular potential was used in calculating all the results shown in subsequent figures. Bottom: the first 32 energy levels E_n vs. ϕ/ϕ_0. The dashed line is E_F for 16 electrons.

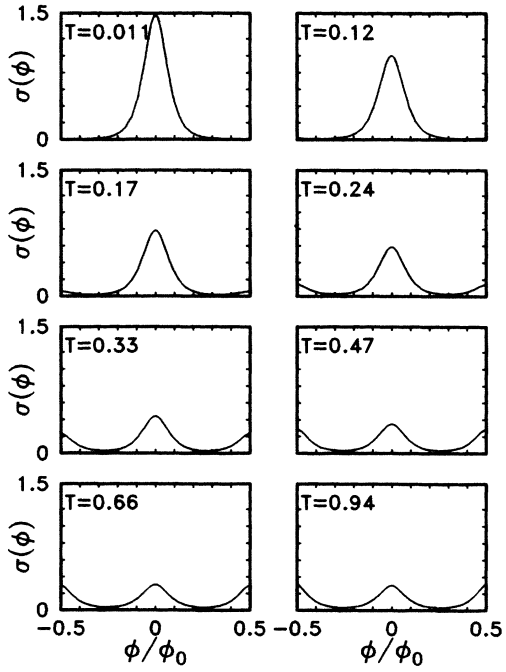

FIG. 2. σ vs ϕ/ϕ_0 at the eight indicated temperatures for $\eta=0.037$.

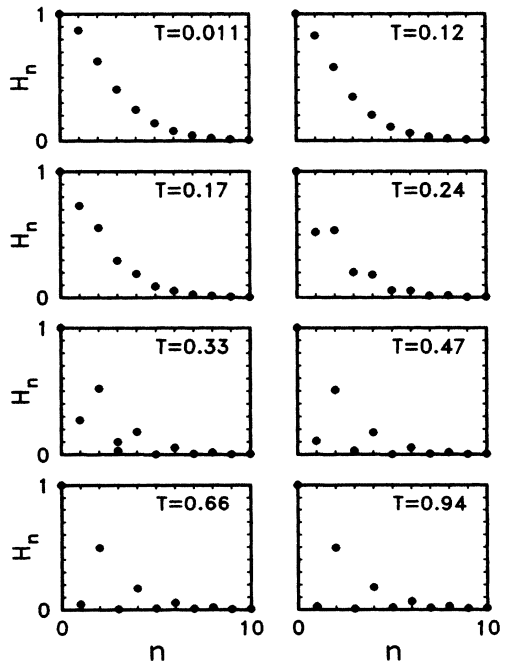

FIG. 3. Amplitudes of the first 10 harmonics, H_n (normalized to H_0), vs n corresponding to the conductivities shown in Fig. 2.

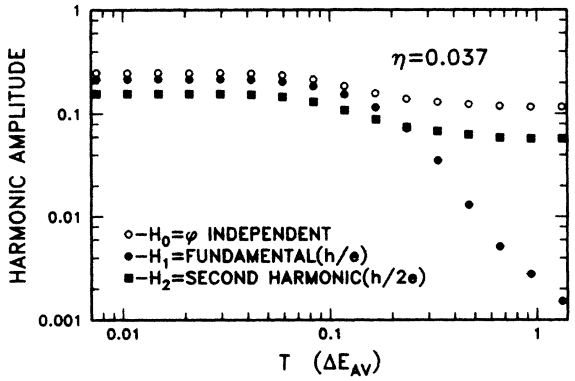

FIG. 4. H_0,H_1,H_2 as functions of temperature T for $\eta=0.037$.

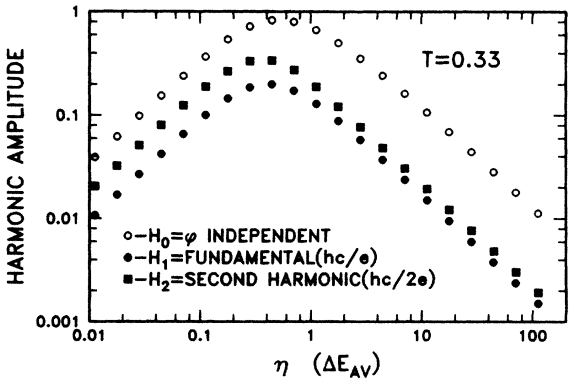

FIG. 6. H_0,H_1,H_2 as functions of η for $T=0.33$.

approach finite limits at high temperatures. The latter behavior is due to the fact that η was kept constant. The dependence of $\sigma(\phi/\phi_0)$ and the harmonics on $\eta=\hbar/\tau_{\text{in}}$ at constant T are shown in Figs. 5 and 6, which again demonstrate the averaging out of the fundamental and odd harmonics with increasing η. Surprisingly, it appears that the strengths of the ϕ-independent part, as well as those of the fundamental and second harmonic decrease with increasing η roughly like η^{-1} and not exponentially, as found in the weak-localization calculation.[11] This behavior appears to be a special property of the strictly 1D model considered.

As mentioned above, the phase of the oscillation in $\sigma(\theta)$ appears to be the correct one for the strictly 1D case with the particular field configuration we have chosen. However, we note that had we considered instead an electric field pointed in the same direction on opposite halves of the loop, corresponding to a voltage applied across the ring at contact points differing in θ by π, then we would expect the phase of the oscillation to be opposite to that found in the present case. This is because for that configuration the appropriate velocity matrix elements come from higher-order terms in the Fourier expansion of the velocity operator. These elements connect pure states but only weakly connect nearly degenerate states i,j which occur at $\phi=0,\pm\phi_0/2$. It follows that the absorption will be minimal at these points and the resulting phase in $\sigma(\theta)$ will agree with the results in Refs. 11 and 24. We have carried out a preliminary calculation which indicates the correctness of the above argument in the 1D case. Whether the argument also applies to a finite thickness multichannel ring remains to be seen.

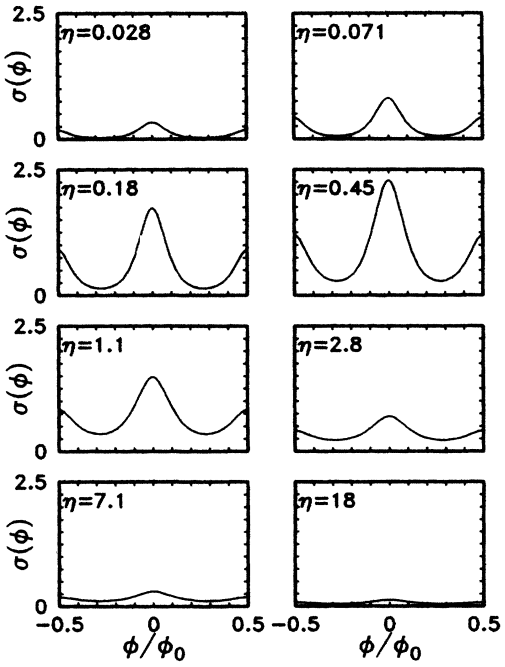

FIG. 5. σ vs ϕ/ϕ_0 at the eight indicated values of η for $T=0.33$.

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APPENDIX

The absorption can be fully treated in the following way. A monochromatic low-frequency emf, $V=-c^{-1}\partial\phi/\partial t$ is introduced, starting from a given level i. In the adiabatic approximation the energies vary in accordance with the time-dependent flux and the relaxation processes try to maintain equilibrium with the bath. This leads to a Debye relaxation-type absorption, previously obtained by Landauer and Büttiker[45] for a dc field, and by Büttiker[46] for an rf field. The contribution of Eq. (3) is obtained thru the admixture of the higher-lying states j in the adiabatic approximation. These are given by

$$a_{ij}=\frac{\hbar e V v_{ij}}{L(E_j-E_i)^2}(e^{i(E_j-E_i)t/\hbar}-1)\ . \tag{A1}$$

The adiabatic approximation is valid in the small V limit because then the a_{ij} are small.

The absorption of Eq. (6) is obtained by assuming that the relaxation processes bring the populations to equilibrium (with random phases) after each collision time τ, and evaluating the energy flow to the bath. The relaxation contribution of Landauer and Büttiker and the direct transition contribution of Eq. (6) are *different* and depend on different parameters. We have only considered the latter contribution. Note that the former, for example, vanishes in the $T\rightarrow 0$ limit.

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