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Effects of channel opening and disorder on the conductance of narrow wires

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The crossover from ballistic to diffusive transport in narrow two-dimensional conductors is studied as a function of Fermi energy and disorder. For an ordered sample, conductance quantization is confirmed. As the disorder is increased, the sharp conductance steps as a function of Fermi energy are rounded and preceded by pronounced dips. The origin of these dips is explained in terms of "level repulsion" between Lyapunov exponents of the total transfer matrix. For even larger disorder, the channel-opening signature in a given sample is obscured by universal conductance fluctuations. However, this structure can be restored, even for samples longer than the elastic mean free path, by ensemble averaging over different realizations of the disorder. The conditions for carrying out experimentally such an ensemble averaging are specified.

Both ballistic and diffusive quantum transport have attracted considerable interest in recent years. The conductance of ballistic constrictions induced in a high mobility two-dimensional (2D) electron gas was discovered experimentally[1-3] to be quantized in multiples of $2e^2/h$, reflecting the discrete number of the conducting channels in narrow constrictions, each channel characterized by a transmission coefficient of unity. At the other end, in the diffusive regime, the so-called universal conductance fluctuations (UCF) were found theoretically and observed experimentally in a large number of systems. Recently, Hirayama, Saku, and Horikoshi[4,5] have observed conductance fluctuations in transport through narrow channels which they attributed to elastic scattering in the constriction region. The link between ballistic[6] and diffusive transport in constrictions is also the subject of this Rapid Communication where we report on a systematic numerical study of the role of disorder in transport through narrow channels at low temperatures. In particular, we show that in the presence of a weak disorder ($l \gtrsim L,M$ where l is the elastic mean free path and L,M are the channel length and width in atomic units, respectively) the jumps characterizing conductance quantization start to smear and are preceded by pronounced dips in the conductance each time a new channel is about to be opened (enhanced scattering). For a stronger disorder ($L,M > l$, but still in the delocalized regime), UCF dominate the conductance and obscure the characteristic structure due to channel opening. This structure can be restored, even for moderate disorder, by ensemble averaging over different realizations of the disorder, since this procedure averages out the UCF and only the channel-opening structure remains. Experimentally this procedure amounts to either a measurement at temperatures much higher than the Thouless energy, $V_T = \hbar D/L^2$ (D is the diffusion coefficient), or to an average over magnetofingerprints at many values of the magnetic field covering a range larger than ϕ_0/LM, where ϕ_0 is the quantum flux unit (we assume that the relevant dimensions are smaller than the phase coherence length).

In our simulations we use the two-terminal[7] Landauer[8-10] formula for the conductance between two particle reservoirs bridged by the narrow system under consideration. The assumptions and limitations associated with this formula are discussed elsewhere.[10-12] Reference 7 shows that conductance steps follow from this formula for an ideal system. We employ two methods previously used to study transport through disordered conductors. To study the behavior of the Lyapunov exponents of the total transfer matrix we adopt a method based on the Oseledec theorem which was first used in this context by Pichard[13] and is also documented in Ref. 14. The samples studied by this method consisted of 2D strips, 15 sites wide and up to 10000 sites long. To extract the exponents of an infinite sample from the finite ones, an extrapolation procedure was employed as detailed in Ref. 15. The Lyapunov exponents method fails to yield the precise conductance of a finite length sample. To that end we have adopted the Green's-function method first used by Fisher and Lee[16] (see also Lee and Stone).[17] Using that method, the conductance of squares up to 15×15 sites was calculated accurately. The Hamiltonian in both cases was a nearest-neighbors two-dimensional tight-binding Hamiltonian with diagonal disorder (Anderson model).

$$H = \sum_{n,m} |n,m\rangle \varepsilon_{nm} \langle n,m| + \sum_{\substack{n,m \\ n',m'}}{}' |n,m\rangle V \langle n'm'| , \qquad (1)$$

where the prime indicates sum over nearest neighbors only. The site energies ε_{nm} were assumed to be uniformly distributed in the range $[-W/2, W/2]$. Energies will be

given in units of V, where the zero-disorder bandwidth is $B=8$.

The results presented here were obtained for rigid boundary conditions in the transverse direction. Similar calculations for periodic boundary conditions yielded identical results (except for the exact values for the energies corresponding to channel opening) implying that the effects described below do not crucially depend on boundary conditions.

The dimensionless conductance g of a 15×15 square as a function of energy, for an increasing amount of disorder is depicted in Fig. 1. For $W=0$ (ordered case) g varies in the expected steplike fashion where each step corresponds to an opening of a new conducting channel as is well known by now. As the disorder is decreased the average conductance decreases monotonically. For $W\sim4$, $g\sim1$, in agreement with previous studies of localization in 2D systems.[18] The average conductance is sensitive to the energy near the band edge and becomes practically energy independent closer to the band center. This point is further discussed later. The fluctuations are extremely sensitive to the disorder. For $W=0.5$, where g is reduced by only 20% compared with the ideal case, the conductance steps are already substantially rounded and are preceded by distinctive dips. For a somewhat larger disorder, when the elastic mean free path becomes shorter than the sample's length, the steps are not discernible (see Fig. 1) since the UCF are now fully developed.

The results depicted in Fig. 1 characterize transmission through a specific realization of the disorder. The results of an ensemble averaging over 50 realizations are shown in Fig. 2. We find that the averaging process eliminates most of the UCF and reveals the structure due to channel opening which can now be seen even for a mean free path

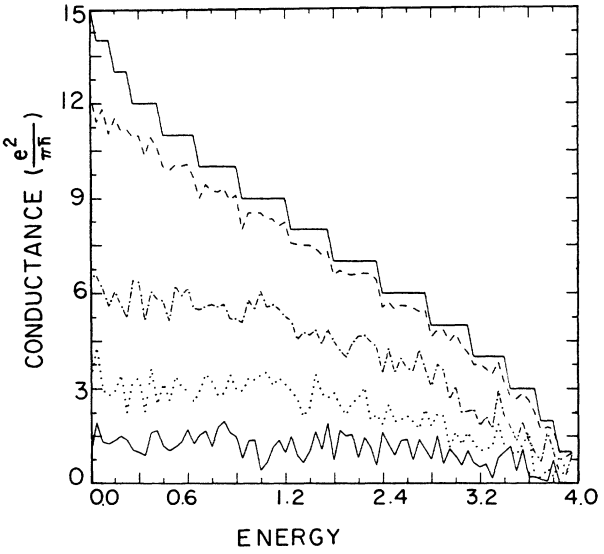

FIG. 1. Conductance $g=\mathrm{tr}(tt^+)$ as function of energy, disorder $W=0$, 0.5, 1.5, 2.5, and 4.0 corresponding to mean free paths (calculated in 2D and effective-mass approximation) of ∞, 100, 11, 5, and 1.5, respectively (upper curves for small disorder). Sample geometry 15×15, calculation using Green's function.

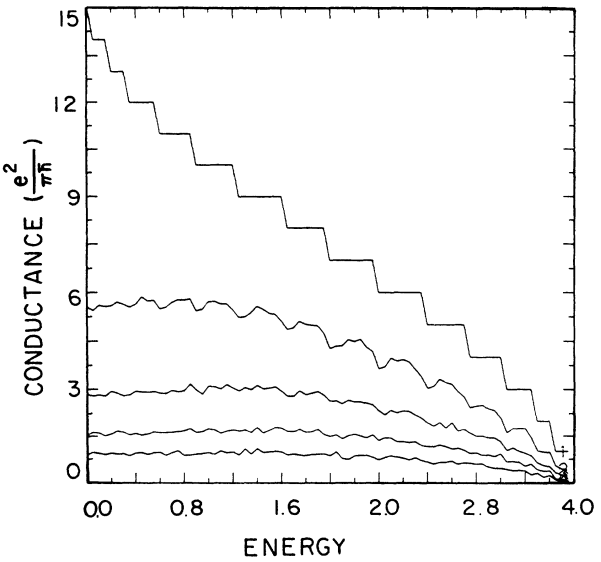

FIG. 2. Conductance $g=\mathrm{tr}(tt^+)$ as function of energy, ensemble averaged over 50 different samples having the same geometry 15×15 and the same disorder was taken for each of the curves. $W=0$, 1.5, 2.5, 3.5, and 4.5 (upper curves for smaller disorder). Calculation using Green's function.

which is a few times smaller than the sample's dimensions. We emphasize that such an averaging can be easily realized experimentally by using temperatures larger than the Thouless parameter $V_T=\hbar D/L^2$ (and smaller than the energy separation between the different channels), by scanning the Fermi energy over an energy range within the above interval, or by averaging over different magnetoprints taken at magnetic fields covering many intervals of ϕ_0/LM. To verify that such an energy interval indeed exists we notice that the energy spacing between adjacent transverse states is roughly given by $\delta E=\pi E_F/k_F w$ (where w is the channel width). Substituting $v_F l/2$ for D one thus obtains $V_T/\delta E=wl/\pi L^2\ll1$, a condition which can easily be satisfied experimentally by choosing the right dimensions and disorder.

Next we consider the conductance saturation as the Fermi energy is increased (for $W>0$). The two-terminal conductance of a finite sample is given by[13]

$$g=\mathrm{tr}(tt^+)=\sum_{i=1}^{M}\frac{2}{\cosh(2L/\xi_i)+1}\,, \tag{2}$$

where ξ_i is the decay length of the ith eigenfunction of the total transfer matrix. As conjectured by one of us[19] (see also Ref. 20), the $1/\xi_i$ are roughly equally spaced (Wigner repulsion) such that $1/\xi_i\sim i/Ml$. For $L>l$ it follows then from Eq. (2) that only $M_{\mathrm{eff}}\approx lM/L\approx g$ channels contribute to the conduction and opening of new channels with $\xi<L$ will not increase the conductance. These features are clearly observed in both Figs. 1 and 2. As the disorder is increased, $M_{\mathrm{eff}}\approx g$ is reduced and the energy at which the conductance saturates shifts towards the band edge.

Finally, we turn to discuss the pronounced dips in the conductance each time a new channel is about to be turned on. The Lyapunov exponents of a strip of 15×10000 sites are depicted in Fig. 3 for $W=1.5$. It is

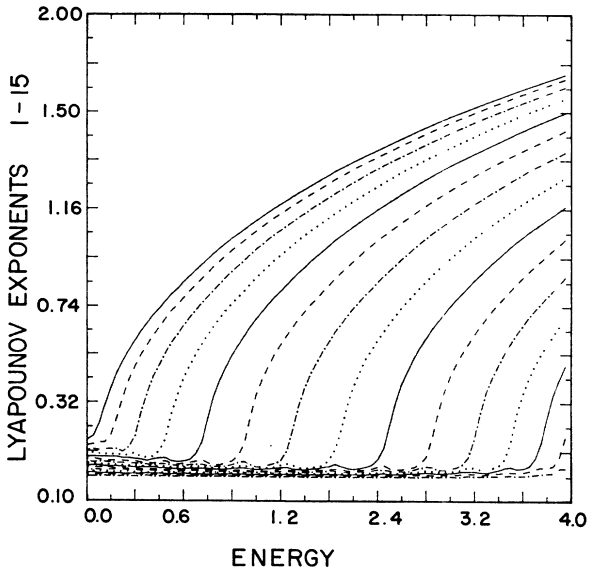

FIG. 3. Lyapunov exponents 1-15 (starting from the right-hand side of the figure) as functions of energy. Calculation using a transfer matrix for a strip of 15×10000 sites and disorder $W=1.5$.

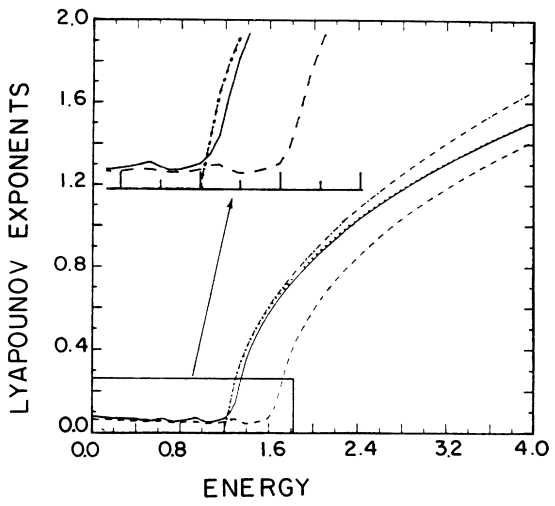

FIG. 4. Lyapunov exponents as function of energy calculated using a transfer matrix. Dashed and solid lines for Lyapunov exponents 9,10 ($W=1.5$); dotted line for Lyapunov exponent 10 ($W=0$); dash-dotted line for the function $(\varepsilon_F-E_{ci}-2)^{1/2}$. Inset shows the blowup of the region of vanishing of the exponents.

clear from Fig. 3 that any channel opening is accompanied by an increase in the Lyapunov exponents of other states and in particular the adjacent ones. The elastic mean free path is much shorter than L ($l\approx10$) thus excluding the possibility of any resonances of the type discussed, for example, by Szafer and Stone.[6] We argue that the origin of the increase in the Lyapunov exponents each time a new channel is opened is due to enhanced scattering from all other channels (and particularly neighboring ones) to the new one. Since the longitudinal energy of a barely open channel is small, this channel is localized and reflects many of the incoming electrons to backwards propagating states. Such a mechanism will indeed result in conductance dips each time a new channel is opened. The effect also exists as the evanescent channel is about to be opened. Such dips have been observed experimentally by Hirayama and co-workers[4,5] and during the final preparation of this paper, similar effects were found analytically by Bagwell[21] for a model with a single attractive δ-function impurity.

More detailed information is given in Fig. 4 where four curves appear as a function of band energy: dashed and solid lines for Lyapunov exponent 9,10 (out of 15 shown in Fig. 3), Lyapunov exponent 10 for an ordered system in a dotted line, and the fourth curve, in a dash-dotted line, for the function $(\varepsilon_F-E_{ci}-2.0)^{1/2}$ where $E_{ci}\equiv\cos[\pi i/(m+1)]$ is the transverse energy of the ith state and $i=10$. [The last curve is the first-order expansion of $\cos(k_i)$ where k_i is the longitudinal momentum.] In the ordered case the k_i's are the Lyapunov exponents. It is seen that Lyapunov exponent 10 of the ordered system coincides with that of the disordered system over much of the range so they have practically the same "effective critical exponent" of $\frac{1}{2}$ even for relatively strong disorder $W=1.5$. The "resonance" in Lyapunov exponent 9 appears when channel 10 is opened resulting in a conductance dip. When the energy is further increased the localization length of the new channel increases and becomes comparable to L (for a short enough system).

To summarize, a systematic numerical study was done on how disorder modifies the conductance steps due to channel opening and smears them via the UCF. A suitable ensemble averaging (feasible experimentally) can average out the latter and make the characteristic structure due to channel opening visible even for $l<L$. These structures may exist in experiments looking at UCF and it is an interesting question to what extent they might increase the size of the latter.

Note added. After submitting this paper, the authors learned about theoretical calculations on a related problem by Kramer[22] as well as experimental results by Gao *et al.*[23] The subband opening effects observed in this work are in qualitative agreement with our results.

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