Nanowires with Surface Disorder: Giant Localization Lengths and Quantum-to-Classical Crossover

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We investigate electronic quantum transport through nanowires with one-sided surface roughness. A magnetic field perpendicular to the scattering region is shown to lead to exponentially diverging localization lengths in the quantum-to-classical crossover regime. This effect can be quantitatively accounted for by tunneling between the regular and the chaotic components of the underlying mixed classical phase space.

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Transport through a disordered medium is a key issue in solid state physics which comprises countless applications in (micro-) electronics and optics [1]. The ubiquitous presence of disorder plays a prominent role for the behavior of transport coefficients governing, e.g., the metal-insulator transition [2]. The interest in disordered media has recently witnessed a revival due to new experimental possibilities to study the "mesoscopic" regime of transport where a quantum-to-classical crossover gives rise to a host of interesting phenomena [3].

In most investigations a static disorder is assumed to be present in the *bulk* of a material. The strength and distribution of the disorder potential determine whether transport will be ballistic, diffusive, or suppressed in the localization regime [1,3]. In nanodevices the reduction of system sizes leads, however, to an increased surface-to-volume ratio, for which *surface roughness* can represent the dominant source of disorder scattering. While random matrix theory (RMT) is successful in describing bulk disordered systems [4], its application to wires with surface disorder is not straightforward [5].

In the present Letter we study electronic quantum transport through a nanowire in the presence of one-sided surface disorder and a magnetic field. We show both numerically and analytically that by increasing the number of open channels N in the wire, or equivalently, by increasing the wave number k_F, the localization length ξ increases exponentially. Using a numerical approach that allows to study extremely long wires we show an increase by a factor 10^7 (Fig. 1). Such a giant localization length falls outside the scope of RMT predictions, $\xi \propto N$, previously studied for this system [6]. Instead it can be understood in terms of the underlying mixed regular-chaotic classical motion in the wire. We find that the conductance through the wire is controlled by tunneling from the regular to the chaotic part of phase space. This process, often referred to as "dynamical tunneling" [7], has been actively studied in quantum chaos and plays an important role in the context of classically transporting phase-space structures [8–12]. Here we establish a direct quantitative link between the exponential increase of the localization length in mesoscopic systems and the suppression of tunneling from the regular to the chaotic part of phase space in the semiclassical limit.

We consider a 2D wire with surface disorder to which two leads of width W are attached (Fig. 1, inset), with a homogeneous magnetic field B perpendicular to the wire present throughout the system. We simulate the disorder by a random sequence of vertical steps. The wire can thus be assembled from rectangular elements, referred to in the following as modules, with equal width l, but random

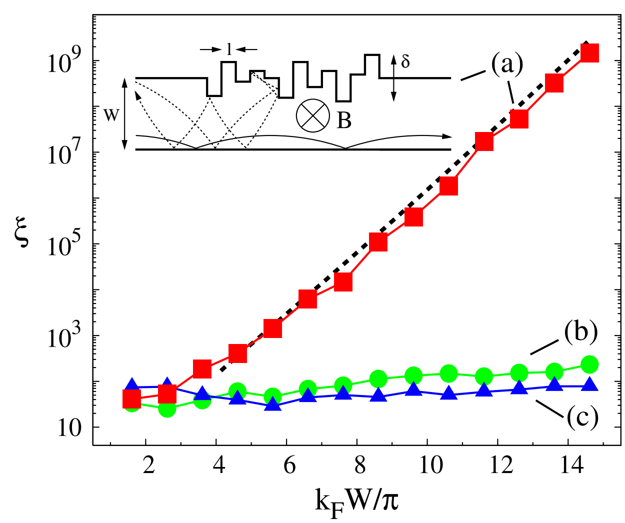

FIG. 1 (color online). Localization length ξ for a wire with surface roughness vs $k_F W/\pi = 1/h_{\mathrm{eff}}$. Results are compared for wires with (a) one-sided disorder (OSD) with $B \neq 0$ (red ■), (b) OSD with $B = 0$ (green ●), and (c) two-sided disorder with $B \neq 0$ (blue ▲). In (a) an exponential increase of ξ is observed in excellent agreement with Eq. (8) which has no adjustable parameters (dashed line).

heights h, uniformly distributed in the interval $[W - \delta/2, W + \delta/2]$. This particular representation of disorder allows for an efficient numerical computation of quantum transport for remarkably long wires $L \to \infty$ by employing the modular recursive Green's function method [13]. We first calculate the Green's functions for $M = 20$ rectangular modules with different heights. A random sequence of these modules is connected by means of a matrix Dyson equation. Extremely long wires can be reached by implementing an "exponentiation" algorithm [14]: Instead of connecting the modules individually, we iteratively construct different generations of "supermodules", each consisting of a randomly permuted sequence of M modules of the previous generation. Repeating this process leads to the construction of wires whose length increases exponentially with the number of generations [15].

The transmission (t_{mn}) and reflection amplitudes (r_{mn}) for an electron injected from the left are evaluated by projecting the Green's function at the Fermi energy E_F onto all lead modes $m, n \in \{1, \ldots, N\}$ in the entrance and exit lead, respectively. Here $N = \lfloor k_F W/\pi \rfloor$ is the number of open lead modes and k_F the Fermi wave number. We obtain the localization length ξ in a wire composed of L modules (i.e., length Ll) by analyzing the dimensionless conductance $g = \mathrm{Tr}(t^\dagger t)$ in the regime $g \ll 1$, extracting ξ from $\langle \ln g \rangle \sim -L/\xi$. The brackets $\langle \cdots \rangle$ indicate the ensemble average over 20 different realizations of disorder and 3 neighboring values of wave numbers k_F.

For increasing k_F, we adjust the magnetic field B such that the cyclotron radius $r_c = \hbar k_F/(eB)$ remains constant. This leaves the classical dynamics invariant and allows for probing the quantum-to-classical crossover as $k_F \to \infty$. We choose $r_c = 3W$ and a disorder amplitude $\delta = (2/3)W$ such that we obtain a large regular region in phase space (see below) and use a module width $l = W/5$. We find for one-sided disorder an exponential increase of the localization length ξ (Fig. 1), while ξ remains almost constant when either (i) the magnetic field is switched off or (ii) a two-sided disorder is considered. The latter clearly rules out that the observed giant localization length is due to edge states of the quantum Hall effect [3].

Before giving an analytic determination of the exponentially increasing localization length, we provide an explanation invoking the mixed classical phase-space structure which captures the essential features of this increase.

The classical dynamics inside the disordered wire is displayed by a Poincaré section in Fig. 2(b), for a vertical cut at the wire entrance ($x = 0$) with periodic boundary conditions in the x direction. The resulting section (y, p_y) for $p_x > 0$ shows a large regular region with invariant curves corresponding to skipping motion along the lower straight boundary of the wire. Close to the upper disordered boundary ($y > W - \delta/2$) the motion appears to be chaotic for all p_y. A corresponding Poincaré section for $p_x < 0$ (not shown) is globally chaotic. The lowest transverse

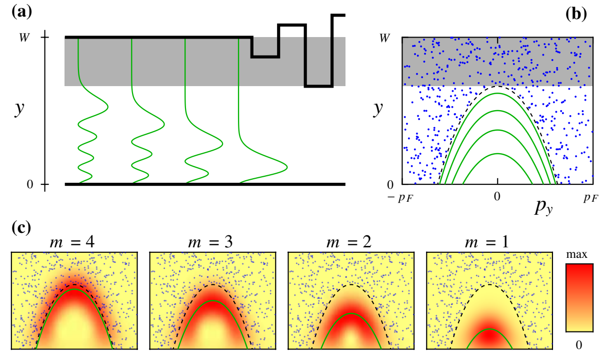

FIG. 2 (color online). (a) Nanowire with the regular transverse modes (green) $m = 4$, 3, 2, 1 for $k_F W/\pi = 14.6$. The gray shaded part indicates the y range affected by disorder. (b) Poincaré section showing a large regular island with outermost torus (dashed), a chaotic sea (blue dots), and quantized tori corresponding to the regular modes (green). (c) Poincaré-Husimi functions of these modes and their quantizing tori.

modes [Fig. 2(a)] of the incoming scattering wave functions overlap primarily with the regular island [Fig. 2(b)]. Only their exponential tunneling tail through the diamagnetic potential barrier (in Landau gauge)

$$V(y) = \tfrac{1}{2} m_e \omega_c^2 (y - y^0)^2 - E_F \tag{1}$$

touches the upper disordered surface at $y > W - \delta/2$. In Eq. (1), m_e is the electron mass, ω_c the cyclotron frequency, and y^0 the guiding center coordinate. These regular modes can be semiclassically quantized as [16,17]

$$\frac{A}{h} = \frac{B\mathcal{A}}{h/e} = (m - 1/4) \quad \text{with} \quad m = 1, 2, \ldots, \tag{2}$$

where A is the area in the Poincaré section enclosed by a quantized torus and $\mathcal{A} = r_c A/p_F$ is the area in position space enclosed by a segment of a skipping orbit. One finds $A = p_F r_c[\arccos(1-\nu) - (1-\nu)\sqrt{1-(1-\nu)^2}]$ for $0 \le \nu \le \nu_{\max} \le 1$, where νr_c is the y position at the top of the cyclotron orbit. The size A_{reg} of the regular island is found for $\nu = \nu_{\max} = (W - \delta/2)/r_c$. The Poincaré-Husimi projections (i.e., projections onto coherent states of the transverse eigenfunctions) show, indeed, a density concentration near the quantized tori residing in the regular region of phase space [Fig. 2(c)].

The lowest mode $m = 1$ in the center of the island has the smallest tunneling rate [8,18,19]

$$\gamma_1 \sim \exp\left(-C \frac{A_{\mathrm{reg}}}{h}\right) \tag{3}$$

to the chaotic sea with some constant C (see below). Its temporal decay $\exp(-\gamma_1 t)$ together with its velocity $v_1 = \hbar k_x/m_e$ lead to an exponential decay as a function of propagation length x, $\exp(-\gamma_1 x/v_1)$. This gives a localization length $\xi \sim \gamma_1^{-1}$ [10]. When increasing k_F, while keeping the cyclotron radius r_c fixed, the classical dynamics remains invariant while the island area scales as $A_{\rm reg} = a_{\rm reg}A_{\rm PS}$. Here $A_{\rm PS} = 2p_F W$ is the area of the Poincaré section and $a_{\rm reg}$ is the relative size of the island. This semiclassical limit is thus equivalent to decreasing the effective Planck's constant $h_{\rm eff} := h/A_{\rm PS} = (k_F W/\pi)^{-1}$ and results in an exponential increase of the localization length

$$\xi \sim \exp\left(C\frac{a_{\rm reg}}{h_{\rm eff}}\right), \tag{4}$$

for $h_{\rm eff} \to 0$, qualitatively explaining Fig. 1(a). Moreover, this exponential increase should set in when the first mode fits into the island, i.e., for $A_{\rm reg}/h \approx 1$. For the parameters of Fig. 1(a) we have $\nu_{\rm max} = 2/9$, resulting in the critical value $k_F W/\pi \approx 3.5$, which is in very good agreement with the numerical result. By contrast, for two-sided disorder or for $B = 0$ no regular island with skipping orbits exists and ξ shows no exponential increase; see Fig. 1.

We now turn to an analytical derivation of the localization length using the specifics of the scattering geometry (Fig. 1 inset). To this end we first calculate the transmission amplitude t_{11} of the transverse regular mode $m = 1$ by considering its consecutive projections from one module to the next

$$t_{11} \approx \prod_{j=1}^{L-1} \int_0^{W+\delta/2} \chi_{h(j)}(y)\chi_{h(j+1)}(y)dy, \tag{5}$$

where $\chi_{h(j)}(y)$ is the mode wave function in module j with height $h(j)$. Equation (5) amounts to a sequence of *sudden approximations* for the transition amplitude between adjacent surface steps. As the wave function is exponentially suppressed at the upper boundary, the scale lk_F introduced by the corners drops out of the calculation. For simplicity, a few technical approximations have been invoked, whose accuracy can be checked numerically: (i) terms in the transmission from one module to the next that involve reflection coefficients and are typically smaller by a factor of 5 are neglected, (ii) contributions from direct coupling between different island modes are neglected, and (iii) the factor $(2y - y^0_{h(j)} - y^0_{h(j+1)})$ from the orthonormality relation for the χ functions [13] is omitted in the above integral as its contribution is negligible.

The modes pertaining to different heights h can be written as $\chi_h(y) = [\chi_\infty(y) - \varepsilon_h(y)]/N_h$, where $\chi_\infty(y)$ is the mode wave function if there was no upper boundary, $\varepsilon_h(y)$ is the correction that is largest at the upper boundary [where $\chi_h(h) = 0$], and N_h is a normalization factor. Keeping only terms of order $O(\varepsilon_h)$ and using a WKB approximation for $\varepsilon_h(y)$ around $y = h_{\rm min} = W - \delta/2$ leads to

$$t_{11} \approx (1-\sigma)^{2L/M} \quad \text{with} \quad \sigma = \frac{\chi^2_\infty(h_{\rm min})}{k_F\sqrt{V(h_{\rm min})/E_F}}. \tag{6}$$

According to Eq. (6) the coupling strength is quantitatively determined by the tunneling electron density at $y = h_{\rm min}$ in the classically forbidden region of the 1D diamagnetic potential, Eq. (1). The conductance in the regime $g \ll 1$ is now given by

$$g = |t_{11}|^2 \approx \exp(-4\sigma L/M), \tag{7}$$

resulting in a localization length $\xi = M/(4\sigma)$. Using a WKB approximation for $\chi_\infty(y)$ we find

$$\xi(h_{\rm eff}) \approx (ah_{\rm eff}^{-2/3} - b)\exp[ch_{\rm eff}^{-1}(1 - dh_{\rm eff}^{2/3})^{3/2}], \tag{8}$$

with coefficients $a = (16\pi^5)^{1/3}\zeta M\eta\rho^{-1/3}$, $b = -2\pi z_0\zeta M$, $c = \pi(32/9)^{1/2}\eta^{3/2}\rho^{-1/2}[1 + (3/20)\eta\rho^{-1}]$, $d = -z_0\rho^{1/3}/(2^{1/3}\pi^{2/3}\eta)$. Here $z_0 \approx -2.338$ is the first zero of the Airy function $\mathrm{Ai}(z)$, $\zeta = \int_{z_0}^\infty \mathrm{Ai}(z)^2 dz$, $\eta = h_{\rm min}/W$, and $\rho = r_c/W$ are dimensionless parameters [20]. Equation (8) is in very good quantitative agreement with the numerically determined localization length [Fig. 1(a)]. We conclude that tunneling from the regular phase-space island is primarily due to interaction of each regular mode with the rough surface rather than via successive transitions from inner to outer island modes.

We note that the constant C in Eqs. (3) and (4) is found to be $C = 2\pi[1 + (289/960)\eta\rho^{-1}]$, which differs from $C = 2\pi$ [19] and $C = 3 - \ln 4$ [18] derived for other examples of dynamical tunneling from a resonance-free regular island to a chaotic sea. We also note that the scaling behavior of ξ in Eq. (8) is reminiscent of previously obtained results for diffusive 2D systems (see [1]).

For the case of a constant magnetic field B, increasing k_F increases the cyclotron radius, $r_c \propto k_F$, and the classical dynamics is no longer invariant. In particular, the area of the regular island $A_{\rm reg} \sim \sqrt{k_F}$ shrinks compared to $A_{\rm PS} \sim k_F$ as skipping motion is increasingly suppressed. Nevertheless, the arguments leading to Eqs. (4) and (8) remain applicable and yield a localization length that increases dramatically as $\xi \sim \exp(\mathrm{const}\sqrt{k_F})$ in agreement with numerical observations (not shown).

Now we turn to the behavior of the conductance for wires of lengths smaller than the localization length. Modes with larger m have larger amplitudes near the rough surface and thus couple more strongly to the chaotic part of phase space. They have, consequently, larger tunneling rates γ_m and smaller localization lengths $\xi_m \sim \gamma_m^{-1}$. The successive elimination of modes as a function of the length L of the wire results in a sequence of plateaus [Fig. 3(a)]. For $L > \xi_m$ the mode m no longer contributes to transport, as can be seen by its individual contribution to the transmission in Fig. 3(b). This disappearance of regular modes is reflected in the averaged Poincaré-Husimi distributions calculated from incoherent superpositions of all modes entering from the left and scattering to the right. Also shown are the complementary distributions obtained for backscattering from right to right. For small L these Poincaré-Husimi functions are outside the regular island, while with increasing L they begin to "flood" it [11]. This

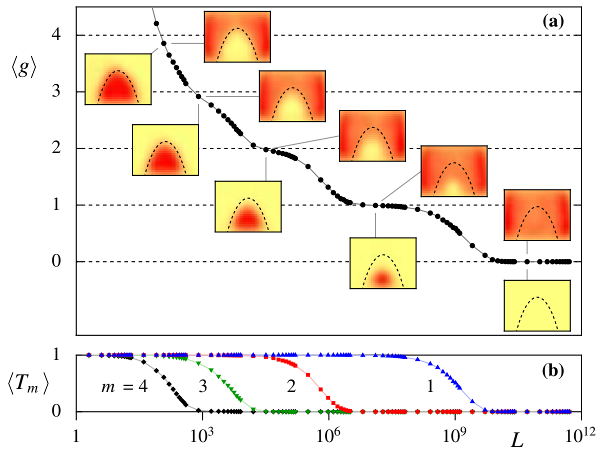

FIG. 3 (color online). (a) Averaged conductance $\langle g \rangle$ vs length L of the wire. The stepwise decrease is accompanied by the disappearance of the regular modes and the flooding of the island region by chaotic states. The Poincaré-Husimi distributions to the left (right) of the curve correspond to scattering from left to right (backscattering from right to right). (b) Transmission $\langle T_m \rangle$ of the incoming mode m vs L.

process is complete for lengths $L \gg \xi$. The complementarity of the Husimi distributions illustrates that tunneling between the regular island and the chaotic sea proceeds symmetrically in both directions, as required by the unitarity of the scattering matrix.

Summarizing, we have presented a numerical computation and an analytical derivation for the exponential increase of the localization length in a two-dimensional system of a quantum wire with one-sided surface disorder. Our approach, based on a mixed phase-space analysis, also explains the increase of ξ over 1 order of magnitude under increase of the magnetic field observed in Ref. [6]. It sets in for a magnetic field for which the regular island is large enough to accommodate at least one quantum mechanical mode. Clearly, the RMT result, $\xi \propto N$, which ignores the mixed phase-space structure, no longer applies. Instead, we find that the giant localization length (Fig. 1) in this disordered mesoscopic device is determined by the tunneling from the regular to the chaotic region, the rate of which is exponentially suppressed in the semiclassical regime.

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