Conductance fluctuations near the ballistic-transport regime

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The fluctuations in the electric conduction of a short disordered region are studied theoretically. The ensemble-averaged conductance and its fluctuations are calculated analytically in the single-site approximation. For a small number of impurities, the mean square of the fluctuations increases in proportion to the number of impurities, but is independent of the system size; i.e., each impurity contributes independently to the fluctuations. Numerical simulations confirm the analytical results. The amplitude of the fluctuations can be larger than the universal values in diffusive conductors when the impurity scattering potential is sufficiently strong. In terms of random matrix theory, the enhancement can be understood by a reduced spectral rigidity of the transmission matrix eigenvalues. [S0163-1829(96)00839-9]

I. INTRODUCTION

Quantum interference effects on transport in microstructures have been thoroughly investigated in the last decade.^{1,2} Universal conductance fluctuations (UCF's) of the order of the quantum unit of conduction e^2/h are a fundamental consequence of phase-coherent transport in disordered metals.³⁻⁶ In the diffusive limit, the amplitude of the fluctuations does not depend on the microscopic details of the disorder but only on the symmetry of the Hamiltonian, and can be thus classified into three universality classes. Recently, a random matrix theory⁷ of transport based on the Landauer-Büttiker scattering formalism^{8,9} has been invoked to explain the universality.¹⁰⁻¹² In this framework, the eigenvalues of the transmission matrix for disordered systems can be interpreted in terms of classical fictitious charges with a logarithmic repulsion, which has a strictly geometric origin. The universality of the conductance fluctuations can be traced back to the "spectral" rigidity caused by this long-range repulsion without involving the microscopic parameters of the system.

This approach is valid for conductors with a sufficiently large degree of disorder. The size of disordered region (L) must be sufficiently larger than the elastic mean free path of an electron at the Fermi energy (l_F). When this condition is fulfilled, the conductors are in the diffusive transport regime. Only in this regime does the symmetry of the Hamiltonian (e.g., orthogonal, unitary, and symplectic) govern the statistics of the transport properties. The situation is more complicated for conductors where L is of comparable magnitude with l_F , i.e., for the near-ballistic transport regime, in which universality may not taken to be granted. This was explicitly shown for transport through a disordered region much shorter than the average distance between the scatterers.¹³ This model represents a rough metallic heteropoint contact¹⁴ as relevant for the perpendicular giant magnetoresistance in magnetic multilayers.¹⁵⁻¹⁹ The diagrammatic calculation of the conductance fluctuations was carried out for a two-

dimensional system ("impurity necklace") in the Born approximation. The results revealed nonuniversal fluctuations, depending strongly on microscopic parameters like the impurity density, and scattering potential, which was caused by a predominantly attractive interaction between the eigenvalues of the transmission matrix. Experiments in this direction are now in progress by investigating transport through narrow disordered regions in the two-dimensional high-mobility electron gas.²⁰

A nonuniversal enhancement of the fluctuation is not an exclusive phenomenon of a disordered interface, however, but a general property of the nearly ballistic regime. Previously an enhancement of the fluctuations close to the ballistic limit was found for mesoscopic quantum wires.^{21,22} Phenomenological parameters called an "effective fluctuating domain" and "effective channels" were introduced to explain the enhancement of the fluctuations obtained in numerical simulations.²¹

In this paper, we study conductance fluctuations near the ballistic regime both analytically and numerically. Our work is motivated by the belief that it should be possible to derive an expression for the fluctuations by conventional perturbation theory, which should help to understand the numerical experiments fully. In the analytical method, we consider a wide strip of two-dimensional electron gas (width $W \gg l_F$) with a small number of impurities (N_i), and calculate the fluctuations using the Landauer-Büttiker conductance formalism and the single-site approximation.²³ Exact numerical simulations are performed on the two-dimensional single-band tight-binding model by the recursive Green-function method.^{24,25} For small N_i the fluctuation amplitudes are found to increase proportionally to $\sqrt{N_i}$, in disagreement with the Born approximation, which predicts a linear dependence.¹³ The amplitude of the fluctuations does not depend on the thickness of the disordered region. When the number of impurities is small, each impurity appears to contribute to the mean-square fluctuations independently. However, this statement is no longer true in the limit of many

impurities, when the amplitude of the fluctuations approaches the universal values. The numerical results demonstrate the enhancement of the fluctuations, which can be understood by a reduced spectral rigidity of the transmission matrix in the nearly ballistic regime as compared with the diffusive regime.¹³ Although the present results are obtained for a two-dimensional system, an extension to three-dimensional systems is straightforward.

The outline of this paper is as follows. In Sec. II, the transmission matrix is derived from the Lippmann-Schwinger equation. The conductance fluctuations are calculated within the single-site approximation in Sec. III. In Sec. IV, we perform numerical calculation in order to confirm the validity of the analytical results. In Sec. V we compare the fluctuations near the ballistic regime with that in the diffusive regime, and discuss the main results in terms of a purely classical model, which reproduce some features of the quantum mechanical results. The conclusions are summarized in Sec. VI.

II. TRANSMISSION COEFFICIENT

Let us consider the Hamiltonian in the two-dimensional continuum,

$$H(\mathbf{r}) = H_0(\mathbf{r}) + V(\mathbf{r}), \quad (1a)$$

$$H_0(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2(\mathbf{r}), \quad (1b)$$

$$V(\mathbf{r}) = \sum_{\mathbf{r}_i} V \delta(\mathbf{r} - \mathbf{r}_i), \quad (1c)$$

where V and $\mathbf{r}_i = (x_i, y_i)$ denote the potential and the position of the impurities, respectively. We assume that the impurities are distributed randomly. The system is unbounded in the direction of the electric current (x direction). In the direction normal to the current (y direction), the system width is W , and we use periodic boundary conditions. The eigenfunctions of $H_0(\mathbf{r})$ are given by

$$\phi_0^l(\mathbf{r}) = \alpha_l(y) e^{ik_l x}, \quad (2a)$$

$$\alpha_l(y) = \frac{1}{\sqrt{W}} e^{ik_y^l y}, \quad (2b)$$

$$E_F = \frac{\hbar^2}{2m} (k_y^l{}^2 + k_l^2) \equiv \frac{\hbar^2}{2m} k_F^2. \quad (2c)$$

Here E_F is the Fermi energy, and k_l and k_y^l are the momenta in the x and the y directions, respectively.

In order to calculate the wave function, we use the Lippmann-Schwinger equation

$$\psi^l(\mathbf{r}) = \phi_0^l(\mathbf{r}) + \int d\mathbf{r}' G_0(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') \psi^l(\mathbf{r}'). \quad (3)$$

Here $\psi^l(\mathbf{r})$ is an eigenfunction of $H(\mathbf{r})$. The unperturbed Green function $G_0(\mathbf{r} - \mathbf{r}')$ satisfies the equation

$$[E_F - H_0(\mathbf{r})] G_0(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \quad (4)$$

and is calculated to be

$$G_0(\mathbf{r} - \mathbf{r}') = -i \frac{m}{\hbar^2} \sum_{k_y} \frac{\alpha_l(y) \alpha_l^*(y')}{k_l} e^{ik_l |x - x'|}, \quad (5)$$

where k_l is the wave number which satisfies Eq. (2c). We assume that k_l is real and positive for propagating channels and is positive imaginary ($i\kappa_l$ with $\kappa_l > 0$) for evanescent channels. The divergent integral over wave numbers in Eq. (5) is assumed to be regularized by a suitable ultraviolet cutoff.

The wave function $\psi^l(\mathbf{r})$ can be expressed by the linear combination of $\phi_0^l(\mathbf{r})$'s in terms of the transmission and reflection coefficients $\tilde{t}_{l,l'}$ and $\tilde{r}_{l,l'}$ as

$$\psi^l(\mathbf{r}) = \begin{cases} \sum_{l'} \tilde{t}_{l,l'} \alpha_{l'}(y) e^{ik_{l'} x} & \text{for } x > L \\ \alpha_l(y) e^{ik_l x} + \sum_{l'} \tilde{r}_{l,l'} \alpha_{l'}(y) e^{-ik_{l'} x} & \text{for } x < 0. \end{cases} \quad (6)$$

We assume that the impurities are confined in a region with length L in the x direction, (i.e., $0 < x_i < L$), and we use the notation l instead of k_y^l for simplicity. Current conservation implies

$$\sum_m [|t_{l,m}|^2 + |r_{l,m}|^2] = 1, \quad (7)$$

with

$$t_{l,m} = \left(\frac{k_m}{k_l} \right)^{1/2} \tilde{t}_{l,m}, \quad (8)$$

$$r_{l,m} = \left(\frac{k_m}{k_l} \right)^{1/2} \tilde{r}_{l,m}. \quad (9)$$

Since we consider short-range impurity potentials [Eq. (1c)], Eq. (3) has a closed form with respect to the position of the impurities (i.e., $\mathbf{r} = \mathbf{r}_j$),

$$\psi^l(\mathbf{r}_j) = \phi_0^l(\mathbf{r}_j) + \sum_{\mathbf{r}_i} G_0(\mathbf{r}_j - \mathbf{r}_i) V \psi^l(\mathbf{r}_i). \quad (10)$$

Equation (10) is an exact relation between the $\psi^l(\mathbf{r}_i)$'s.

In this study, we concentrate on the electric transport through a constriction or wire which contains a small number of impurities. In what follows, we use a single-site approximation to estimate the wave function. This means that in the second term on the right-hand side of Eq. (10), we take into account only the contribution of the impurity at $\mathbf{r}_i = \mathbf{r}_j$, and neglect effects of other impurities. Multiple-scattering processes at one impurity are included in the approximation, but those involving many impurities are not taken into account. It is therefore evident that the approximation is valid for systems which contain a small number of impurities, and exact for a single impurity ($N_i = 1$). A more precise criterion for the validity of this approximation which also involves the scattering potential is derived below. The wave function at the impurities in this approximation is given by

$$\psi^l(\mathbf{r}_j) \approx \frac{\phi_0^l(\mathbf{r}_j)}{1 - G_0(0)V}. \quad (11)$$

FIG. 1. Feynman diagrams for the single-particle Green function in the single-site approximation.

Using Eq. (11), Eq. (3) becomes

$$\psi^l(\mathbf{r}) = \phi_0^l(\mathbf{r}) + \sum_{\mathbf{r}_i} G_0(\mathbf{r} - \mathbf{r}_i) V \left(\frac{\phi_0^l(\mathbf{r}_i)}{1 - G_0(0)V} \right). \quad (12)$$

The transmission coefficients are obtained by multiplying Eqs. (12) and (6) by $\alpha_m^*(y)$, and integrating with respect to y . The coefficient of $e^{ik_m x}$ in the expression for $x > L$ is

$$\tilde{t}_{l,m} = \delta_{l,m} - i \frac{m}{\hbar^2} \frac{V}{1 - G_0(0)V} \sum_{\mathbf{r}_i} \frac{\alpha_l(y_i) \alpha_m^*(y_i)}{k_m} e^{i(k_l - k_m)x_i}. \quad (13)$$

It is possible to obtain the coefficient $\tilde{r}_{l,m}$ from the expression for $x < 0$,

$$\tilde{r}_{l,m} = -i \frac{m}{\hbar^2} \frac{V}{1 - G_0(0)V} \sum_{\mathbf{r}_i} \frac{\alpha_l(y_i) \alpha_m^*(y_i)}{k_m} e^{-i(k_l - k_m)x_i}. \quad (14)$$

In order to understand the physical meaning of the present approximation as defined by Eq. (11), the single-particle Green function²⁴

$$t_{l,m} = i\hbar \left(\frac{\hbar k_l}{m} \frac{\hbar k_m}{m} \right)^{1/2} G_{l,m}(x, x') \Big|_{x' > L}^{x < 0} \quad (15)$$

is calculated as

$$G_{l,m}(x, x') = G_l^0(x, x') \delta_{l,m} + \frac{V}{1 - G_0(0)V} \times \sum_{\mathbf{r}_i} G_l^0(x, x_i) \alpha_l(y_i) \alpha_m^*(y_i) G_m^0(x_i, x'), \quad (16)$$

$$G_l^0(x, x') = -i \frac{m}{\hbar^2} \frac{1}{W} \frac{1}{k_l} e^{ik_l|x-x'|}. \quad (17)$$

The scattering processes taken into account in Eq. (16) are illustrated diagrammatically in Fig. 1. Thick and thin lines denote the full and unperturbed Green functions, respectively. The shaded triangle is the self-energy part, and broken lines connected with a cross in a circle denote impurity scattering. We see that the self-energy in Eq. (16) agrees with the conventional (non-self-consistent) single-site

approximation.²³ In the limit of a single impurity ($N_i \rightarrow 1$), Eq. (16) is an exact relation for the single-particle Green function. Physically, the effect of the impurity ensemble on the total wave function is obtained by summing up the contributions from each impurity incoherently.

For simplicity, we introduce the following short-hand notation for the transmission coefficient and the real-space Green function

$$t_{l,m} \equiv \delta_{l,m} - i c_{l,m} \beta, \quad (18)$$

$$c_{l,m} \equiv \frac{m}{\hbar^2} \frac{1}{\sqrt{k_l k_m}} \frac{1}{W} \sum_{\mathbf{r}_i} e^{i(k_y^l - k_y^m)y_i} e^{i(k_l - k_m)x_i}, \quad (19)$$

$$\beta \equiv \frac{V}{1 - G_0(0)V}, \quad (20)$$

$$G_0(0) \equiv -i\hbar_1 - h_2, \quad (21)$$

$$h_1 \equiv \frac{m}{\hbar^2} \frac{1}{W} \sum_{k_y^l} ' \frac{1}{k_l}, \quad (22)$$

$$h_2 \equiv \frac{m}{\hbar^2} \frac{1}{W} \sum_{k_y^l} '' \frac{1}{\kappa_l}. \quad (23)$$

Only the coefficients $c_{l,m}$ depend on the configuration of the impurity positions. The summations in Eqs. (22) and (23) are over all propagating (primed summation) and evanescent channels (double-primed summation), respectively. h_1 and h_2 are real and positive.

III. CONDUCTANCE AND CONDUCTANCE FLUCTUATIONS

The conductance (g) and the reflectance (r) (in units of e^2/h) are given by the Landauer-Büttiker formula(s)

$$\langle g \rangle = 2 \sum_{l,m} ' \langle t_{l,m}^* t_{l,m} \rangle, \quad (24)$$

$$\langle r \rangle = 2 \sum_{l,m} ' \langle r_{l,m}^* r_{l,m} \rangle, \quad (25)$$

where $\langle \rangle$ denotes the ensemble average over all different impurity configurations and the spin degree of freedom of an electron gives rise to the factor 2. With Eqs. (18), (19), and (20), the conductance becomes

$$\langle g \rangle = 2 \left\{ \sum_l ' - i \sum_l ' (\langle c_{l,l} \rangle \beta - \langle c_{l,l}^* \rangle \beta^*) + \sum_{l,m} ' |\beta|^2 \langle c_{l,m}^* c_{l,m} \rangle \right\}. \quad (26)$$

The average of the diagonal elements is

$$\langle c_{l,l} \rangle = \frac{m}{\hbar^2} \frac{1}{k_l} \frac{1}{W} \left\langle \sum_{\mathbf{r}_i} \right\rangle = \frac{m}{\hbar^2} \frac{1}{k_l} \frac{N_i}{W}, \quad (27)$$

where N_i is the number of impurities. We have to average the third term on the right-hand side of Eq. (26) consistently

with the basic approximation in Eq. (11). In other words, the vertex correction of the two-particle Green function must satisfy the current conservation law

$$g + r = 2\tilde{W}, \quad (28)$$

$$\tilde{W} \equiv \sum_l' \quad (29)$$

$$= \frac{W}{2\pi} \int_{-k_F}^{k_F} dk_y^l = \frac{Wk_F}{\pi}, \quad (30)$$

where $\tilde{W}$ is the number of propagating channels for each spin degree of freedom. The second-order term of $c_{l,m}$ reads

$$\langle c_{l,m}^* c_{l,m} \rangle = \left(\frac{m}{\hbar^2} \right)^2 \frac{1}{k_l k_m} \frac{1}{W^2} \left\langle \sum_{\mathbf{r}_i} \sum_{\mathbf{r}_j} e^{i(\mathbf{k}_l - \mathbf{k}_m)(\mathbf{r}_i - \mathbf{r}_j)} \right\rangle, \quad (31)$$

where we introduced the notation $\mathbf{k}_l = (k_l, k_y^l)$. In the spirit of the single-site approximation, we only consider the contribution of $\mathbf{r}_i = \mathbf{r}_j$,

$$\langle c_{l,m}^* c_{l,m} \rangle \approx \left(\frac{m}{\hbar^2} \right)^2 \frac{1}{k_l k_m} \frac{1}{W^2} N_i. \quad (32)$$

It is easy to show that otherwise g and r would not satisfy the current conservation, Eq. (28). To lowest order in N_i , the final expression for the conductance is

$$\langle g \rangle = 2 \left(\tilde{W} - N_i \frac{\xi^2}{1 + \xi^2} \right), \quad (33)$$

$$\xi \equiv \frac{h_1 V}{1 + h_2 V}, \quad (34)$$

which agrees with the results of Ref. 23. Again, in the few impurity limit ($N_i \rightarrow 1$) the above results are exact. However, for $N_i > 1$ the results are not valid for large ξ anymore. The total transmission probability of the l th channel is given by

$$T_l = \sum_m' \langle t_{l,m}^* t_{l,m} \rangle = 1 - \frac{m}{\hbar^2} \frac{1}{k_l} \frac{N_i}{W} \frac{1}{h_1} \frac{\xi^2}{1 + \xi^2}. \quad (35)$$

Consider the propagating channel (l_0) with the largest kinetic energy in the y direction (grazing incidence). Let us define the smallest transmission T_{l_0} , which, as a probability, must be positive:

$$T_{l_0} = 1 - \gamma N_i \frac{\xi^2}{1 + \xi^2} \geq 0, \quad (36)$$

$$\gamma \equiv \frac{1}{k_{l_0}} \frac{1}{\sum_m' \frac{1}{k_m}}. \quad (37)$$

The numerical factor γ is smaller, but not much smaller than unity. For T_{l_0} to be positive, $N_i \xi^2$ should not be much larger than unity. This is a necessary, but not sufficient, condition for the validity of the single-site approximation. On the other hand, it is a rather strict condition for the global transport

properties, which might still be well described even when the approximation fails for the grazing incident states. Note that Eq. (36) always holds for $N_i = 1$, as it should. In the strong-scattering limit ($|h_2 V| \gg 1$) we may use the single-site approximation only when N_i is not much larger than unity, which agrees with the condition mentioned in the beginning. For weak scattering ($|h_2 V| \ll 1$), however, the results are more generally valid, since only $\gamma N_i \xi^2$ should not be much larger than unity. The criterion $\gamma N_i \xi^2 = O(1)$ also holds for intermediate and strong scattering, but is unnecessarily restrictive for the latter. The term h_1 in Eq. (34) is the negative imaginary part of the real-space diagonal Green function which is equivalent to the density of states at the Fermi energy multiplied by π . When the scattering potential of the impurities is much smaller than the inverse of the density of states at the Fermi energy, we may also use the single-site approximation for a larger number of impurities.

The square of the conductance is given by

$$\langle g^2 \rangle = 4 \left\langle \sum_{l,m}' t_{l,m}^* t_{l,m} \sum_{\mu,\nu}' t_{\mu,\nu}^* t_{\mu,\nu} \right\rangle. \quad (38)$$

We have to average the third- and fourth-order terms of the coefficients $c_{l,m}$ and $c_{\mu,\nu}$. The average can be carried out in the same way as in Eq. (32). The details are explained in the Appendix, and here we show only the example

$$\begin{aligned} & \left\langle \sum_{l,m}' c_{l,m}^* c_{l,m} \sum_{\mu,\nu}' c_{\mu,\nu}^* c_{\mu,\nu} \right\rangle \\ &= \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^4 \sum_{l,m}' \sum_{\mu,\nu}' \frac{1}{k_l k_m k_\mu k_\nu} \\ & \times \left\langle \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_2} \sum_{\mathbf{r}_3} \sum_{\mathbf{r}_4} e^{i(\mathbf{k}_l - \mathbf{k}_m)(\mathbf{r}_1 - \mathbf{r}_2)} e^{i(\mathbf{k}_\mu - \mathbf{k}_\nu)(\mathbf{r}_3 - \mathbf{r}_4)} \right\rangle. \end{aligned} \quad (39)$$

We consider only the situations $\mathbf{r}_1 = \mathbf{r}_2$ and $\mathbf{r}_3 = \mathbf{r}_4$ in the summation over the impurity sites, since the conductance must satisfy the current conservation law. The result is

$$\left\langle \sum_{l,m}' c_{l,m}^* c_{l,m} \sum_{\mu,\nu}' c_{\mu,\nu}^* c_{\mu,\nu} \right\rangle = h_1^4 \left\langle \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_3} \right\rangle \quad (40)$$

$$= h_1^4 \begin{cases} N_i: & \mathbf{r}_1 = \mathbf{r}_3 \\ N_i^2: & \mathbf{r}_1 \neq \mathbf{r}_3. \end{cases} \quad (41)$$

The final expression for the squared conductance is

$$\langle g^2 \rangle = \langle g \rangle^2 + 4N_i \left(\frac{\xi^2}{1 + \xi^2} \right)^2. \quad (42)$$

The (root-mean-square) conductance fluctuations δg in units of e^2/h are given by the equation

$$\delta g = \sqrt{\langle g^2 \rangle - \langle g \rangle^2} \quad (43)$$

$$= 2\sqrt{N_i} \left(\frac{\xi^2}{1 + \xi^2} \right). \quad (44)$$

FIG. 2. Pairs of bubble diagrams describing the conductance fluctuations. (a), (b), and (c) vanish, and (d) contributes to fluctuations in the lowest order of impurity scattering.

These results can be understood by the diagrams in Fig. 2, which lead to lowest order in the number of scattering events. Each “bubble” diagram consists of a pair of the retarded (+) and advanced (−) Green functions. Only bubbles which are connected by impurity lines contribute to the fluctuations. In this sense, the term proportional to N_i^2 in Eq. (41) is absorbed in $\langle g \rangle^2$, since it is composed of unconnected bubbles. The diagrams in Figs. 2(a)–2(c) vanish, since the imaginary part of the retarded and the advanced Green function have opposite signs. This must be so because they violate the current conservation law. To lowest order in the number of impurities only the bubble in Fig. 2(d) contributes to the fluctuations.

It turns out that in almost ballistic samples each impurity contributes to the fluctuations independently, and that the mean-square fluctuations increase proportionally to the number of impurities, and the root-mean-square fluctuations like $\sqrt{N_i}$. The amplitude of the fluctuations does not depend on the size of the system as long as the number of impurities is kept constant. In Sec. IV these analytical results are corroborated by numerical simulations.

Note that we did not include either the diffuson or the cooperon ladder diagrams, which are crucial to describe the UCF in the diffusive regime. Some of the lower-order ladder diagrams are illustrated in Fig. 3. These graphs contribute to

FIG. 3. Ladder diagrams in the Born approximation. These are higher order terms compared to Fig. 2(d).

higher order in the number of impurities to the fluctuations than the graph in Fig. 2(d), and may therefore be disregarded in the nearly ballistic limit.

In the Born approximation, however, the graphs in Fig. 3 are the lowest-order diagrams, because the graph in Fig. 2(a) vanishes and Fig. 2(d) is a multiple-scattering diagram on the same impurity which is not included in the Born approximation. The conductance fluctuations in the Born approximation scale like $N_i \xi^2$, which is of higher order than $\sqrt{N_i} \xi^2$. We see that the single-site approximation is indispensable to describe correctly the fluctuations in the quasiballistic regime, and that the Born approximation gives qualitatively wrong results.

At the end of this section, we consider the amplitude of the conductance fluctuations compared to the universal values in the diffusive regime. The maximum value of the fluctuations in the present method is restricted by the condition that $N_i \xi^2$ should not be much larger than unity. This means that the fluctuations in the nearly ballistic regime can be larger than the universal values, but the present theory cannot predict the magnitude of the enhancement.

IV. NUMERICAL SIMULATION

In order to confirm the validity of the analytical results, we perform numerically exact simulations on the two-dimensional single-band tight-binding model. The Hamiltonian reads

$$H_2 = -t \sum_{(\mathbf{r}_i, \mathbf{r}_j)} c_{\mathbf{r}_i}^\dagger c_{\mathbf{r}_j} + \sum_{\mathbf{r}_i}' \epsilon_i c_{\mathbf{r}_i}^\dagger c_{\mathbf{r}_i}, \quad (45)$$

where the summation $(\mathbf{r}_i, \mathbf{r}_j)$ runs over nearest-neighbor sites on the two-dimensional square lattice, $c_{\mathbf{r}_i}^\dagger$ ($c_{\mathbf{r}_i}$) is the creation (annihilation) operator of an electron at $\mathbf{r}_i$, and t denotes the nearest-neighbor transfer integral. In the second term, $\sum_{\mathbf{r}_i}'$ denotes the summation with respect to N_i impurity lattice sites. Site disorder is introduced by choosing ϵ_i randomly in the range of

$$-v/2 \leq \epsilon_i \leq v/2. \quad (46)$$

By choosing not only the impurity position but also its potential in a random fashion, we minimize possible finite-size effects in the simulations. In what follows, energy is measured in units of the transfer integral t , and length is measured in units of the lattice constant. We use the recursive Green function method to calculate the conductance.^{24,25}

In Fig. 4, we show the conductance fluctuations as a function of v for several choices of N_i . The length and width of the disordered region are chosen as $L=W=50$ sites. The Fermi energy is fixed at $E_F = -0.5$ relative to energy zero at the band center. Figures 4(a), 4(b), and 4(c) are results for $N_i = 10, 20$, and 30 , respectively. Symbols denote the numerical data averaged over a number of samples (typically 4000). The lines represent results for the single site approximation which are obtained as follows. First, we calculate the unperturbed Green function (i.e., h_1 and h_2) at the Fermi energy. Then we estimate the average

$$2\sqrt{N_i} \left\langle \frac{\xi^2(\epsilon_i)}{1 + \xi^2(\epsilon_i)} \right\rangle \equiv 2\sqrt{N_i} \frac{1}{v} \int_{-v/2}^{v/2} du \frac{\xi^2(u)}{1 + \xi^2(u)}, \quad (47)$$

where $\xi(\epsilon_i) \equiv h_1 \epsilon_i / (1 + h_2 \epsilon_i)$ is site dependent. The fluctuations increase with increasing v and the analytical results agree with the numerical data.

In Fig. 5, we show the conductance fluctuations as a function of $\sqrt{N_i}$ for several choices of v . Straight lines are guides for the eyes. The maximum number of impurities (N_C) which satisfies the condition $N_i \langle \xi^2(\epsilon_i) \rangle \leq 1$ are estimated to be 167, 40, 17, and 10 for $v = 0.5, 1.0, 1.5$, and 2.0 , respectively. The fluctuations increase like $\sqrt{N_i}$ for $N_i < N_C$ and deviate from this relation around $N_i \sim N_C$. From the discussion in Sec. III we can understand this to be caused by the strong scattering potential.

We show the fluctuations for larger N_i and v in Fig. 6 as a function of $\sqrt{N_i}$. Again, the fluctuations deviate from the linear relation when the scattering becomes strong. The numerical data for $v \geq 1.0$ show a maximum, then decrease to the universal value for two-dimensional orthogonal system, i.e., 0.862 (Refs. 3 and 4). We observe a significant enhancement of the fluctuations only when the impurity scattering potential is large.

In Fig. 7 we demonstrate the property that the amplitude of the conductance fluctuation is independent of the system size as expected from the single-site approximation. We show the v dependence of the fluctuations for several choices of system size ($L=M=50, 100, 150$, and 200) and

FIG. 4. Conductance fluctuations as a function of impurity potential. The size of the disordered region is chosen to be $L=50$ and $M=50$, the Fermi energy is at $E_F = -0.5$. Symbols represent numerical results and lines are the analytical results. (a), (b), and (c) are the results for $N_i = 10, 20$, and 30 , respectively.

N_i . The fluctuations do not depend on the size of disordered region, but depend only on the number of the impurities.

We repeated the simulations for several Fermi energies, (e.g., $E_F = -1.0$ and -2.0). The results are qualitatively unchanged. In all cases the numerical results agree well with the analytical results when the number of scatterers is small.

FIG. 5. Conductance fluctuations as a function of the number of impurities. The size of disordered region is chosen to be $L=M=50$, and the Fermi energy is at $E_F=-0.5$.

V. DISCUSSION

The UCF in the diffusive regime is usually discussed by perturbation theory in the Born approximation. We have found here that the Born approximation fails, and that the single-site approximation has to be involved to explain the characteristic behavior of the conductance fluctuations near the ballistic regime. These statements seem to contradict each other. However, in the UCF theory, the ladder sum of the vertex correction characterizes the universal behavior, rather than the nature of the irreducible vertex part. The diffusion and the cooperon show a singularity like $\int d^d \mathbf{q} \mathbf{q}^{-2}$ for small $|\mathbf{q}|$, where $\mathbf{q}$ is the total momentum of two Green functions which run on either side of the ladder. The integral with respect to $\mathbf{q}$ depends on the dimensionality (d), and the singular behavior of the cooperon is suppressed in the presence of the magnetic field. This characteristic feature is independent of the approximations employed for the self-energy or irreducible vertex. In fact, these are assumed to be constant,

FIG. 6. Conductance fluctuations as a function of the number of impurities. The size of the disordered region is chosen to be $L=M=50$, and the Fermi energy is at $E_F=-0.5$.

FIG. 7. System size dependence of the conductance fluctuations. The Fermi energy is held at $E_F=-0.5$. The size of the disordered region is chosen to be $L=M=50, 100, 150$, and 200 .

and do not appear in the final expression of the universal fluctuations at all. For this reason, there should be no essential difference between the two approximations in the framework of the UCF theory, which reflects the essence of the universality. On the other hand, in the nearly ballistic regime, the ladder sums do not have to be calculated in order to obtain the fluctuations, because they give rise to higher-order terms with respect to the number of impurities. In addition, the Born approximation does not take account of the leading-order graph in the single-site approximation. The Born approximation leads to qualitatively wrong results for the fluctuations as a function of the impurity number, at least in a model of short-range impurity scattering.

We expect that the symmetry of the Hamiltonian and the dimensionality does not drastically effect the fluctuations close to the ballistic regime, since the ladder sums do not contribute significantly. Equation (44) remains qualitatively unchanged even in the three-dimensional system and when the time-reversal symmetry is broken by a magnetic field. The electronic structure at the Fermi energy, which depends on the dimensionality and magnetic field, is taken into account through the scattering parameter ξ , since ξ includes the unperturbed Green function. In this way we shall be able to quantify the effects of the time-reversal symmetry and the dimensionality.

The spectral rigidity of the transmission matrix eigenvalues explains the amplitude of the fluctuations in the framework of random matrix theory. We may understand the enhancement of the conductance fluctuations by the fact that the spectral rigidity can be created only by a sufficiently large degree of disorder: the amplitude of the fluctuations is determined by the maximum entropy condition. On the other hand, the fluctuations must vanish in the clean limit since there are no impurities left. In the intermediate regime, fluctuations differ from universal ones in the diffusive regime, because the spectral rigidity should be weakened.¹³ This does not necessarily lead to an enhancement, as shown in Fig. 6, where the numerical data for weak scattering potentials ($v=0.5$) approach the universal value monotonically. However, the data with larger scattering potentials clearly show larger fluctuations. This enhancement occurs only

when the number of impurities is small. Therefore, conductors cannot in general be characterized only by the ratio of a phenomenological mean free path and the system length. For an experimental realization of enhanced fluctuations, mesoscopic conductors containing a small number of impurities with a strong scattering potential, are required. Such samples can be realized by intentionally disordered metallic (hetero) point contacts, since the fluctuations in clean homopoint contacts are very small.¹⁴

The mean-square conductance fluctuations increase proportionally with N_i , which suggests a classical origin of the fluctuations. We have analyzed the classical transmission of particles through a disordered medium. A complete statistical analysis will be published elsewhere. Here we will give only a simple back-of-the-envelope explanation of the physics involved, which agrees with the complete treatment for low impurity densities. The term $\xi^2/(1+\xi^2)$ in Eq. (33) can be interpreted as the effective cross section of each impurity, which can be much larger than its actual potential range. We can then consider the situation where classical particles travel through a sample which contains N_i impurities, which are modeled by hard discs with diameter $\xi^2/(1+\xi^2)$. In this model the overlap of the impurities is the source of the fluctuations. Let us take the averaged conductance for N_i impurities to be $\langle g_{N_i} \rangle$ and add one more impurity to the system. The conductance for the system with N_i+1 's impurities is estimated as

$$\begin{aligned} \langle g_{N_i+1} \rangle = & \frac{N_i}{\bar{W}} \frac{\xi^2}{1+\xi^2} \langle g_{N_i} \rangle \\ & + \left(1 - \frac{N_i}{\bar{W}} \frac{\xi^2}{1+\xi^2} \right) \left(\langle g_{N_i} \rangle - \frac{\xi^2}{1+\xi^2} \right). \end{aligned} \quad (48)$$

The first term is the contribution when the (N_i+1) th impurity overlaps with another impurity and the second term is the contribution when it occupies an empty site. The square-averaged conductance can be estimated in the same way, and the classical conductance fluctuations are given by the equation

$$\delta g_{\text{classic}} \sim \left(\frac{N_i}{\bar{W}} \right)^{1/2} \frac{\xi^2}{1+\xi^2} - \frac{N_i}{\bar{W}} \left(\frac{\xi^2}{1+\xi^2} \right)^2. \quad (49)$$

The classical fluctuations increase with $\sqrt{N_i}$, which agrees with the conductance fluctuations in the near-ballistic regime, and decrease again when the overlap becomes large for high-impurity densities.

It follows that we can understand part of the physics in terms of a classical analogy. Still there is a crucial difference between the classical model and the quantum mechanical results, viz. the factor $\bar{W}$ in the denominator of Eq. (49). In the classical regime the fluctuations vanish when the system width is increased, while keeping N_i constant, whereas in quantum mechanics they remain constant. Due to quantum mechanics the (coherent) wave functions extend through the system under consideration irrespective of the system width. We may therefore conclude that quantum coherence is responsible for the conductance fluctuations even in the nearly ballistic regime. The question is thus legitimate whether the conductance also shows an oscillatory behavior as a function

of a weak magnetic field, which allows the measurement of sample-to-sample fluctuations the diffusive regime on a single sample. It is therefore important to check the ergodic hypothesis of the UCF theory, i.e., whether our predicted enhancement of the sample-to-sample fluctuations will be faithfully represented by magnetoconductance fluctuations. At present, we are investigating this hypothesis by numerical simulations. The results will be reported elsewhere.

A crucial assumption for the analytical treatment of the problem is the short-range nature of the scattering potentials. It is likely that the fluctuations in the quasiballistic regime will also depend sensitively on the range of the potentials. The single-site approximation is always superior to the Born approximation, but the difference vanishes in the regime of many weak scatterers. We do not know an easy way to treat conductance fluctuations in the presence of general scattering centers, or determine under what conditions the error of the Born approximation becomes tolerable. A failure of the Born approximation for the distribution function of the transmission matrix eigenvalues $P(T)$ in Ref. 13 might shed some light on the problem: The Born approximation fails to describe the important, completely transmitting states for a small number of impurities. These completely transmitting states exit because the wave functions can adjust themselves to avoid the few points representing the short-range scatterers. This is not possible when the potentials of the individual impurities overlap, which lets us expect that the Born approximation should perform better in that limit. The same might hold for the conductance fluctuations.

VI. CONCLUSION

In conclusion, we have studied the conductance fluctuations near the ballistic transport regime both analytically and numerically using the Landauer-Büttiker conductance formula. The conductance fluctuations are calculated for a system which contains a small number of impurities (N_i) with a short-range scattering potential. We employ the single-site approximation in analytical calculations, and use the numerically exact recursive Green function method in numerical simulations. The single-site approximation explains the characteristic features of the fluctuations in this regime. The analytical results agree well with the numerical data.

Quantum interference is responsible for the fluctuations in the nearly (quasi) ballistic as well as diffusive regimes. In the former regime the conductance fluctuations increase proportionally with $\sqrt{N_i}$ and do not depend on the size of disordered region, which means that each impurity contributes to the fluctuations independently. The numerical results show that when the system contains a small number of impurities with a large scattering potential the amplitude of the fluctuations can be larger than the UCF. The enhancement of the fluctuations can be understood by the reduced spectral rigidity of the transmission matrix compared to the diffusive regime. When the scattering events become frequent enough to randomize transport, the fluctuations approach the universal values.

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APPENDIX: DERIVATION OF CONDUCTANCE FLUCTUATION

Equation (38) is rewritten with Eqs. (18), (19), and (20) as follows:

$$\langle g^2 \rangle = \left\langle \sum_{l,m} ' \sum_{\mu,\nu} ' (\delta_{l,m} + i c_{l,m}^* \beta^*) (\delta_{l,m} - i c_{l,m} \beta) \times (\delta_{\mu,\nu} + i c_{\mu,\nu}^* \beta^*) (\delta_{\mu,\nu} - i c_{\mu,\nu} \beta) \right\rangle \quad (A1)$$

$$\begin{aligned} &= \sum_l ' \sum_{\mu} ' \left\langle 1 - i(c_{l,l} + c_{\mu,\mu})(\beta - \beta^*) \right. \\ &\quad + \sum_m ' |c_{l,m}|^2 |\beta|^2 + \sum_{\nu} ' |c_{\mu,\nu}|^2 |\beta|^2 \\ &\quad + c_{l,l} c_{\mu,\mu} (2|\beta|^2 - \beta^2 - \beta^{*2}) \\ &\quad - i \left(c_{l,l} \sum_{\nu} ' |c_{\mu,\nu}|^2 + c_{\mu,\mu} \sum_l ' |c_{l,m}|^2 \right) |\beta|^2 (\beta \\ &\quad \left. - \beta^*) + \sum_m ' \sum_{\nu} ' |c_{l,m}|^2 |c_{\mu,\nu}|^2 |\beta|^4 \right\rangle. \end{aligned} \quad (A2)$$

We have to calculate the averages

$$\langle c_{l,l} c_{\mu,\mu} \rangle, \quad (A3)$$

$$\langle c_{l,l} |c_{\mu,\nu}|^2 \rangle \quad (A4)$$

in addition to Eqs. (27), (32), and (41). Equation (A3) is explicitly written

$$\langle c_{l,l} c_{\mu,\mu} \rangle = \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^2 \frac{1}{k_l k_{\mu}} \left\langle \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_2} \right\rangle \quad (A5)$$

$$= \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^2 \frac{1}{k_l k_{\mu}} \left\{ \begin{array}{l} N_i: \mathbf{r}_1 = \mathbf{r}_2 \\ N_i^2: \mathbf{r}_1 \neq \mathbf{r}_2. \end{array} \right. \quad (A6)$$

The average in Eq. (A4) can be carried out in the same way as Eq. (41),

$$\langle c_{l,l} |c_{\mu,\nu}^* c_{\mu,\nu}|^2 \rangle = \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^3 \frac{1}{k_l k_{\mu} k_{\nu}} \left\langle \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_2} \sum_{\mathbf{r}_3} e^{i(\mathbf{k}_{\mu} - \mathbf{k}_{\nu})(\mathbf{r}_2 - \mathbf{r}_3)} \right\rangle \quad (A7)$$

$$= \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^3 \frac{1}{k_l k_{\mu} k_{\nu}} \left\langle \sum_{\mathbf{r}_1} \sum_{\mathbf{r}_2} \right\rangle \quad (A8)$$

$$= \left(\frac{m}{\hbar^2} \frac{1}{W} \right)^3 \frac{1}{k_l k_{\mu} k_{\nu}} \left\{ \begin{array}{l} N_i: \mathbf{r}_1 = \mathbf{r}_2 \\ N_i^2: \mathbf{r}_1 \neq \mathbf{r}_2. \end{array} \right. \quad (A9)$$

The square average of the conductance becomes

$$\langle g^2 \rangle = 4 \left[\tilde{W}^2 - 2 \tilde{W} N_i \frac{\xi^2}{1 + \xi^2} + N_i^2 \left(\frac{\xi^2}{1 + \xi^2} \right)^2 \right] + 4 N_i \left(\frac{\xi^2}{1 + \xi^2} \right)^2. \quad (A10)$$

When the system contains only one impurity, we can easily show that

$$\langle g^2 \rangle = \langle g \rangle^2. \quad (A11)$$

There is no conductance fluctuation in this case, because we use periodic boundary condition in the y direction.

The current conservation law in Eq. (28) is useful to check the calculations. The square of Eq. (28) becomes

$$g^2 + 2gr + r^2 = \tilde{W}^2. \quad (A12)$$

This relation must be true even after the ensemble average. The averages $\langle r^2 \rangle$ and $\langle gr \rangle$ can be calculated in the same way as above. We can see that $\langle r^2 \rangle$, $\langle gr \rangle$, and $\langle g^2 \rangle$ satisfy Eq. (A12) within the single-site approximation.

In the analytical model, we assume that the impurity potential V is a constant for all impurities. Often the impurity potentials are used which vanish on average,

$$\langle V_i^{2n} \rangle = V^{2n}, \quad (A13)$$

$$\langle V_i^{2n+1} \rangle = 0, \quad (A14)$$

where n is the natural number. It is easy to show that our expressions for the fluctuations are still valid by setting the real part of the Green function shown in Eq. (21) to zero, (i.e., $h_2 = 0$).

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