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Numerical Studies of Shot Noise in 3D Disordered Systems

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Shot noise power in 3D disordered conductors has been studied by means of numerical simulations. The Anderson model of disordered conductor, Green's function technique and Fisher-Lee relations have been employed to calculate the transmission matrix **t**, its eigenvalues T_n, the conductance $G = \mathrm{Tr}(\mathbf{t}\mathbf{t}^+)$ and the shot noise power $S = \mathrm{Tr}(\mathbf{t}^+\mathbf{t}) - \mathrm{Tr}(\mathbf{t}^+\mathbf{t})^2$ for various degrees of disorder. To explain the results of simulations, Nazarov's microscopic theory describing the correction to the distribution of transmission eigenvalues has been applied. It was found that the crossover from the ballistic to the diffusive region is well described by the relation obtained by random matrix theory. In the weakly localized regime the correction to the shot noise power is different from the 1D result. Namely, $S = G/3 + 0.209$. At the localization–delocalization transition we have observed $S \cong 0.57G$.

Introduction Over the past few years a growing interest in shot noise studies of disordered conductors is being observed [1–3]. A very convenient quantity to characterize properties of disordered systems with respect to shot noise is the Fano factor $F \equiv \left(\sum_n T_n(1-T_n)\right)/\sum_n T_n = S/G$, where S and G are the dimensionless shot noise power and quantum conductance, respectively, and T_n are eigenvalues of the transmission matrix square $\mathbf{t}^+\mathbf{t}$. In the 1D case the transition from ballistic to diffusive regime has been proven to be described by the relation [4]

$$F = \frac{1}{3}\left(1 - \frac{1}{1 + L/l}\right), \tag{1}$$

where L is the size of the system and l is the mean free path. On both sides of this crossover the above formula gives the well known results. In the ballistic regime ($l \gg L$) F tends to 0 due to all eigenvalues being close to unity. On the other side, in the metallic diffusive limit, where $L \gg l$, we have $F = 1/3$ which is also a well known fact [1]. All these results have been obtained within the framework of random matrix theory, which in principle, works in 1D systems.

The aim of this paper is to present new results concerning the influence of disorder on the shot noise in 3D disordered conductor. The main result presented here is the weak localization quantum correction to shot noise power $\delta S \equiv S - G/3 \cong 0.209$ in 3D, which turns out to be significantly larger than that observed in reduced dimensionalities. We also show that for critical disorder (W = 16.5) the Fano factor takes the value of $F \cong 0.574$. Both these results have been obtained by means of Monte Carlo simulations and then confirmed by the use of the microscopic theory of WL

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corrections to the distribution of transfer matrix eigenvalues [5] and conjecture about linear distribution of variables $\lambda_n = \operatorname{arccosh}(1/\sqrt{T_n})$ at localization–delocalization transition [6].

The paper is organized as follows: after the introduction a description of the model used in numerical studies comes together with the details of the computational procedure. Next, the results of simulations are shown followed by the discussion. At the end some final conclusions are given.

Model and Numerical Details We have used the Anderson model of disorder described by the one-electron tight-binding Hamiltonian with hopping restricted to nearest neighbors only,

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{V} = \sum_{\mathbf{n}} |\mathbf{n}\rangle\, \varepsilon_{\mathbf{n}}\, \langle \mathbf{n}| + t \sum_{\mathbf{n},\mathbf{m}} |\mathbf{n}\rangle\, \langle \mathbf{m}|\,. \tag{2}$$

Diagonal disorder was introduced by taking site energies $\varepsilon_{\mathbf{n}}$ randomly with uniform probability density of $1/W$. The elements t_{mn} of transmission matrix $\mathbf{t}$ were evaluated with the help of Fisher-Lee relations [7],

$$t_{mn} = \sum_{j \in L_1} \sum_{k \in L_2} i\chi_n(j)\, \sqrt{v_n}\, \mathbf{G}_{kj}(L_1, L_2)\, \sqrt{v_m}\, \chi_m(k)\,, \tag{3}$$

where χ_n, χ_m are transverse components of envelope functions, v_n, v_m are longitudinal velocities of incoming and outgoing waves, respectively, and the sums run over all sites in leads L_1 (left) and L_2 (right) that lie on the sample-to-lead edge. To determine the Green's function $\mathbf{G}$ the Dyson equation $\mathbf{G} = (\mathbf{I} - \mathbf{G}_0\mathbf{V})^{-1}\mathbf{G}_0$, where $\mathbf{G}_0 = (E\mathbf{I} - \mathbf{H}_0)^{-1}$ was employed [8]. Having the matrix $\mathbf{t}$ evaluated the eigenvalues T_n of $\mathbf{t}^{+}\mathbf{t}$ were calculated by the standard LAPACK procedure. Eventually the dimensionless shot noise power S and quantum conductance G have been calculated as $S = \sum_n T_n(1 - T_n)$ and $G = \sum_n T_n$. All calculations have been done for the energy E close to the band center, $E = 0.5t$. The simulations have been performed for many configurations of disorder potential of which the results were then averaged and marked by '$\langle\ \rangle$'.

Results and Discussion The results of the simulations are depicted in Fig. 1 in the form of $\langle S\rangle$ versus $\langle G\rangle$ plots which allow us to study distinct transport regimes. Data for small disorder ($W < 8$) are grouped in Fig. 1a. An additional line, $\langle S\rangle = \langle G\rangle/3$, is added to distinguish the features of diffusive region. Data for $4 \le W \le 7$ follow this line even for small sizes. For $W \le 3$ data are situated below this line. We interpret this situation as the crossover to ballistic regime. This is proven in Fig. 2 where data from Fig. 1a for $1 \le W \le 3$ have been replotted in $(1 - 3F)^{1/3}$ versus L coordinates. They follow straight lines with the slope corresponding to (disorder-dependent) mean free path. Our results confirm that relation (1) describes the crossover from the ballistic to the diffusive region also in 3D systems.

In the weakly localized regime, $G > 1$, the data in Fig. 1b tend to approach the line $\langle S\rangle = \langle G\rangle/3 + 0.209$ (see also Fig. 3). This behavior is similar to that observed in reduced dimensionalities, however with the exception of constant term. Namely, in 1D and 2D the relations $\langle S\rangle = \langle G\rangle/3 + 4/45$ [4] and $\langle S\rangle = \langle G\rangle/3 + 0.124$ [9] have been found. The significant rise in constant term is not accidental nor caused by numerical imperfections. To prove it we recall the microscopic theory of weak localization correc-

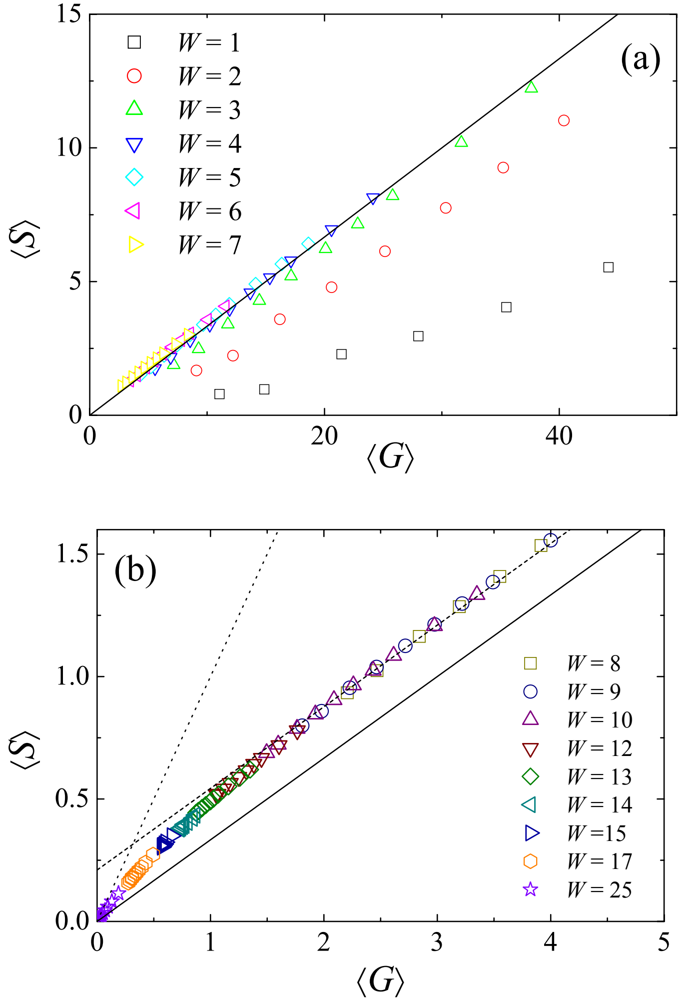

Fig. 1 (online colour). Dimensionless shot noise power $\langle S\rangle$ versus conductance $\langle G\rangle$ for a) $1 \le W \le 7$ and b) $8 \le W \le 25$. The meanings of the symbols are given in the legends. Solid lines are the plots of $\langle S\rangle = \langle G\rangle/3$, which is the metallic diffusive limit. The dashed line is the plot of $\langle S\rangle = \langle G\rangle/3 + 0.209$ which is the weak localization result. The dotted line is the (strong) localization limit $\langle S\rangle = \langle G\rangle$. For $W \le 15$ ($W \ge 17$) the increase of L, causes increase (decrease) of $\langle G\rangle$

tions to eigenvalues of the matrix $\mathbf{t}^{+}\mathbf{t}$ [5]. This theory gives the function $\delta F(\phi)$ generating moments of the WL correction to transmission eigenvalues [5]

$$\delta F(\phi) \equiv \delta \mathrm{Tr}\left(\frac{\mathbf{t}^{+}\mathbf{t}}{1+\sin^2\dfrac{\phi}{2}\mathbf{t}^{+}\mathbf{t}}\right) = -\frac{2\phi}{\sin\phi}\sum_s \frac{1}{s^2-\phi^2}, \tag{4}$$

where for 3D geometry $s^2 = \pi^2(n_x^2 + n_y^2 + n_z^2)$ and n_x, n_y, n_z are integer numbers labeling discrete diffusion modes. Further, x is the direction of transport and n_x starts from 1

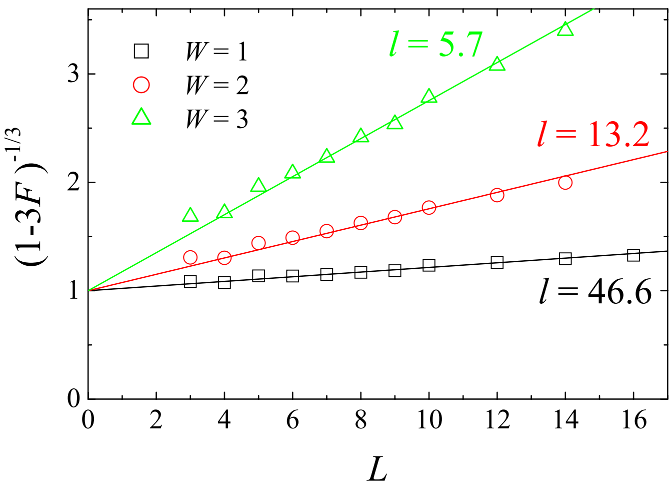

Fig. 2 (online colour). Data from Fig. 1a replotted in different coordinates. The mean free paths are estimated from the slopes of the approximating lines

whereas n_y, n_z range from 0 to ∞. We get

$$\delta\mathrm{Tr}\,(\mathbf{t}^{+}\mathbf{t}) = \delta F(0) = 2\sum_s s^{-2}\,, \qquad \delta\mathrm{Tr}\,(\mathbf{t}^{+}\mathbf{t})^2 = 4\,\mathrm{d}\delta F(0)/\mathrm{d}\phi^2 = 4\sum_s s^{-4}\,, \qquad (5)$$

which, if combined, give eventually $\delta S = 8\sum_s s^{-2}$. Numerical evaluation in 3D gives $\delta S \equiv 0.20936\ldots$, in excellent agreement with our numerical simulations in Figs 1b and 3. It is interesting to examine r.m.s. fluctuations of shot noise power. The random matrix theory predicts r.m.s. $\mathrm{S} = \sqrt{\langle \mathrm{S}^2\rangle - \langle \mathrm{S}\rangle^2} = \sqrt{46/2385} \cong 0.123$ in 1D case [4]. In 3D r.m.s. S saturates at considerable higher level of approximately 0.2. This is apparent in Fig. 4 where results from simulations are depicted against the horizontal line in the background, which is 1D limit.

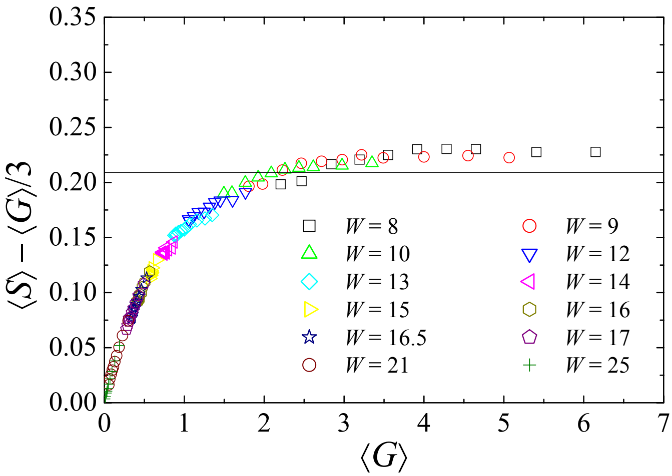

Fig. 3 (online colour). Data from Fig. 1 with additional data series rearranged in $\langle S\rangle - \langle G\rangle/3$ versus $\langle G\rangle$ coordinates. The solid line is the weak localization limit

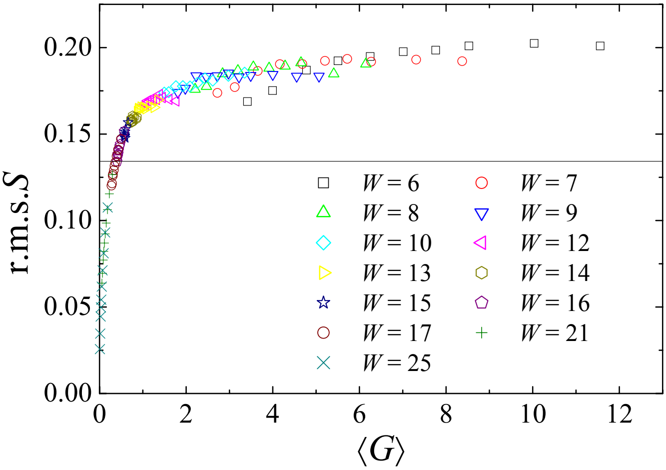

Fig. 4 (online colour). r.m.s. fluctuations of shot noise power S versus $\langle G \rangle$. The horizontal line is the random matrix theory limit of $\sqrt{46/2385}$ [4]

The unique feature of noninteracting 3D systems is disorder induced localization–delocalization transition. It is interesting to look into the behavior of shot noise power as critical disorder $W_C \cong 16.5$ is approached [6]. In Fig. 5 the Fano factor versus the system size L is depicted for a variety of disorder, covering ballistic, diffusive, weakly and strongly localized regimes. For $W \leq 3$ the trajectories approach from below the asymptotic dashed line at 1/3 which is the theoretical limit for metallic diffusive wires. With increasing disorder the data approach the same asymptotic limit but from above. It takes place up to $W = 14$. At even stronger disorder a very interesting behavior is

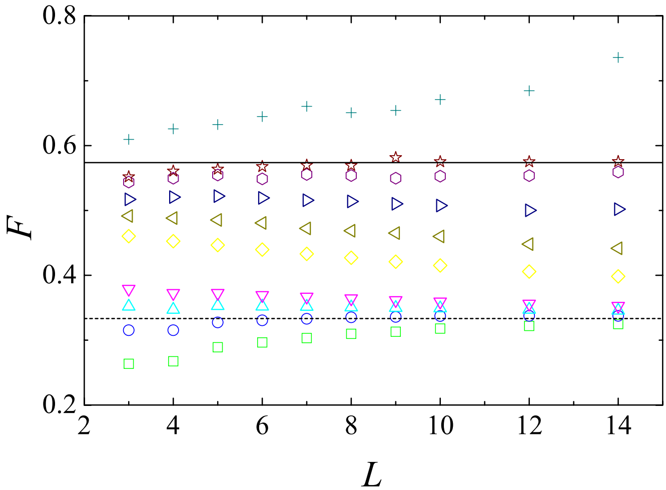

Fig. 5 (online colour). Fano factor F versus system size L for various disorder degrees W. The meaning of the symbols is as follows: square $W = 3$, circle $W = 4$, uptriangle $W = 5$, downtriangle $W = 6$, diamond $W = 10$, lefttriangle $W = 12$, righttriangle $W = 14$, hexagon $W = 16$, star $W = 17$, cross $W = 25$

apparent. Namely, a nearly constant Fano factor of $F \cong 0.57$ is observed for $16 \leq W \leq 17$. Further increase in disorder, $W > 17$, causes the system to cross into a strongly localized regime where, due to all channels being closed ($T_n \to 0$), F reaches theoretical upper limit of 1.

The value of the Fano factor $F \cong 0.57$ we have found at metal-insulator transition calls for comparison with existing knowledge. We recall that the probability density of the variable $\lambda = \operatorname{arccosh}(1/\sqrt{T})$ at the transition point was found to be nearly linear, $P(\lambda) \propto \lambda$ [6]. The Fano factor at the transition point can be estimated as

$$F = \frac{\langle T(1-T)\rangle}{\langle T\rangle} = \frac{\int\limits_0^\infty \cosh^{-2}\lambda\left(1-\cosh^{-2}\lambda\right)\lambda\,\mathrm{d}\lambda}{\int\limits_0^\infty \lambda\cosh^{-2}\lambda\,\mathrm{d}\lambda} \approx 0.57378$$

which is in agreement with our numerical result in Fig. 5.

Summary Numerical simulations of the shot noise power in disordered 3D systems show that the crossover from ballistic to diffusive regime follows the same relation as for the 1D case. In the weakly localized regime the shot noise power S exceeds the one-third suppression value by $\delta S = 0.20936$. At localization–delocalization transition the Fano factor takes the value of $F \cong 0.574$.

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