Conductance fluctuations and boundary conditions

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The conductance fluctuations for various types for two- and three-dimensional disordered systems with hard wall and periodic boundary conditions are studied, all the way from the ballistic (metallic) regime to the localized regime. It is shown that the universal conductance fluctuations (UCF) depend on the boundary conditions. The same holds for the metal to insulator transition. The conditions for observing the UCF are also given.

The influence of the boundary conditions (bc) on critical phenomena in disordered mesoscopic systems has been demonstrated by studies of the conductance distribution[1–3] and energy level statistics.[4] The ensemble average of the logarithm of the conductance, $\langle \ln(g) \rangle$, is smaller for hard wall boundary conditions than for periodic boundary conditions. The variance $\langle \ln^2(g) \rangle - \langle \ln(g) \rangle^2$, on the other hand, is larger for hard wall than for periodic boundary conditions. The distribution of nearest neighbor energy level separations $P(s)$ becomes more Wigner-Dyson-like for periodic boundary conditions. Thus, systems with periodic boundary conditions exhibit a "more metallic" behavior than those with hard wall boundary conditions. Different boundary conditions also lead to different values for the universal conductance fluctuations (UCF) in the diffusive metallic regime where the mean free path l is much smaller and the localization length ξ_l much bigger than the system size. The variation of ensemble fluctuations of the conductance as the disorder increases throughout the metallic regime has been studied,[6,7] but the influence of the boundary conditions in the ballistic regime where l exceeds the system size, and close to the localized regime where ξ_l becomes comparable with the system size, has not been studied in detail. Also, the role of the correlation length in samples with a true metal-insulator-transition (MIT)—i.e., in systems where the localization length is "infinite" in the metallic regime—has not been discussed. We present here numerical studies of cubic systems and squares with spin-orbit scattering—all of which have a true MIT—for both hard wall and periodic boundary conditions in the direction(s) perpendicular to transport.

We are using the tight-binding model with the Hamiltonian

$$\mathcal{H} = \sum_{n,\tau} |n\tau\rangle \varepsilon_n \langle n\tau| + \sum_{n,\tau,n',\tau'} |n\tau\rangle V_{n,n'} \langle n'\tau'|, \quad (1)$$

where n, n' are nearest neighbor lattice sites on a square or cubic lattice. For systems with spin-orbit interactions τ and τ' take on values of $+1$ or -1 and the hopping integrals $V_{n,n'}$ are 2×2 matrices; without spin-orbit interactions, the hopping integrals are scalar and the spin "variables" have only one value. We take the site energies ε_n (independent of τ) to be random variables, chosen from an interval

$[-W/2; W/2]$ with a uniform probability distribution. The parameter W serves thus as a measure of disorder strength. The conductance is calculated using the transfer matrix method and the Landauer formula.[8]

We have used the analytical derivation of Lee *et al.*[9] to calculate theoretical values for the UCF for both types of boundary conditions. In order to change the boundary conditions to periodic, one needs to make the following changes [references to equations are from the Appendix of Lee *et al.* (1987)[9]]: in the eigenfunctions Q_m to the diffusion equations, the cosines in the transverse directions [Eq. (A9)] must be replaced by exponentials with a factor of 2π instead of π in the argument; this will lead in effect to a factor 4 in the m_x^2 and m_y^2 terms in the modified eigenvalues $\tilde{\lambda}_m$ [Eq. (A13)], and to a summation over all integers (including negative ones) for m_x and m_y in Eqs. (A15), (A16), (A24), and (A25). The results are presented in Table I. The values are only half those given by Lee *et al.* due to a factor 2 in the definition of g. Also, our result for the three-dimensional case is slightly higher, probably due to our calculating the involved sums to a higher precision. The boundary conditions have of course no effect for the quasi-one-dimensional case. The values given here are those for the standard deviation σ_g for the orthogonal universality class of random matrix theory. The
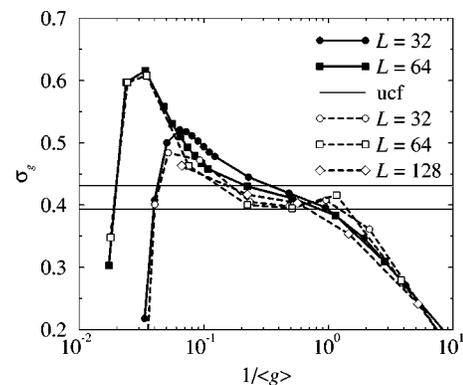

FIG. 1. Standard deviation σ_g of the conductance for squares of $L \times L$ lattice sites. Full symbols: hard wall bc; open symbols: periodic bc. Note that the bc seem to have little effect outside the plateau region. The two horizontal lines indicate the theoretical values for the UCF for hard wall (top) and periodic (bottom) bc.
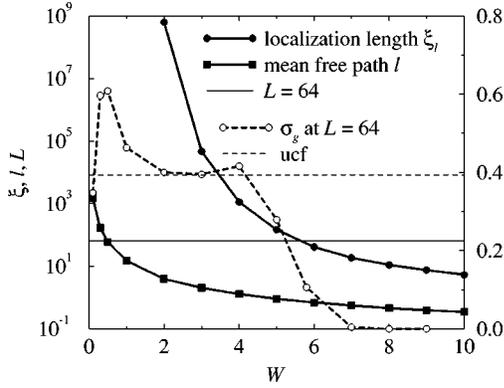
FIG. 2. Standard deviation of a square of 64×64 lattice sites together with the mean free path l and the localization length ξ_l.

TABLE I. The universal conductance fluctuation values for different bc and dimensionality of the system.

bc	Q1D	2D	3D
hard wall	0.365	0.431	0.559
periodic	0.365	0.393	0.471

values for the other universality classes[10] are obtained by dividing the variance, i.e., σ_g^2, by the universality class parameter β, where $\beta = 1,2,4$ for the orthogonal, unitary, and symplectic universality classes respectively.

In Fig. 1 we show the standard deviation of the conductance in ensembles of 10 000 samples for different system sizes (squares with $L \times L$ lattice sites) and boundary conditions (open symbols: periodic boundary conditions; filled symbols: hard wall boundary conditions) as a function of the inverse of the average conductance. It is well known that in a two-dimensional disordered tight-binding model all the states are exponentially localized.[5] The typical structure[6,7] of the fluctuations with increasing disorder strength can be seen: after an initial strong increase in the ballistic regime (large $\langle g \rangle$) it reaches a peak value which becomes more pronounced for larger systems; then the fluctuations drop back to the universal value and finally decrease again in the strongly localized regime. The boundary conditions have apparently no influence on the behavior outside the region of UCF in this case. Notice that for the case of periodic boundary conditions for the large system size of $L = 128$, σ_g approaches the theoretical value of 0.393 given by the lower horizontal line.

In Fig. 2 the same data is plotted for a two-dimensional disordered system of size $L = 64$ with periodic boundary conditions. In the same plot the mean free path and the localization length as a function of disorder strength W are given. Both the mean free path and the localization length were obtained from the numerical results of Economou *et al.*[5] The localization length was obtained[5] by the transfer matrix

method, while the mean free path was obtained by the coherent potential approximation[5] (CPA). Notice that ξ_l is always larger than l. So for a given system size ($L = 64$ in this case), there is a finite region where $l \ll L \ll \xi_l$. Only in this region there is a plateau visible at the correct UCF value. For $W \lesssim 1$, l is larger than L, and we are in the ballistic regime where one observes a monotonic increase of σ_g followed by the characteristic maximum as the system enters the crossover between the ballistic regime and the regime characterized by UCF.

Figure 3 shows that the same overall behavior is observed also for three-dimensional systems. As there is a MIT (indicated by vertical lines in Fig. 3) where the conductance distribution and therefore also its standard deviation become universal, i.e., independent of system size (though still depending on the boundary conditions[1-3]), this value is approached after leaving the region of UCF. A direct comparison of the results shows again that the boundary conditions have only minimal effect outside that region. The additional peak noticeable in some of the periodic boundary conditions data are due to a near degeneracy of eigenenergies for very small disorder.

In Fig. 4 we plot the data for one of the systems again as a function of W, together with the mean free path l and the correlation length ξ_c. In the three-dimensional disordered case, the mean free path and the correlation length ξ_c were again obtained[11] by the CPA and the transfer matrix method. The size of the cube is $L = 16$ and periodic boundary conditions were used. In the three-dimensional case, l drops as the disorder strength W increases, while ξ_c increases as W increases. The plateau in σ_g is seen only when $l \ll L$ and $\xi_c \lesssim L$, so that we expect a *wider* plateau for larger systems. The fluctuations begin to approach the critical value as soon as $L \approx \xi_c$. In the three-dimensional case too, when $W \lesssim 2$, l is larger than L and the ballistic regime is observed, followed by the maximum in the crossover regime.

Finally, Fig. 5 shows data for square systems with spin-orbit interactions. We have chosen the Evangelou-Ziman
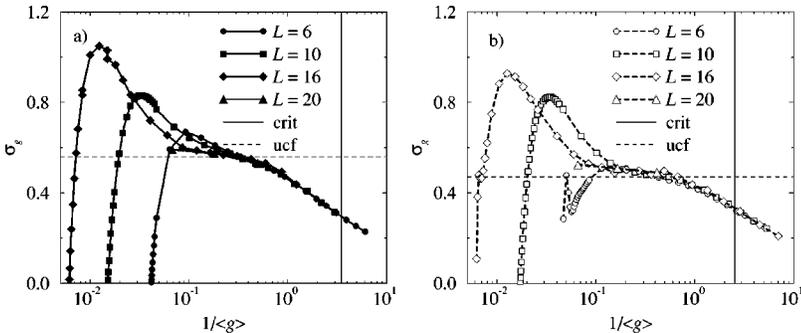

FIG. 3. The standard deviation for systems of $L \times L \times L$ lattice sites: (a) hard wall bc; (b) periodic bc. The horizontal lines indicate the UCF values; the vertical lines indicate the MIT.
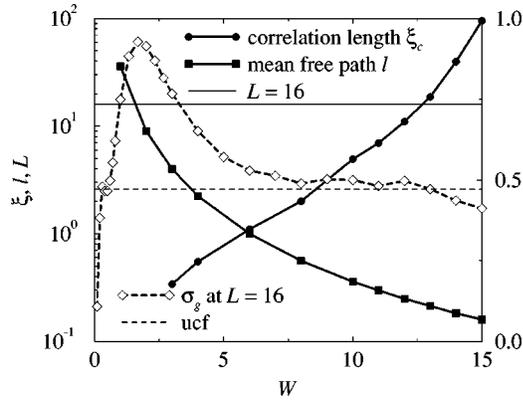
FIG. 4. The standard deviation of a cube with $16 \times 16 \times 16$ lattice sites together with the mean free path l and the correlation length ξ_c.
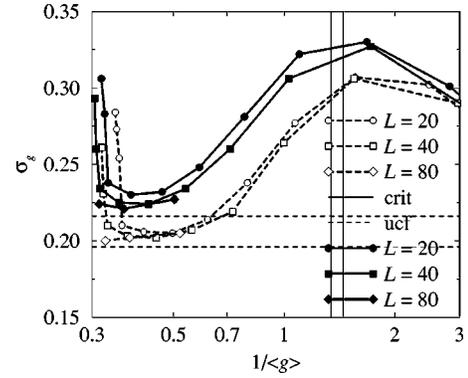

FIG. 5. The standard deviation for square systems of $L \times L$ lattice sites with spin-orbit interaction (Evangelou-Ziman model) for hard wall (solid symbols) and periodic (open symbols) bc. The two horizontal dashed lines indicate the theoretical values for the UCF for hard wall (top) and periodic (bottom) bc.

model,[12] where even in the absence of diagonal disorder there is disorder in the hopping matrices $V_{n,n'}$, which accounts for the fact that the fluctuations do not vanish for small diagonal disorder. Apparently, boundary conditions have a noticeable influence on the fluctuations even outside the region of UCF, but this is likely due to the peculiar overall structure in this case, most significantly the fact that the UCF value is much smaller than the critical value, causing another increase in the standard deviation as one approaches the MIT.

In conclusion, we have investigated the conductance fluctuations for various types of systems with both hard wall and periodic boundary conditions from the ballistic regime to the localized regime. The boundary conditions seem to have a

relevant influence on the conductance fluctuation only in the region of UCF and at the critical point of the MIT. In true metallic systems, the fluctuations begin to deviate from the UCF value and approach the critical value as soon as the correlation length approaches the system size.

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