ON THE 'NONUNIVERSAL' CONDUCTANCE OF AN ALMOST IDEAL QUANTUM WIRE

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High quality quantum wires conductance measurements have revealed an unexpected feature: the quantization step of the conductance is apparently system dependent. We show that even a single impurity (modelled by a short range potential) in a wire leads to enhanced backscattering and affects the conductance steps. We construct a random matrix model which shows similar behaviour with the size of conductance step dependent on a single parameter.

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1. Introduction

The conductance of mesoscopic devices, the so called quantum dots or quantum wires, exhibits a number of universal features such as the quantization of the average conductance or the magnitude of the conductance fluctuations. For the ideal one-dimensional (1D) quantum wire the dc conductance G is quantized in units of $G_0 = 2e^2/h$ (the factor 2 is due to electron spin) [1], $G = G_0 M_1$ with M_1 being equal to the number of transverse modes supported by the wire. Thus the dimensionless conductance $g = G/G_0$ changes by integer steps when M_1 increases.

Similarly, the integer conductance steps are predicted when the ideal wire is coupled coherently to broad leads [2]. Additionally, one expects in such a situation an appearance of resonant structures at the beginning of each step at low temperatures. For higher temperatures, due to effective

averaging, the sharp resonant structures disappear and conductance steps become smooth [2]. The presence of strong disorder destroys the steps, leading to the so called universal conductance fluctuations [3] with variance of the order of G_0. Let us mention also that if transition from wire to leads is not sharp but smooth, the conductance steps are not affected as follows from [4].

On the other hand, recent experiments, carried out on high quality wires coupled to broad leads [5] revealed smaller quantization steps of the height $\gamma < 1$, with γ varying from sample to sample and reaching 0.86 at low temperatures. This result is in apparent contradiction with the predictions of [2] mentioned above. No clear explanation of the experimental results is available, as far as we know. In [5] three different theoretical possibilities for the explanation of the data are discussed. The difficulties with the standard random matrix theory (RMT) approach and the Luttinger liquid theory [6] are emphasized. The authors give their own explanation in terms of the competition between the scattering from 2D into the edge modes. It has been pointed out [5, 7] that such a behaviour may be an evidence of a coherent backscattering between the 1D wire and the 2D leads. In such a case the conductance becomes $G = G_0 T$ where T is a M_1-dependent transmission coefficient. Still it is not clear how the dimensional argument comes into play in view of Szafer and Stone result [2] — the backscattering from the interface between a narrow wire and the broader lead in the ideal case does *not* lower the conductance steps. On the other hand the lowering of the conductance steps may be also considered as an evidence for the importance of electron–electron interactions [5].

The purpose of this work is to show that the experimental results may be reproduced by an assumption of a weak residual disorder (*e.g.* due to defects in the almost ideal wire). Such model is proposed and analyzed in Section 2. We do not claim, that the effect discussed is the sole source of the unusual conductance steps observed in [5]. Rather we would like to point out that any additional (in respect to ideal pure system [2]) backscattering in the narrow wire (not necessarily on the interface between wire and leads) may decrease the size of conductance steps. This point of view is supported by results coming from an appropriate model based on random matrices and presented in Sections 3 and 4. We summarize our findings in Section 5.

2. Conductance quantization in 'non-ideal' wire

We want to discuss the effects due to impurities, so we consider a very simple model of a wire — a strip of length, L (in x direction) and the width W with $W \ll L$ (compare Fig. 1). The Dirichlet boundary conditions are assumed for the electron wavefunctions on horizontal strip boundaries at

$y = 0$ and $y = W$ (hard walls). The corresponding Schrödinger equation reads (in $e = \hbar = m = 1$ units)

$$\left\{ \frac{k_x^2}{2} + \frac{k_y^2}{2} + P(x,y) + Fy \right\} \psi(x,y) = E\psi(x,y), \tag{1}$$

where E is the energy of the electron travelling along the strip and $P(x,y)$ is the additional potential (*e.g.* the disk impurity introduced below) acting in the wire region $0 < x < L$ only. By changing E we may change the number of open channels, M_1. Alternatively, to reproduce more closely an experimental situation [5], we fix the energy, E, but we add a static electric field across the strip. By increasing its amplitude F, we can decrease the number of open channels M_1 due to the presence of potential across the strip, $V = Fy$. To see this, realize, that outside of the perturbation region (where $W = 0$) the Schrödinger equation separates into the scattering motion in x direction and the bound motion in y coordinate. The latter corresponds either to square well (for $F = 0$) or to the triangular well (in the presence of the electric field). The electron entering (leaving) the interaction region has its energy split into "translational energy" corresponding to the x coordinate motion and the "transverse" quantized motion. For a given total energy E only a finite number M_1 of transverse motion levels are accessible. These M_1 possibilities defines, of course, the number of open channels. The dimensionless conductance $g = G/G_0$ is calculated from the

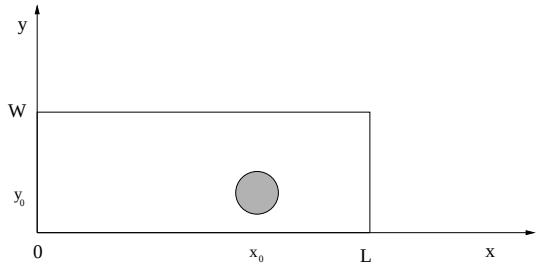


Fig. 1. Model wire considered in this section of length L and width $W \ll L$. We discuss the conductance of such a quasi-1D wire in the presence of an impurity modelled by a disk scatterer placed at a random position (x_0, y_0).

Landauer formula [8] (see also [9,10])

$$g = \mathrm{Tr}(\boldsymbol{t}\boldsymbol{t}^\dagger), \tag{2}$$

where $\boldsymbol{t}$ is the transmission matrix through the 'sample' relating the incoming and the outgoing solutions [actually a submatrix of the full S matrix, see

Eq. (5) below]. The impurity is introduced by placing inside the strip a disk potential of radius R at some random position (x_0, y_0). The potential inside the disk region is assumed to be equal to a positive constant V_0 with V_0 greater than the energy E of the incoming electron, *i.e.*, $P(x, y) = V_0$ for $(x - x_0)^2 + (y - y_0)^2 < R^2$ and $P(x, y) = 0$ elsewhere. The Schrödinger equation (1) is then solved using the finite element method and the result is averaged over several realizations of the position of the impurity in the strip. The width W of the strip is set to 1: $W = 1$. Fig. 2a compares the

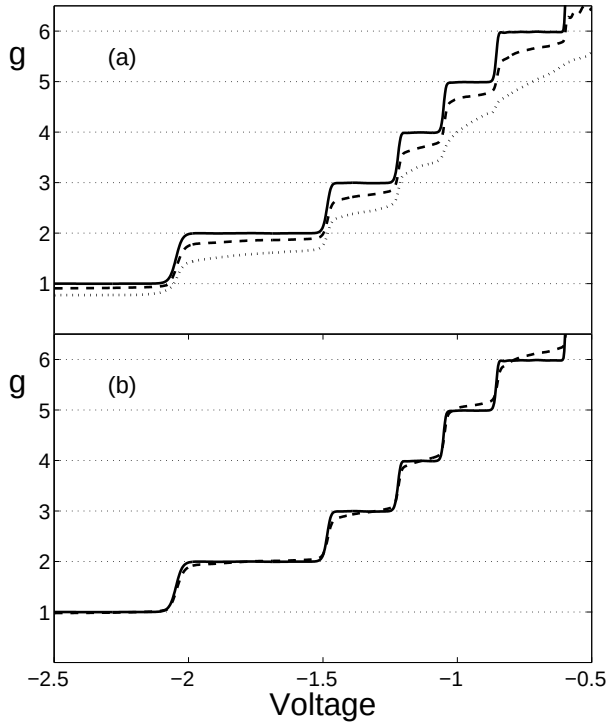


Fig. 2. Panel (a) displays mean dimensionless conductance, g, as a function of the applied voltage V. The case without impurity is plotted by full line. Broken line displays the conductance for the system with one impurity of radius 0.05 and dotted line corresponds to the case with one impurity having radius 0.1. Panel (b) compares the conductance of the system without impurity (full line) with that for the system with one impurity of the radius 0.05, but multiplied by a factor 1.12 (broken line)

conductance as a function of the applied voltage for the ideal strip and for the strip with a single impurity and two different ranges R. Observe that the presence of the impurity does not destroy the conductance steps; they are lowered and become less sharp. This effect is quite dramatic if more then one

impurity is present. For a better comparison of details of the steps with and without the impurity, we multiply the conductance in the presence of the impurity for $R = 0.05$ by a factor 1.12 so as the lowest step is approximately equal to unity. The result (Fig. 2b) show that with increasing number of open channels the steps, in the presence of the impurity, become larger and less sharp, in full agreement with experimental results [5].

It is worth stressing that the electron transport through the strip is only weakly affected by a single scattering center of the size much smaller that the width of the strip, W. The perturbation makes the process not fully ballistic and the backscattering leads to lowering of the conductance steps. We are, however, in quite a different regime than those in the typical "ballistic" chaotic cavity, where multiple scattering events dominate. In the latter case the average conductance is roughly halved in comparison to the maximal allowed value (proportional to number of open channels, M_1). For example, for the average conductance of a quantum dot coupled to the outside world by two leads each of which supports M_1 open channels one obtains [11]

$$g = \frac{M_1^2}{2M_1 - 1 + 2/\beta}, \tag{3}$$

where $\beta = 1$ for time reversal invariant systems and $\beta = 2$ when this symmetry is broken strongly.

For disordered systems (including the example just above) the rapid progress in the understanding of the electron transport has been obtained within the random matrix theory (RMT) approach, recently reviewed in detail by Beenakker [10]. In the next Section we show that by a slight modification of this approach we can also account for the noninteger conductance steps.

3. RMT Heidelberg-like approach

We consider a standard Heidelberg scattering matrix approach [12, 13] expressing the scattering matrix S as

$$S = 1 - 2\pi i W^\dagger (E_F - H + i\pi W W^\dagger)^{-1} W, \tag{4}$$

where H is the internal Hamiltonian of the system represented by a matrix of rank N while W is a $N \times M$ matrix representing the coupling between the N internal states and M scattering channels in the leads. Assuming two identical leads one gets $M = 2M_1$.

In the application to a chaotic cavity scattering one assumes that the number of internal states, N, around the Fermi energy, E_F, is much larger than M. Taking typical RMT assumptions about the statistical properties

of H and W one may then derive a number of predictions concerning the statistical properties of S and of the measurable observables. As shown by Brouwer [14], such an approach is equivalent (for $M \ll N$), to making RMT assumptions concerning directly the unitary S matrix itself. For example, if H pertains to the Gaussian Orthogonal Ensemble (GOE) and W are composed of real random vectors (the situation appropriate for time reversal invariant systems), then the $M \times M$ matrix S belongs to the corresponding circular orthogonal ensemble of unitary matrices (COE) in the limit $N \to \infty$. Similarly, if time reversal symmetry is broken and H pertains to Gaussian Unitary Ensemble (GUE), the corresponding S matrix shows statistical properties typical for the Circular Unitary Ensemble (CUE).

It is thus justifiable to derive transport properties by making statistical predictions for S matrices themselves. Such an approach yields, *e.g.*, Eq. (3). The advantage of the former, Heidelberg approach is that it allows also to calculate energy dependent quantities such as correlators or time delays, while the direct RMT approach to S matrices says nothing about the dependence on the scattering energy, E_F.

Consider now the experimental system of [5]. The 1D almost ideal wire placed between two 2D leads takes the place of the internal scattering system in the Heidelberg approach with N being now the number of states in the internal wire around E_F or the number 'internal channels'. Note that really the Hamiltonian describing the internal wire supports an infinite number of states. Most of them do not contribute to conductance being vanishingly small (evanescent) on the left or right side of the 1D wire. The important N "states" are the N scattering channels through the 1D wire if it were coupled incoherently to leads. So N can be even only. Moreover there is no ground to assume that the internal matrix H pertains to GOE (the wire is almost ideal). We shall show below that the conductance steps are *not* very sensitive to the detailed statistical properties of H. Since the leads are assumed to be two dimensional, $M = 2M_1$ should be much *larger* than N. Note that the limit $N \ll M$ is the opposite to that taken in the standard transport theory [10].

The structure of the S matrix, Eq.(4), indicates that N out of M of its eigenphases may be nontrivial and different from 0 (*i.e.* the remaining M–N eigenvalues of S are equal to unity). This is due to the fact that the part coupling the channels to the internal states has at most the rank N. Representing S by reflection and transition matrices

$$S = \begin{pmatrix} \boldsymbol{r} & \boldsymbol{t} \\ \boldsymbol{t}' & \boldsymbol{r}' \end{pmatrix} \tag{5}$$

and using scaling arguments one realizes that the dimensionless conductance g, Eq. (2), may depend only on one parameter $c = N/M$. Further we shall

expect that the average conductance increases in steps when N changes. The size of the steps may depend on c.

To test this qualitative picture we have simulated the conductance of the system by averaging the transmission obtained over several random realizations of H and W. In all the simulations $E_F = 0$ while we have varied N, M, as well as assumed different statistical properties of H. Specifically, we shall assume either GOE case or the situation when the eigenvalues of H are uncorrelated. The latter case we shall call the Poissonian ensemble (PE) since the nearest neighbour statistics takes then a Poissonian form. The $N \times M$ coupling matrix W is composed of N mutually orthonormal random vectors of length M. The average is obtained by taking 1000 different realizations of a given system. Fig. 3(a) shows the average transmission (dimensionless conductance) obtained keeping a fixed value of $c = N/M$ and increasing N by two. Observe that regardless of the properties of the internal matrix H the qualitative behaviour of the conductance is quite similar, it increases in steps smaller than unity, the value of the step being dependent on c and to a much lesser extend on the statistical properties of H. Panel (b) shows the behaviour of the system while keeping fixed the number of 'internal channels' N and increasing M. Observe that the conductance steps actually *decrease* with M for M large. It is the number of 'internal channels', N, which limits the conductance value. The dependence on M is much weaker and indicates that for larger M the backscattering plays a larger role leading to decrease of the conductance steps.

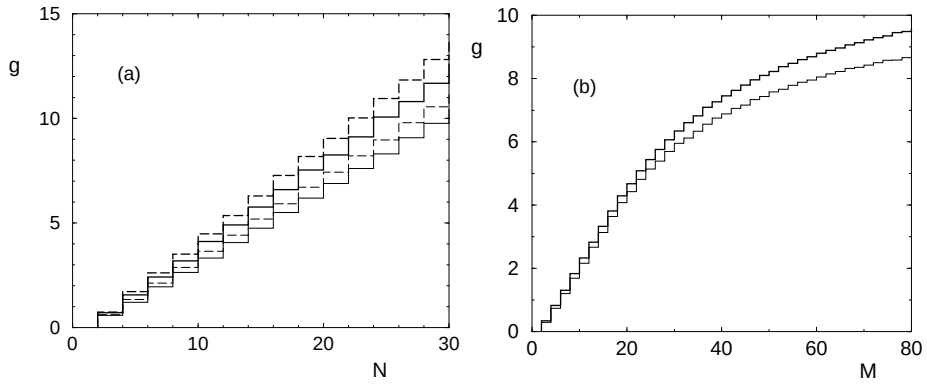


Fig. 3. Panel (a) displays mean dimensionless conductance $g = G/G_0$ evaluated as a function of the number of internal states N for $c = 0.5$ (thick lines) and 0.3 (thin lines). The full line corresponds to the Poissonian case, broken lines represent results obtained for GOE. Panel (b) shows g as a function of the number of channels M with N fixed to 20. Thick (thin) line corresponds to GOE (PE) case, respectively.

Fig. 3 shows already that the experimental observations of [5] may be at least qualitatively explained by the simple RMT model. To exemplify this point further we have assumed that the density of states changes according to a triangular potential well (as in the experiment) when the applied voltage is varied. After choosing the free parameter in the model, *i.e.*, c, the conductance dependence on the applied voltage reproduces fairly accurately the Fig. 2 of [5] (see Fig. 4).

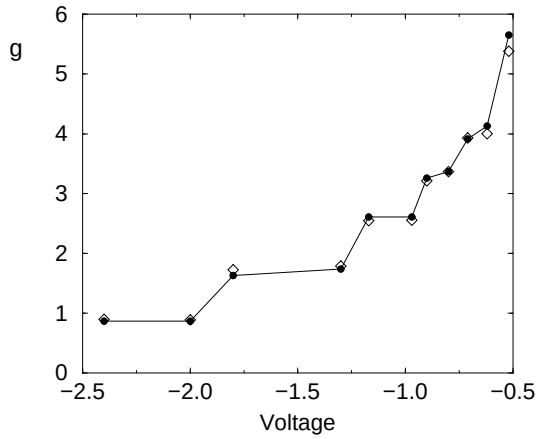


Fig. 4. Dependence of the dimensionless mean conductance on the applied voltage V. Filled dots connected by the line (to guide the eye) represent the results obtained in our model calculations with Poissonian internal matrix. The number of the channels M and internal states N depends on the voltage V as $M = [[(a - 3.7/V)]]$; $N = [[-3.7/V]]$ with $a = 8.8$. Here $[[x]]$ represents even integer number being most close to x. Diamonds correspond to the experimental results obtained in [5].

Let us point out that the results obtained are very weakly dependent on the statistical properties of the internal Hamiltonian H. For a given value of c, the conductance quantization step, observed when N is varied, increases slightly as the statistical properties of H change from PE ($\beta = 0$) to GOE ($\beta = 1$) or the picket fence spectrum corresponding to the levels repulsion parameter $\beta \to \infty$. The quantization step size remains practically unaffected (within the statistical significance of our data) if we consider the case of broken time reversal symmetry, *i.e.*, with H belonging to GUE.

Typically for the RMT approach, our simple model cannot account for the changes of the conductance steps with the temperature, T. Such temperature changes are indicators of the importance of the electron–electron (e–e) interactions [5]. It seems thus quite intuitive to blame this interaction also for the non-integer conductance steps. In this respect the fact that our model, being a single particle approach, also yields c dependent conductance

steps is quite surprising. Apparently, the step size can be reconstructed from RMT, *i.e.* a single particle approach (where at least a part of e–e interaction may be in principle included via Hartree or mean field approach). On the other hand, as shown in the previous section, the lowering of the steps is also obtained by a single electron model with impurity for which the RMT model presented should be appropriate.

4. RMT approach to S matrix

Accepting that the model presented yields reasonable predictions concerning the conductance steps one can ask whether in the studied, $N \ll M$ case similar predictions may be obtained using RMT assumptions directly for the S matrix. Naturally, the standard approach [10] has to be modified since the S matrix, must have $M - N$ unity eigenvalues.

We are thus going to mimic the scattering matrix by a $M \times M$ unitary matrix

$$S = U \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \cdots & \cdots & \vdots \\ 0 & 0 & 1 & \cdots & \cdots & \vdots \\ 0 & \cdots & 0 & e^{i\varphi_1} & 0 & 0 \\ \cdots & \cdots & 0 & 0 & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & e^{i\varphi_N} \end{pmatrix} U^{\dagger}. \tag{6}$$

The diagonal matrix of eigenvalues D consists of $M - N$ unit eigenvalues and N eigenvalues $\exp(i\varphi_i)$. The nontrivial eigenphases φ_i are distributed according to the joint probability distribution

$$P_{\beta}(\varphi_{1,\cdots,}\varphi_N) \sim \prod_{k<l}^{N} \sin^{\beta}[(\varphi_k - \varphi_l)/2],$$

characterized by the level repulsion parameter $\beta \in [0, \infty]$. Random unitary rotation matrix U is drawn uniformly with respect to the Haar measure on M dimensional unitary space and pertains to CUE. Such an assumption concerning U is correct for a broken time-reversal invariance, the situation not realized in the experiment [5]. It is known, however, from the standard RMT of scattering (in the $M \ll N$ limit) that the dependence of the conductance on the symmetry is relatively small for disordered wires and appears only on the level of weak localization corrections [10] through the eigenphases repulsion parameter β. Thus the results obtained should only weakly depend on detailed properties of U. This assumption is even more justified by the numerical results, mentioned above, that revealed that the

size of conductance step is not sensitive to the change from GOE to GUE within the Heidelberg model.

The total conductivity in the system is given by a sum of the individual transmission coefficients

$$g = \sum_{l=M/2+1}^{M} \sum_{m=1}^{M/2} |S_{lm}|^2. \tag{7}$$

There exist $M^2/4$ elements of the matrix S, contributing to the total conductance. Each element of this sum can be written as

$$S_{lm} = \sum_{k=1}^{N} U_{kl}^* U_{km} (e^{i\varphi_k} - 1),$$

with $l \neq m$. The double average $\left\langle \left\langle |S_{lm}|^2 \right\rangle_U \right\rangle_D$, over N random phases of the diagonal matrix D and over random rotation matrix U, consists of N diagonal and $N(N-1)$ off-diagonal terms. The averages over unitary matrices U distributed according to the Haar measure are known [15]. For each diagonal term

$$Q_d := \langle |U_{kl}^*|^2 |U_{km}|^2 \rangle = \frac{1}{M(M+1)}, \tag{8}$$

while off-diagonal elements contribute as

$$Q_{\text{off}} := \langle \text{Re}[U_{k_1 l}^* U_{k_2 l}^* U_{k_1 m} U_{k_2 m}] \rangle = -\frac{1}{M(M^2-1)}. \tag{9}$$

The average conductivity is thus given by

$$g = \frac{M^2}{4} (N P_d Q_d + N(N-1) P_{\text{off}} Q_{\text{off}}), \tag{10}$$

where P_d and P_{off} denote prefactors corresponding to the averages over the phases φ. For N diagonal terms this average does not depend on the ensemble and gives the prefactor $P_d = \left\langle |1 - e^{i\varphi}|^2 \right\rangle_\beta = 2$ for any value of β. For the off-diagonal terms the average over uncorrelated phases of the Poisson ensemble ($\beta = 0$) gives $P_{\text{off}} = \left\langle \left(1 - e^{i\varphi_1}\right) \left(1 - e^{i\varphi_2}\right) \right\rangle_{\beta=0} = 1$. Summing all terms together we obtain the average conductance for the Poissonian case

$$g_{\text{P}} = \frac{MN}{4(M^2-1)} (2M - N - 1). \tag{11}$$

For $N = 2$ the phase averages are simple for any distribution of phases characterized by the level repulsion parameter β. Off-diagonal elements carry a factor occurring from the phase average

$$P_{\rm off} = \left\langle {\rm Re}\left(1 - e^{i\varphi_1}\right)\left(1 - e^{i\varphi_2}\right)\right\rangle_\beta = 1 + f_2,$$

where

$$f_2 = \frac{\int\limits_0^{2\pi} \cos\psi \sin^\beta \frac{\psi}{2}\, d\psi}{\int\limits_0^{2\pi} \sin^\beta \frac{\psi}{2} d\psi} = -\frac{\beta}{\beta+2}. \tag{12}$$

Since their contribution $Q_{\rm off}$ is negative, increasing parameter β increases the average conductance according to

$$g_\beta = \frac{M^2}{4}(2P_d Q_d + 2(1+f_2)Q_{\rm off}) = \frac{M}{2\left(M^2-1\right)}\left(2M - 3 + \frac{\beta}{\beta+2}\right), \tag{13}$$

which in the limiting case of equidistant phases ($\beta \to \infty$) reduces to $g_\infty = M/(M+1)$.

In a similar way one obtains the phase average for off-diagonal elements for $N = 3$. Since in this case the average f_3 reads

$$\begin{aligned} f_3 &= \frac{\int\limits_0^{2\pi}\left(\int\limits_0^{\phi} \cos\psi \sin^\beta\frac{\psi}{2}\, \sin^\beta\left(\frac{\phi-\psi}{2}\right) d\psi\right)\sin^\beta\frac{\phi}{2} d\phi}{\int\limits_0^{2\pi}\left(\int\limits_0^{\phi} \sin^\beta\frac{\psi}{2}\, \sin^\beta\left(\frac{\phi-\psi}{2}\right) d\psi\right)\sin^\beta\frac{\phi}{2} d\phi} \\ &= -\frac{\beta}{2\beta+2} \end{aligned} \tag{14}$$

one gets an explicit formula

$$g_\beta = \frac{M^2}{4}(3P_d Q_d + 6(1+f_3)Q_{\rm off}) = \frac{3M}{2\left(M^2-1\right)}\left(M - 2 + \frac{\beta}{2(\beta+1)}\right). \tag{15}$$

Performing an average over the phases φ for arbitrary β becomes more difficult for larger N, but one may compute the average over the phases in

the limiting case of the most rigid, crystalline spectrum ($\beta \to \infty$). Making use of the identity

$$\sum_{k=1}^{N} \sum_{j=k+1}^{N} (1 + \cos((k-j)2\pi/N) = N^2/2 - N$$

we obtain the average over the phases for off–diagonal elements $P_{\rm off} = 1 - 1/(N-1)$, what substituted into (10) yields the mean conductivity

$$g_{\rm C} = \frac{MN}{4\,(M^2-1)}\,(2M - N)\,. \tag{16}$$

Observe that the dependence of the conductivity on the distribution of the phases $\{\varphi_k\}$ is weak and vanish in the limit of large N (with $M >> N$ preserved). Results for distribution typical of COE and CUE (with $\beta = 1$ and $\beta = 2$) should lie between the two limits. We have verified this assertion by performing numerical calculations. Random unitary matrices, pertaining to COE or CUE, where generated according to the algorithm presented in [16].

Using the above formulae one may calculate the conductance steps for fixed $c = N/M$. In the limit of large N, the step γ (when N increases by two) is equal to $\gamma_{\rm P} = 1 - 1/c$ for the Poissonian case and $\gamma_{\rm C} = 1 - 1/2c$ for the crystalline spectrum. Clearly, also the model constructed to mimic the S matrix directly is capable to yield the prediction for the conductance step size smaller than unity. Finally let us mention that while both the

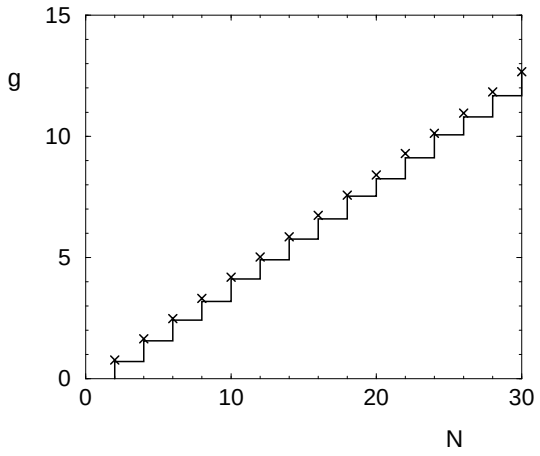


Fig. 5. The mean conductance obtained for $c = 0.3$ in the Poissonian case is plotted as a function of N (full line) and compared with the Eq. (11) (crosses).

approaches, the Heidelberg method (presented in the previous section) and the direct modelling of the S matrix properties yield similar predictions for $N \ll M$, *i.e.* give conductance steps smaller than unity, the models seem not to be equivalent (as it is in the opposite case of $M \ll N$ — see [14]). For example, assuming in the former approach that the internal H pertains to GOE does not assure that the nontrivial eigenphases of the S matrix obey the appropriate COE statistics (as we have checked numerically). Still, as shown in Fig. 5, for $N \ll M$ and fixed c both models yield quite similar prediction for the average conductance (and thus the size of the quantization steps). This robustness of the nonuniversal step size to the details of the random model assumed suggests strongly that the phenomenon is quite general and occurs whenever the number of open channels M exceeds the number of internal states.

5. Summary and conclusions

We have shown that a single impurity placed inside the wire may significantly lower the conductance step size, γ, from its unity value for an ideal wire. This results has been obtained in a continuous, solvable model consisting of a circular disk placed inside the otherwise ideal wire (modelled by a 2D strip). This results is supported by model Random Matrix Theory calculations, both using the Heidelberg approach and the direct assumptions on the S matrix ensemble. The lowering of the conductance steps does not depend on the details of the model, the only requirement being that the number of internal states, N, is much smaller than the number of open channels, M.

The RMT model proposed may be applicable also to other situations. Consider a chaotic quantum dot (with many thousands of levels) coupled by two almost ideal 1D leads to the broad connectors. Provided the coherence length exceeds the length of 1D leads we expect coherent backscattering on the border between the leads and the connectors. Then the number of original channels in the 1D leads determines the number of extended states, N, in the system: quantum dot + leads. This number may be quite small. All other levels of the quantum dot remain localized and do not contribute to the conductance. As the number of channels in the connectors, M, is large, the situation $N \ll M$ is recovered. Then even small impurity in the leads may lower the conductance steps in the system. Let us also mention a related study by Bascones *et al.* [17], in which another random matrix model was used to describe the conductivity in a system consisting of a narrow neck coupled to two wide ideal leads.

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