Transport through waveguides with surface disorder

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We show that the distribution of the conductance in quasi-one-dimensional systems with surface disorder is correctly described by the Dorokhov-Mello-Pereyra-Kumar equation if one includes direct processes in the scattering matrix $S$ through Poisson’s kernel. Although our formulation is valid for any arbitrary number of channels, we present explicit calculations in the one channel case. Ours result is compared with solutions of the Schrödinger equation for waveguides with surface disorder calculated numerically using the $R$-matrix method.

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The prediction of statistical properties of transport through disordered systems is one of the fundamental problems in mesoscopic physics [1-2]. The transmission coefficient, the dimensionless conductance if we are concerned with electronic devices, or in general any scattering quantity varies from sample to sample due to fluctuations on the microscopic configuration of disorder. Then, its distribution over an ensemble of systems macroscopically equivalent, but microscopically different, is of most interest [1]. Transport through quasi-one-dimensional waveguides (quantum wires in the electronic case) with bulk disorder has been tackled theoretically yielding to a Fokker-Planck equation, known as Dorokhov-Mello-Pereyra-Kumar (DMPK) equation [2,3]. This equation gives the evolution of the probability density distribution of the transfer (scattering) matrix $M(S)$ when the length $L$ of the system increases. The parameter appearing as time scale in the DMPK equation is the diffusion time across the disordered region. This leads to a natural assumption, the isotropic model of uniformly distributed random phases for $M(S)$ [1]. In the jargon of nuclear physics, it means that there are not prompt responses that could arise from direct processes in the system [2].

An analytical solution of the DMPK equation, for any degree of disorder, was found in the absence of time-reversal symmetry ($\beta = 2$ in Dyson’s scheme [4]), by mapping the problem to a free-fermion model [5,6]. In the presence of time-reversal invariance ($\beta = 1$), solutions are known only in the localized [6] and metallic regimes [11]. Those solutions were recently checked with extensive numerical Monte Carlo simulations [11,12]. It was also found in those references that waveguides with surface disorder are correctly described by the solutions of the DMPK equation in the localized regime. Interestingly, the solutions of the DMPK equation does not fit with the numerical results for surface disorder in the crossover to--nor in--the metallic regime.

Up to now, a complete theory that include wires or waveguides with rough surfaces is missing. In this letter we show that systems with surface disorder are correctly described by the DMPK equation as the direct processes, due to short-direct trajectories connecting both sides of the waveguides, are taken into account. We introduce prompt responses in a global approach as explained below. The direct processes are quantified by the ensemble average $\langle S \rangle$ of the $S$-matrix, known in the literature as the optical $S$-matrix [13,14]. Our theoretical results are compared with numerical calculations based on the $R$-matrix theory [15] to solve the Schrödinger equation for the one-channel case.

The waveguide with surface disorder is sketched in Fig. 1. It consists in a flat waveguide of width $W$ that support $N$ open modes (or channels) with a region of surface disorder of length $L$. The scattering problem is studied in terms of a $2N \times 2N$ scattering matrix $S$ which has the structure

$$ S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}, \quad \text{(1)} $$

where $r$ ($r'$) and $t$ ($t'$) are the reflection and transmission matrices for incidence on the left (right) of the disordered region. The dimensionless conductance $T = G/G_0$, where $G_0 = 2e^2/h$, is obtained from $S$ as $T = \text{tr}(t t^\dagger)$, according with Landauer’s formula.

From Fig. 1 it is clear that there could be direct transmission since there are trajectories, like $\gamma$, connecting both sides of the waveguide without any bounce in the rough surface although other trajectories like $\gamma'$ connect randomly both sides. In order to verify this statement we perform a numerical computation for the particular case $N = 1$. We choose $W = 1$; length $L = 100$ is divided into 100 pieces. To implement the surface disorder the ending point of each piece is a random number between 0 and a constant $\delta$ that measures the strength

\[ L \]

\[ R \]

\[ S \]

\[ T \]

\[ W \]
of the disorder. The ending points of each piece are connected with a spline interpolation to form a smooth disordered surface. The different realizations are done choosing different random displacements. We use a reaction matrix based method to solve the Schrödinger equation \[ 1 \] in the scattering region with zero derivative at the leads. The basis states can be found using a metric for which scattering geometry transforms to a rectangular region. Finally, the scattering wavefunction is expanded into a 2 \( N \) scattering matrix \( S \) and both, \( S \) and \( S_0 \), can be parameterized in a polar representation; for instance

\[
S_0 = \begin{pmatrix} u_0^{(1)} & 0 \\ 0 & u_0^{(2)} \\ \sqrt{I - \tau_0} & \sqrt{\tau_0} \\ \sqrt{I - \tau_0} & \sqrt{\tau_0} \\ 0 & u_0^{(3)} \\ 0 & u_0^{(4)} \end{pmatrix},
\]

and both, \( S \) and \( S_0 \), can be parameterized in a polar representation; for instance

\[
S_0 = \begin{pmatrix} r_0 & t_0' \\ t_0 & r_0' \end{pmatrix},
\]

where \( \mathbb{I}_{2N} \) is the unit matrix of dimension \( 2N \) and \( t_p \) can be chosen as \( t_p = t_p' \), where \( t_p' \) is a \( 2N \times 2N \) matrix which satisfies \( t_p' t_p'^\dagger = \mathbb{I}_{2N} - (S)_K (S)_K^\dagger \mathbb{I}_{2N} \). Here, \( (S)_K \) is the average of \( S \) taken with Poisson’s kernel, being the Jacobian of the transformation \[ 2 \]. The actual measured direct processes are quantified by \( \langle S \rangle \) which is linearly related to \( (S)_K \) (see below). Then \( S_0 \) is a matrix that describes all the scattering process as \( S \) with exception of the direct processes. It has a microscopic configuration of disorder that gives rise to \( (S)_0 = 0 \). Note that \( S \) is reduced to \( S_0 \) when \( \langle S \rangle_K = 0 \) such that \( \langle S \rangle = 0 \). Then the properties of the conductance in the “metallic” regime of the waveguide with surface disorder can be obtained from the localized regime by adding the direct processes. This means that the scattering matrices \( S \) and \( S_0 \) of the waveguide in the “metallic” and localized regimes, respectively, are related through Eq. \[ 2 \]. Since the distribution of \( S_0 \) is given by the solution of the DMPK equation in the localized regime, the distribution of \( S \) can be obtained from the distribution of \( S_0 \) taking into account the Jacobian of the transformation \[ 2 \].

As in Eq. \[ 1 \], \( S_0 \) has the structure

\[
S_0 = \begin{pmatrix} r_0 & t_0' \\ t_0 & r_0' \end{pmatrix},
\]

and both, \( S \) and \( S_0 \), can be parameterized in a polar representation; for instance

\[
S_0 = \begin{pmatrix} u_0^{(1)} & 0 \\ 0 & u_0^{(2)} \\ -\sqrt{I - \tau_0} & \sqrt{\tau_0} \\ \sqrt{I - \tau_0} & \sqrt{\tau_0} \\ 0 & u_0^{(3)} \\ 0 & u_0^{(4)} \end{pmatrix},
\]

FIG. 2: Dimensionless conductance \( T = G/G_0 \) as a function of \( E/E_0 \), where \( E_0 = \hbar^2 \pi^2/2m \), of a waveguide with (a) surface disorder and direct transmission and (b) surface disorder but without direct transmission. The insets show the respective waveguides. In (a) the conductance shows three regimes. In (b) the conductance shows a localized phase only.

FIG. 3: Distribution of the conductance (histogram) for an ensemble of 10 bent waveguides with surface disorder. It agrees with the solution of the DMPK equation in the localized regime (solid line).
where $\tau_0$ is a diagonal matrix whose elements are the eigenvalues $\{\tau_{0n} \in [0,1]\}$ of the matrix $\tau_{0j}^{(j)}$ and $u_0^{(j)}$, $j = 1, 2, 3, 4$, are $N \times N$ unitary matrices for $\beta = 2$, with the additional conditions $u_0^{(3)} = u_0^{(4)^T}$ and $u_0^{(4)} = u_0^{(2)^T}$ for $\beta = 1$. In the isotropic model each $u_0^{(j)}$ is distributed according to the invariant measure of the unitary group, $d\mu(u_0^{(j)})$. The probability distribution of $S_0$ can be written as

$$dP_{s_0}^{(\beta)}(S_0) = \frac{P_{s_0}^{(\beta)}(\{\tau_{0n}\})}{p_\beta(\{\tau_{0n}\})}d\mu_\beta(S_0),$$  

(5)

where $s_0 = L/\ell_0$ with $\ell_0$ the elastic mean free path without direct processes. $P_{s_0}^{(\beta)}(\{\tau_{0n}\})$ is the solution of the DMPK equation, which depends on the elements of $\tau_0$ only, and

$$d\mu_\beta(S_0) = p_\beta(\{\tau_{0n}\}) \frac{N}{\beta} \prod_{j=1}^N d\tau_0 \prod_{j=1}^N d\mu(u_0^{(j)}).$$  

(6)

(see Ref. 1) is the invariant measure of $S_0$ where

$$p_\beta(\{\tau_{0n}\}) = C\beta \prod_{a<b} \tau_{0a} - \tau_0^b \prod_{c=1}^N \tau_0^{(\beta - 2)/2}. \quad (7)$$

A similar parameterization as Eq. (4) holds for $S$ and for its probability distribution we have

$$dP_S^{(\beta)}(S) = \frac{P_S^{(\beta)}(S)}{p_\beta(\{\tau_0\})}d\mu_\beta(S), \quad (8)$$

where $d\mu_\beta(S)$ has a similar expressions as Eqs. (5) and (7) suppressing the label "0". Now, $P_S^{(\beta)}(S)$ include the phases and it is obtained from the equation $dP_S^{(\beta)}(S) = dP_{s_0}^{(\beta)}(S_0)$, which gives our main result,

$$P_{s_0}^{(\beta)}(S) = V_\beta^{-1} p_\beta(\{\tau_{0n}\}) P_{s_0}^{(\beta)}(\{\tau_{0n}(S)\}) \times \left[ \det \left( \mathbb{1} - \frac{1}{2N} \langle S \rangle_K - \langle S \rangle_K^* \right) \right]^{(2N\beta + 2 - \beta)/2}, \quad (9)$$

where $V_\beta^{-1}$ is a normalization constant. The last term on the right hand side is the Jacobian of the transformation, known as Poisson's kernel. Here, we are postulating that this Jacobian is valid not only when $S_0$ is uniformly distributed but also for $S_0$ with uniformly distributed random phases. However, the average of $S$ that appears in the Jacobian is not the actual value of $\langle S \rangle$. In fact, it is satisfied the one-to-one correspondence $\langle S \rangle = \langle S \rangle_K + \langle S_f \rangle$, where $\langle S_f \rangle$ is the average of the fluctuating part of $S$, as can be easily seen inverting Eq. (5) to write $S$ as $S = \langle S \rangle_K + S_f$. We have verified by numerically simulating DMPK $S_0$’s, and hence $S$ that, for a given value of $\langle S \rangle_K$, $\langle S \rangle$ coincides with $\langle S \rangle - \langle S \rangle_K$. Note that if $\langle S \rangle_K = 0$ (at the same time $\langle S_f \rangle = 0$), $S = S_0$ and $P_{s_0}^{(\beta)}(\{\tau_{0n}\})$ reduces to $P_{s_0}^{(\beta)}(\{\tau_{0n}\})$. Finally, in Eq. (4), it remains to write the $\tau_{0n}$’s in terms of $S$ using Eq. (2). As we mention before, we choose $t_p = t_p'$ once we calculate $t_p'$ numerically from the measured value of $(S)$; in general it can be done by diagonalizing $t''_p t_p'$. Then the distribution of the conductance $T$ can be obtained by multiple integration of Eq. (4). An example is given below.

The case $\beta = 1$ with $N = 1$. In what follows we are concerned with the $\beta = 1$ symmetry only and the index $\beta$ becomes irrelevant such that we can suppress it everywhere. In this case, $S_0$ is the $2 \times 2$ matrix [see Eq. (3)]

$$S_0 = \begin{pmatrix} -\sqrt{1 - \tau_0 e^{2i\phi_0}} & \sqrt{\tau_0 e^{(\phi_0 + \pi)}} \\ \sqrt{\tau_0 e^{(\phi_0 + \pi)}} & \sqrt{1 - \tau_0 e^{2i\phi_0}} \end{pmatrix} \quad (10)$$

where $0 \leq \phi_0, \psi_0 < 2\pi$ and $0 \leq \tau_0 \leq 1$. At the level of $S_0$, $\tau_0$ becomes the dimensionless conductance $T_0$, such that $\tau_0$ is replaced by $T_0$ everywhere. Eq. (6) gives

$$d\mu(S_0) = \frac{dT_0}{2\sqrt{T_0}} \frac{d\phi_0}{2\pi} \frac{d\psi_0}{2\pi}. \quad (11)$$

where we used that $p(T_0) = 1/2\sqrt{T_0}$.

As we mention above, the probability distribution of $S_0$ is given by the solution of the DMPK equation. Although the solution in any phase can be used, we use the one in the localized regime which is well known. In this phase, the variable $x_0$, defined by $T_0 = 1/cosh^2 x_0$, is Gaussian distributed, with

$$P_{0s_0}(x_0) = \frac{1}{\sqrt{\pi s_0}} \exp \left[ -\frac{1}{s_0} (x_0 - s_0^{-2})^2 \right], \quad (12)$$

with $s_0 = -4 \ln(T_0)$. Equivalent expressions to Eqs. (10) and (11) are valid for $S$ without the label "0". Those are used to write $T_0$ in terms of $S$ using Eq. (2) for a given $\langle S \rangle_K$. We will consider only the case $\langle S \rangle_K = w \sigma_x$, where $\sigma_x$ is one of the Pauli matrices and $w$ is a complex number. For $t''_p$ we choose $t''_p = \sqrt{1 - |w|^2} \text{diag}(e^{i\theta_1}, e^{i\theta_2})$, where $\theta_1$ and $\theta_2$ are arbitrary phases. From Eq. (2) we get

$$T_0 = \frac{(1 + |w|^2)\sqrt{T} e^{i\eta} - w^* e^{2i\eta} - w^2}{1 - 2w^* \sqrt{T} e^{i\eta} + w^2 e^{2i\eta}}, \quad (13)$$

where $\eta = \phi + \psi$. We note that the result is independent of the arbitrary phases $\theta_1$ and $\theta_2$. Finally, by direct substitution of $\langle S \rangle_K$, Eq. (12) and Eq. (13) into Eq. (10), we obtain the result for $P_{s_0}(\tau, \phi, \psi)$, from which the distribution of $T$ is obtained by integration over the variables $\phi$ and $\psi$ in the range $0$ to $2\pi$. Since $\phi$ and $\psi$ always appear in the combination $\eta = \phi + \psi$ one integration can...
be done easily. The result is

\[
P_{s_0}(T, \eta) = \frac{1}{2\pi} \frac{1}{\sqrt{s_0}} \exp \left[ -\frac{1}{s_0} \left( \cosh^{-1} \frac{1}{\sqrt{T_0}} - s_0 \frac{1}{2} \right)^2 \right] \\
\times \frac{1}{2\sqrt{T}} \frac{1}{\sqrt{T_0(1-T_0)}} \left( 1 - |\eta|^2 \right)^3 \frac{1}{1 - 2\sqrt{T}e^{i\eta} + \sqrt{T}e^{2i\eta}}.
\]

The remaining integration over the variable \(\eta\) can be done numerically. The results for \(s_0 = 10\) and \(w = 0.2, 0.5\) and 0.8 are shown in Fig. 4a, as well as one random matrix simulation (10^6 realizations) for clarity of the figure. The simulation was done for three values of the disorder parameter: \(w = 0.2\) (dashed), 0.5 (continuous), 0.8 (long-dashed). The crosses are random matrix simulations (10^4 realizations). For clarity we present only the case \(w = 0.5\). The agreement is excellent. (b) Comparison between theory (random matrix simulations) and numerical solutions of Schrödinger equation as described in the text (histogram). Here, \(s_0 = 33.6\) and \(w = 0.93\). The agreement is excellent but the experimental \(\langle S \rangle\) does not fit the theoretical one.

To conclude, we obtained the distribution of the conductance for waveguides with surface disorder. The direct transmission between both sides of the waveguide was taken into account in a global way. The results for the one channel case agree with numerical simulations, as well as with a numerical experiment made with R-matrix method. When the direct processes are increased the distribution moves from localized to metallic. Then, the direct processes could be the cause of the disagreement between the Dorokhov-Mello-Pereyra-Kumar equation and the numerical results recently obtained.

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