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A Monte Carlo approach to determine conductance distributions in quasi-one-dimensional disordered wires

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Abstract

A detailed analysis of the statistical distribution of conductance P(g) of quasi-one-dimensional disordered wires in the metal-insulator crossover is presented. The distribution P(g) is obtained from a Monte Carlo solution of the Dorokhov, Mello, Pereyra and Kumar (DMPK) scaling equation, showing full agreement with 'tight-binding' numerical calculations of bulk disordered wires. Perturbation theory is shown to be valid even for mean dimensionless conductance values $\langle g \rangle$ of the order of 1. In the crossover from diffusive to localized regimes ($\langle g \rangle \langle 1 \rangle$, P(g) presents a characteristic shape different from that observed in surface disordered wires. © 2005 Elsevier Ltd. All rights reserved.

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1. Introduction

The study of disordered systems plays a relevant role in Solid-State Physics (as well as in many other research areas) since well-ordered systems are exceptional situations, and the presence of disorder is a familiar situation to be taken into account when analysing actual physical systems (in many cases fabricated or synthesised with limited precision). When studying disordered physical systems, it is generally accepted that physical measurements on a single sample are well described by the quantities averaged over an ensemble of systems. The reason for this belief is that systems are self-averaging, which constitutes a central piece of the 'macroscopic' description of the system.

At sufficiently small length scales this macroscopic description fails, and a microscopic approach must then be taken into consideration. In particular, the macroscopic approach breaks down at surprisingly large length scales for disordered systems. It has been needed to develop a new approach to describe small and disordered systems. This description, in which the whole distribution function of the physical quantities is taken into account, is so-called the 'mesoscopic' approach.

One of the most extensively studied phenomena in mesoscopic physics is the behaviour, at low temperatures, of the statistical distribution of the dimensionless conductance P(g) of a disordered system as a function of its length L. The magnitude g is defined as $g = G/G_0$, where G is the conductance of the system and $G_0 = 2e^2/h$ the quantum of conductance (e being the electron charge and h the Planck constant). Large values of the conductance variance (var(G)) and different transport regimes were found for increasing length of a disordered system [1,2]. For lengths smaller than the elastic mean free path, $l_{\rm e}$, the electron transport through the system is ballistic, and the conductance distribution depends on the microscopic details characterising the system (system geometry, effective potential acting on the electrons). For L values larger than $l_{\rm e}$, electron transport becomes diffusive (entering into the diffusive or metallic regime). The signature of the diffusive regime is that P(g) presents a Gaussian shape with the same

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value of the conductance variance, irrespective of the sample length, the mean value of the conductance and microscopic details of the system. This property is known as universal conductance fluctuations (UCF) [1,3,4]. For even longer systems, transport enters in a new regime called localized or insulating regime in which the conductance decays exponentially with the system length and P(g) is lognormal [5]. However, the transition of P(g) from Gaussian to log-normal shaped distributions when the quasi-1D system evolves from metallic to insulating regimes is not yet well understood.

During the last years there has been an increasing interest in the study of P(g) at the crossover region (from diffusive to localization regimes) motivated by the numerical and analytical support for the existence of a universal distribution at the metal-insulator transition [6], the evidence of a broad distribution of the critical conductance at the integer quantum Hall transition [7,8] and the anomalous conductance distributions recently found in gold wires [9]. The understanding of the crossover region is not only important in electronic systems but could also play an important role to determine the onset of localization in photonic systems [10].

For quasi-one-dimensional (Q1D) systems, where there is only a smooth crossover from the metallic to insulating regimes, the behaviour of P(g) is highly nontrivial. It has been recently shown [11] that in the crossover region P(g) is highly asymmetric, and is described by an one-sided log-normal distribution. For larger disorder, the tail of the log-normal distribution for g > 1 is cut off by a Gaussian. These distributions have been observed in numerical simulations of different model systems [8,12,13]. In the crossover region (where $\langle g \rangle \approx 1/2$), numerical calculations of surface disordered wires (SDW) [12] have found a striking behaviour quite different from both the log-normal and Gaussian distributions. In particular, P(g)presents a 'cusp-point' at g=1 and is well described by random matrix theory (RMT) for two fluctuating channels [12]. Here we show that P(g) for bulk disordered wires (BDW) presents a sharp feature for $\langle g \rangle \approx 1$, which, however, differs from that observed in SDW. These results strongly contrast with the smooth behaviour of the conductance mean and variance [14] and the distributions of transmission coefficients [15], which were obtained exactly from the non-linear sigma model.

In this work we present a detailed analysis of the metal– insulator crossover based on the scaling approach of Dorokhov, Mello, Pereyra and Kumar (DMPK) [16] in the presence (β =1) or absence (β =2) of time reversal symmetry. By using numerical methods based on Monte Carlo techniques, we have obtained the exact conductance distribution of the DMPK equation all the way from the metallic to the insulating regimes. We have also performed extensive numerical calculations using the 'tight-binding' model for BDW with diagonal disorder (Anderson Model). We will show that the results of the Anderson model in the weak disorder limit are in full agreement with the solution of the DMPK equation. However, we will show that for increasing disorder the distribution P(g) of both, BDW and SDW, differs from the DMPK results.

2. The DMPK approach

The DMPK approach [16] describes the evolution of the join probability distribution of transmission eigenvalues $\wp(T_1,...,T_N;s=L/l_e)$ with increasing wire length *L*, where *N* is the number of open channels where electron transport is allowed. It is more convenient to use the set of *N* variables $(x_{n=1,...,N})$ where $T_n=1/\cosh^2(x_n)$. The distribution $\wp(\mathbf{x}=x_1,x_2,...,x_{N;s})$ is obtained by solving an associated *N*-dimensional Fokker–Planck equation (generalized diffusion equation) obtained from a first-order perturbative analysis of the transfer matrix solution for a disordered system of increasing length. Once $\wp(\mathbf{x};s)$ is determined, it is feasible to find the statistical distribution of the dimensionless conductance $P(g) = P(g = \sum_{n=1,...,N} T_n)$ for any *L* value.

However, the solution of the Fokker–Planck equation leading to $\wp(\mathbf{x};s)$ is a non-trivial exercise. In fact the exact solution $\wp_{\text{exact}}(\mathbf{x};s)$ of the DMPK equation is only known for $\beta = 2$ [4]. However, in the diffusive limit the solution $\wp_{\text{diff}}(\mathbf{x};s)$ (for both $\beta = 1$ [17] and $\beta = 2$) can be written in the general form of a Gibbs distribution $\wp_{\text{diff}}(\mathbf{x}=x_1,x_2,...*x_N;s) \sim \exp[-\beta H_{\text{diff}}(\mathbf{x};s)]$, where $H_{\text{diff}}(\mathbf{x};s)$ is given by:

$$H_{\text{diff}}(x;s) = \sum_{i < j} u_{i,j} + \sum_{i} V(x_i;s)$$
(1a)

$$u_{i,j} = -\frac{1}{2}\ln|\sinh^2(x_j) - \sinh^2(x_i)| - \frac{1}{2}\ln|x_j^2 - x_i^2|$$
(1b)

$$V(x;s) = \gamma (2s\beta)^{-1} x^2 - (2\beta)^{-1} \ln|x \sinh(2x)|$$
(1c)

with $\gamma = \beta N + 2 - \beta$. Following Eq. (1), $H_{\text{diff}}(\mathbf{x})$ may be interpreted as the Hamiltonian function of *N* classical particles located at positions $x_{n=1,...,N}$ where $u_{i,j}$ represents the interaction potential between two particles located at x_i and x_j , and V(x;s) is an effective confining potential.

3. Bulk disordered wires (BDW): a Monte Carlo solution of the DMPK model

Since there is a clear analogy between the solution of the Fokker–Planck and that of the effective *N*-particles systems described by the Hamiltonian described by Eq. (1), we have computed the main statistical properties of P(g) using classical Monte Carlo techniques [18]. This method has been previously used to analyse fictitious Gibbs distributions of eigenvalues of random matrix models [19], but, to our knowledge, it is the first time used to describe electronic transport properties.

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