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Current in a quantum driven thermostatted system with off-diagonal disorder

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HIGHLIGHTS

- We observe no localization effects, for an equilibrium distribution of energies.
- We discuss the occurrence of fluctuations around the Bloch-wavesolutions.
- We discuss the onset of mesoscopic and macroscopic length scales.
- We show a large deviation principle for the transmission coefficient.
- We analyze the dependence of the transmission coefficient on the external field.

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ABSTRACT

We analyze a one dimensional quantum model with off-diagonal disorder, consisting of a sequence of potential energy barriers whose width is a random variable either uniformly or "half-normally" distributed, subjected to an external electric field. We shed light on how the microscopic disorder affects the value of the transmission coefficient and on the structure of the fluctuations around the solutions corresponding to the regular lattice configuration. We also characterize the asymptotic limit obtained by letting the number of barriers diverge. Thus, we explain the novelty of our method with respect to the standard thermodynamic limit discussed in the literature and also evidence the onset of a large deviation principle for the transmission coefficient.

1. Introduction

Nonequilibrium thermodynamics is based on the notion of space and time scales separation and on the assumption of *local equilibrium* [1–6]. The theory of large deviations, in particular, helped us to understand and interpret the role of the fluctuations in nonequilibrium systems [7–10]. On the other hand, recent technological advances on the nanoscale science and technology demand an extension of the theoretical apparatus and foster a statistical mechanical approach to systems of relatively small numbers of degrees of freedom. In such systems the microscopic, mesoscopic and macroscopic scales cannot be sharply separated, and the physical properties of microscopic devices widely fluctuate with respect to their mean values, violating the standard thermodynamic laws which describe macroscopic fields. In this work we face these issues by considering a variant of the original Anderson model, which is the prototype of a disordered solid [11]. In particular, we investigate the role of the microscopic disorder on the transmission coefficient of one dimensional systems consisting of a sequence of N barriers, with random widths, and $N-1$ wells, under the constraint that the sum of the barrier widths and the

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total length of the system are fixed and do not change with N. We then introduce a classical thermostat at given temperature T and an external electric potential $V_\ell - V_r$. Furthermore, we do not introduce simplifying assumptions such as the "tight-binding" approximation introduced by Anderson in his pioneering paper [12] on localization effects in disordered solids. Therefore, our model enjoys a purely off-diagonal disorder [13–15] which concerns only the tunneling couplings among the wells, leaving unaffected the energies of the bound states within the wells. This is not the case of the original tight-binding model, whose random fluctuations only concern the energy of a bound state. In turn, while in Anderson's model increasing the number of barriers corresponds to taking the large system limit, in our case it corresponds to distribute more finely the same amount of insulating material within the fixed length of the system.

The introduction of an external field allows us to extend to "nonequilibrium" the results previously obtained in the analysis of the model treated in Ref. [16], which are recovered, as shown below, in the limit of vanishing external fields. We, thus, investigated the effect induced by this kind of disorder at the mesoscopic scale on the transmission coefficient and we shed light on the structure of its fluctuations. Our results can be summarized as follows.

- There are no localization effects for the equilibrium distribution of energies at temperature $T = 300$ K: positive currents persist even in the large N limit.
- Furstenberg type theorems [11] do not apply. The reason is that the product of the random matrices yielding the transmission coefficient for a given choice of N barriers changes, in order to preserve the length of the system and the sum of the barrier widths, when the $N + 1$-th barrier is introduced.
- The value of the transmission coefficient, averaged over an ensemble of disordered configurations, is close, for large N, to the value corresponding to the ordered sequence of equally spaced barriers and wells, which is bounded away from zero.
- There is a scale for N, above which the (always positive) transmission coefficient does not depend on the specific realization of the disorder, but still depends on N, and there is another scale above which even the dependence on N is eliminated. We call "mesoscopic" the first, and "macroscopic" the latter scale, since it represents macroscopic nanostructured materials. This means that all realizations of the disorder become equivalent in the $N \to \infty$ limit.
- At room temperature, the probability distribution function (PDF) of the time independent transmission coefficients of the different realizations of the system satisfies a principle of large deviations. Furthermore, the peak of this PDF corresponds to the transmission coefficient of the regular realizations.
- Our $N \to \infty$ limit, representing a macroscopic object at given temperature, which is microscopically randomly structured, leads to radically different results from the usual macroscopic limits. In particular, it leads to the experimentally verifiable lack of localization. This is relevant in situations complementary to those described by the standard theories.

2. The model

Our one-dimensional model of a macroscopic semiconductor device consists of an array of N potential barriers and $N-1$ conducting regions (wells), in contact with one electrode which acts as an external thermostat at temperature $T = 300$ K. The particles leaving this thermostat are subjected to an external electric field F; cf. Fig. 1. The barriers have a constant height $V(x) = V$ while their width is either uniformly or "half-normally" randomly distributed. For any N, the widths of the conducting regions take a constant value δ_N. We denote by L the fixed total length of the sample, by L^{is} the fixed sum of the widths of all the barriers (i.e. the total length of the insulating region), and by β the fixed ratio between insulating and conducting lengths, so that

$$L = (1 + \beta)(N - 1)\delta_N \tag{1}$$

holds. To compute the current, we study the steady state Schrödinger Equation (SE):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + (V - eFx)\psi(x) = E\psi(x), \quad x \in [0, L] \tag{2}$$

where m is the mass of the particle, e is the electronic charge and F is the magnitude of the external electric field which takes the values F^{is} inside the barriers and F^{con} in the conducting regions. Due to the electric field, the potential energy decreases monotonically from V_ℓ, on the left boundary, down to V_r, on the right boundary, with a slope given by, respectively, $-eF_{is}$ within the barriers and $-eF_c$ in the conducting regions. Let us also introduce the parameter $r = F_{is}/F_c < \infty$, which allows us to consider the presence of a nonvanishing electric field even within the wells. Therefore, the energy of the electric field acting on the system, denoted by E_v, amounts to

$$E_v = e(V_\ell - V_r) = eF_cL_c(r\beta + 1). \tag{3}$$

The boundary conditions prescribe $A_0 > 0$ for the amplitude of the plane wave entering from the left boundary and $A_{4N+1} = 0$ (no wave enters or is reflected from the right boundary). The barriers are delimited by a set of $2N$ points, denoted by $x_0 = 0, \ldots, x_{2N-1} = L$ in Fig. 1, hereafter called *nodes* of discontinuity of the potential. The left boundary consists of a classical thermostat at temperature T, from which particles emerge at node in x_0 as plane waves, with energies distributed according to the Maxwell–Boltzmann distribution. Differently, no particles come from the electrode on the right.

Thus, denoting by $\mathcal{U}_\ell$ the ℓ-th region, for $\ell \in \{0, 2, \ldots, 2N\}$, the solutions of Eq. (2) take the form

$$\psi_\ell(x) = A_{2\ell}Ai_\ell(x) + A_{2\ell+1}Bi_\ell(x), \quad \text{if } x \in \mathcal{U}_\ell \tag{4}$$