Signature of ballistic effects in disordered conductors

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Statistical properties of energy levels, wave functions and quantum-mechanical matrix elements in disordered conductors are usually calculated assuming diffusive electron dynamics. Mirlin has pointed out [Phys. Rep. 326, 259 (2000)] that ballistic effects may, under certain circumstances, dominate diffusive contributions. We study the influence of such ballistic effects on the statistical properties of wave functions in quasi-one dimensional disordered conductors. Our results support the view that ballistic effects can be significant in these systems.

One of the simplest and yet most widely used models [1,3] for a disordered wire is that of independent electrons moving in a disordered potential described by a \( \delta \)-correlated Gaussian random function \( \nu(r) \) (where \( r = (x, y, z) \) is a spatial coordinate)

\[
\langle \nu(r) \rangle = 0,
\]

\[
\langle \nu(r) \nu(r') \rangle = (2\pi\nu\tau)^{-1} \delta(r - r').
\] (1)

Here \( \langle \cdots \rangle \) is an average over potential realisations, \( \nu = 1/(V\Delta) \) the electronic density of states, \( V \) the volume of the system, \( \Delta \) the mean level spacing, and \( \tau \) the scattering time. The corresponding Hamiltonian is

\[ H = \frac{p^2}{2m} + \nu(r) \] (2)

with mass \( m \) and momentum \( p \). For the model (1,2) it has been proven [2] that on small energy scales (of the order of \( \Delta \)) and for sufficiently weak disorder the quantum-mechanical correlation functions are universal and equivalent to those of random matrix theory (RMT) [4,5]. Moreover, deviations from universal statistics are parameterised by the dimensionless conductance \( g = 2\pi hD/(L^2\Delta) \) where \( D \) is the diffusion constant and \( L \) is the linear extension of the system. In the limit of \( g \to \infty \), fluctuations are of RMT type. Deviations may be calculated perturbatively, as an expansion in \( g^{-1} \) (see for instance [3,6] and references therein).

These important results were established using an effective field theory, the nonlinear \( \sigma \) model (NLSM) [6], valid for \( \lambda_F \ll \ell \) (where \( \lambda_F \) is the Fermi wave length) and on length scales larger than the mean free path \( \ell = \nu_F \tau \) (where \( \nu_F \) is the Fermi velocity). Efetov’s NLSM assumes that the electrons undergo diffusive motion and, within a saddle-point approximation, statistical properties of eigenvalues, wave functions, and matrix elements are characterised by a classical return probability expressed in terms of the diffusion propagator.

It has, however, been suggested that under certain circumstances, ballistic trajectories (i.e., trajectories scattering just once before returning to their starting point) may influence the fluctuations in the model (1,2). At present it is unclear to which extent the fluctuations in (1,2) may differ from those obtained from the diffusive NLSM. It is thus necessary to quantify the significance of ballistic effects using alternative methods.

One possibility would be to derive a more general NLSM for (1,2) incorporating ballistic effects [7]. Very recently, for instance, a ballistic NLSM was used to discuss statistical properties of energy levels and wave functions in ballistic quantum billiards with surface scattering [8].

In this paper, we determine the statistical properties of wave-function amplitudes in the model (1,2) using exact-diagonalisation calculations for one- and quasi-one dimensional (1d and quasi-1d) tight-binding models with random on-site potentials. We determine to which extent the statistics are influenced by ballistic effects. In addition to spatially uncorrelated disordered potentials [corresponding to (1)], we also consider potentials with smoothly varying spatial correlations (Eq. (6) below). In the latter case one expects ballistic contributions to be suppressed. Our results support the view that ballistic effects can be significant in quasi-one dimensional disordered systems.

Formulation of the problem. Within the diffusive NLSM, one finds that deviations from universal statistics are parameterised by the time-integrated return probability [6,7]

\[ P(r, r' ; \omega = 0) \sim g^{-1} \begin{cases} 1 & \text{in quasi-1d,} \\ \log(L/\ell) & \text{in 2d,} \\ L/\ell & \text{in 3d} \end{cases} \] (3)

where \( P(r, r' ; \omega) \) is the diffusion propagator. It was pointed out in [7] that the time-integrated return probability may have additional contributions of the form

\[ P(r, r' ; \omega = 0) \sim \begin{cases} g^{-1} \log(\ell/\lambda_F) & \text{in 2d,} \\ \lambda_F/\ell & \text{in 3d} \end{cases} \] (4)

These arise from ballistic trajectories contributing to the return probability on small length scales. In (4a), the diffusive contribution behaves as \( \sim (\lambda_F/\ell)^2 \) which is much
smaller than \((4b)\). The applicability of the diffusive NLSM is thus questionable, an issue raised in \(B\). In 2d systems, the effects are less drastic but can nevertheless be appreciable. In quasi-1d wires, the ballistic contribution is of the form \((B)\) (when the sample is locally 3d). Then the ratio of \((3a)\) and \((4b)\) determines whether ballistic effects are important or not.

The ballistic contributions \((4a, b)\) are suppressed in the case of a smoothly correlated disordered potential, such as

\[
\langle v(r) \rangle = 0,
\langle v(r)v(r') \rangle = (2\pi\nu)^{-1} f(|r - r'|/\ell_c)
\]

where \(f(x)\) is a dimensionless smooth function decaying on the scale \(x \approx 1\). When the correlation length is much larger than the Fermi wave length, \(\ell_c \gg \lambda_F\), ballistic contributions of the type \((4)\) are negligible.

The following questions arise: How important are ballistic contributions of the type \((4a, b)\) in low-dimensional disordered quantum systems? How exactly are they suppressed when \(\ell_c\) is increased? Under which circumstances is the diffusive NLSM applicable?

**Method.** In order to answer these questions we have performed exact diagonalisation studies of a tight-binding version of \((B)\) on a cubic lattice with lattice spacing \(a_0\)

\[
\hat{H} = \sum_{r,r'} t_{rr'} c^\dagger_r c_{r'} + \sum_r v_r c^\dagger_r c_r. \tag{6}
\]

Here \(c^\dagger_r\) and \(c_r\) are the creation and annihilation operators, the hopping amplitudes are \(|t_{rr'}| = 1\) for nearest-neighbour sites and zero otherwise. We consider \(\delta\)-correlated potentials

\[
\langle v_r v_{r'} \rangle = (W^2/12)\delta_{rr'} \tag{7}
\]

as well as spatially smooth potentials

\[
\langle v_r v_{r'} \rangle = (W^2/12) \exp[-|r - r'|^2/(2\ell_c)^2]. \tag{8}
\]

As usual, the parameter \(W\) characterises the strength of the disorder. As is well known, the eigenvalues \(E_j\) and wave functions \(\psi_j(r)\) of this Hamiltonian, for \(d \geq 2\), on small energy scales and for sufficiently weak disorder \((g \rightarrow \infty)\), exhibit fluctuations described by RMT. Depending on the phases of the hopping amplitudes \(t_{rr'}\), Dyson’s Gaussian orthogonal or unitary ensembles are appropriate \([B]\). We refer to these cases by assigning, as usual, the parameter \(\beta = 1\) to the former and \(\beta = 2\) to the latter.

By diagonalising the Hamiltonian \((B)\) using a modified Lanczos algorithm \([B]\), we have determined the distribution function

\[
f_\beta(E, r; t) = \Delta \left\langle \sum_j \delta(t - |\psi_j(r)|^2 V) g_\eta(E - E_j) \right\rangle \tag{9}
\]
of wave-function amplitudes for 1d and quasi-1d metallic samples. The wave functions are normalised so that \(\langle |\psi_j(r)|^2 \rangle = V^{-1}\) and \(g_\eta(z)\) is a window function of width \(\eta\), centered around \(z = 0\) and normalised to unity.

**Results.** We first discuss results for a chain of length \(L = 2 \times 10^4 a_0\) with periodic boundary conditions, using the smoothly correlated potential \((B)\). Fig. \(1(a)\) shows the \(x\)-averaged distribution functions \(\langle f(E; t) \rangle = \langle f(E, x; t) \rangle_x\) as a function of \(t\) for \(W = 0.5\), \(E = -1\) and for several different values of \(\ell_c\). Our numerical results are fitted by the expression

\[
f(E; t) \approx \frac{\xi}{L \ell_c} \exp \left( -\frac{t \xi}{L} \right) \tag{10}
\]

derived in \([1]\) for a 1d chain of length \(L \gg \xi\). Here \(\xi\) is the localisation length. Eq. \((10)\) describes the exact-diagonalisation results well for \(t \gg L/\xi \exp(-L/\xi)\), as expected \([12]\). Fig. \(1(b)\) shows \(\xi\) as a function of \(\ell_c\). We observe that \(\xi\) increases exponentially fast with \(\ell_c\) for \(\ell_c\) not too large. This is in keeping with second-order perturbation theory \([3]\), valid for small \(W\) where

\[
\xi^{-1} = \frac{W^2}{36 a_0^2} \sum_{x=-\infty}^{\infty} e^{-x^2 a_0^2/(2\ell_c)^2} e^{2i\pi x} \tag{11}
\]

with \(E = 2\cos(k)\). Evaluating the sum over \(x\) using Poisson summation one obtains for \(E = -1\) and large \(\ell_c\)

\[
\xi^{-1} \approx \frac{W^2}{36 a_0^2} \sqrt{\pi \ell_c} \exp[-4\pi^2 \ell_c^2/(9 a_0^2)]. \tag{12}
\]

We observe reasonable agreement between Eqs. \((11)\) and \((12)\) for large \(\ell_c\) and the results of our simulations. For stronger disorder and shorter chains we observe significant deviations from \((11)\) (not shown).

We now discuss results for quasi-1d wires. As is well known, in the limit of large dimensionless conductance, the distribution function \((\hat{B})\) tends to the RMT result

\[
f_{\beta}^{(0)}(t) = \begin{cases} 
\exp(-t/2)/\sqrt{2\pi t} & \text{for } \beta = 1, \\
\exp(-t) & \text{for } \beta = 2.
\end{cases} \tag{13}
\]

The \(\beta = 1\)-distribution is often referred to as the Porter-Thomas distribution \([B]\). Within the diffusive NLSM one obtains for the \(x\)-averaged relative deviations \(\delta f_{\beta}(E; t) \equiv \langle f_{\beta}(E, x; t) \rangle_x / f_{\beta}^{(0)}(t) - 1\)

\[
\delta f_{\beta}(E; t) \approx P \left\{ \begin{array}{ll}
3/4 - 3t/2 + t^2/4 & \text{for } \beta = 1, \\
1 - 2t + t^2/2 & \text{for } \beta = 2
\end{array} \right. \tag{14}
\]

(see \([B]\) and references therein). Here \(P \equiv \langle P(x, x; \omega = 0) \rangle_x\). Eq. \((14)\) is expected to be valid for small values of \(t\) \((t \lesssim P^{-1/2})\). We emphasise that, according to the diffusive NLSM, \(P\) is the same for \(\beta = 1\) and \(2\): it is related to the diffusion propagator, a classical quantity. Interference effects are contained in the coefficients of the polynomials in \(t\).
According to Refs. [2][4], the diffusive NLSM is expected to be valid under the following conditions

\[ 1 \ll \ell / \lambda_F \ll S / \lambda_F^2 \]

where \( S = M a_0^2 \) is the cross-section of the wire.

How may ballistic contributions, such as those given by Eq. (4) affect the prediction (14)? The heuristic argument of Ref. [3] proceeds as follows: in the \( \delta \)-correlated case, short ballistic trajectories contributing to the return probability scatter only once before returning and are thus self-retracing. When fitting \( P \) independently for \( \beta = 1 \) and 2 to Eq. (4), the values \( P_2 \) may differ. In the limit where ballistic effects dominate, \( P_1 / P_2 \to 1/2 \). If ballistic effects are absent (for sufficiently smoothly correlated \( \nu \)) one expects \( P_1 / P_2 = 1 \).

Comparing expressions (4a) and (4b), one sees that in the \( \delta \)-correlated case the diffusive contribution is dominant only for small enough values of \( g \), i.e., when \( g \ll \ell / \lambda_F \). Since \( g = \xi / L \approx S \ell / (\lambda_F^2 L) \), this implies a condition

\[ S / \lambda_F^2 \ll L / \lambda_F \]

or, if \( \lambda_F \approx a_0 \),

\[ M \ll L / a_0 \].

Therefore, we expect the ballistic effects to dominate for large \( M \) and small \( \ell / a_0 \).

We have evaluated \( \delta f_{\beta}(E, t) \) for \( \delta \)-correlated as well as for smooth disordered potentials in a \( L \times \sqrt{S} \times \sqrt{S} \) sample of length \( L \) and cross section \( S \). Our results for the \( \delta \)-correlated case are summarised in Fig. 3. The results for the smooth case (\( \ell / a_0 = 2 \)) are similar and are shown in Fig. 2. In both cases, we have also plotted fits of Eq. (14) to the data, using the parameters \( P_1 \) and \( P_2 \) as fitting parameters. We see from Figs. 2 and 3 that the functional forms of the deviations \( \delta f_{\beta}(E, t) \) are well described by (14). In Fig. 4, the values of \( P_1 / P_2 \) are shown, as obtained from fitting (14) to the data in Figs. 2 and 3 for \( \beta = 1 \) and 2. Despite the fact that the scatter is large, we identify the following trends.

First, in the smoothly correlated case, \( P_1 / P_2 \simeq 1 \) for all values of \( M \). This corresponds to the result derived using the diffusive NLSM. In the case of a smooth potential, large-angle scattering of the electrons is reduced and the contribution of ballistic, self-retracing trajectories to the time-integrated return probability is negligible.

Second, in the \( \delta \)-correlated case we observe a crossover from \( P_1 / P_2 \simeq 1 \) for small values of \( M \) to \( P_1 / P_2 \simeq 1/2 \) for large values of \( M \). The crossover takes place at values of \( M \) of the order of \( L / a_0 \). This is consistent with the heuristic prediction (10) and indicates that ballistic contributions to the return probability are of the form (4b). They dominate the diffusive contribution (3a) for large values of \( M \) and are negligible for small values of \( M \). In the latter case the diffusive NLSM applies, in the former case it does not.

Conclusions. Using exact-diagonalisation calculations of the quasi-1d tight-binding model (6-8), we have determined statistical properties of wave-function amplitudes and compared the results to predictions of the diffusive NLSM. Our results depend on the nature of the spatial correlations of the disordered potential which may be \( \delta \)-correlated or spatially smooth. The conclusions can be summarised in three points. First, in the \( \delta \)-correlated case the diffusive NLSM applies provided the wires are not too thick (\( M \ll L / a_0 \)). This is consistent with the following heuristic ansatz: The classical return probability is assumed to be a sum of diffusive and ballistic contributions. If \( M \ll L / a_0 \), the diffusive contribution (3a) dominates and the diffusive NLSM is applicable. If \( M \gg L / a_0 \), the ballistic contribution (4b) dominates and the diffusive NLSM is not applicable (we find \( P_1 / P_2 \simeq 1/2 \) and not 1 as predicted by the diffusive NLSM). Second, the functional form of the deviations, is still very well approximated by the diffusive NLSM prediction even for thick wires. Third, in the smoothly correlated case, the exact-diagonalisation results agree with the NLSM predictions.

Our results confirm a heuristic discussion of ballistic effects [3]. Their influence on the distribution of wave-function amplitudes is thus qualitatively understood, but a quantitative understanding has not yet been achieved. It would be of great interest to calculate the distribution function \( f_{\beta}(E, x; t) \) using the ballistic NLSM discussed in [4], and to compare to the results summarised in the present paper.

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FIG. 1. (a) The distribution functions $f(E; t)$ for a 1d chain of length $L/a_0 = 2 \times 10^4$, with $W = 0.5$, for different values of $\ell_c/a_0$ (symbols). They have been fitted to Eq. (10) (lines), using $\xi/a_0$ as a fitting parameter. (b) The corresponding localisation lengths $\xi$ as a function of $\ell_c$. Also shown are expressions (11) (full line) and (12) (dashed line).

FIG. 2. Shows $\delta f_\beta(E; t)$ for the model (7), for $\beta = 1$ (●) and $\beta = 2$ (□), for $W \approx 0.7$, $L = 128 a_0$, and for different values of $M$. Also shown are fits to the data according to (14) (lines), with $P$ as a fitting parameter.

FIG. 3. The same as Fig. 2 but for the model (8), for $\beta = 1$ (●) and $\beta = 2$ (□), $\ell_c/a_0 = 2.0$, and $W = 0.5$.

FIG. 4. $P_1/P_2$ versus $\sqrt{M}$ for $\delta$-correlated (□) and smooth (●) potentials. The parameters are as in Figs. 2 and 3.