Localization Length in Quasi One Dimensional Disordered System Revised

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In the weak disordered regime we provide analytical expressions for the electron localization lengths in quasi-one dimensional (Q1D) disordered quantum wire with hard wall and periodic boundary conditions. They are exact up to order $W^2$ ($W$ being the disorder strength) for an arbitrary number of channels. Detailed numerical analysis of the Anderson localization, based on Kubo’s formula for conductivity, show excellent agreement with analytical calculations. We establish relationship between various lengths in Q1D systems.

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Introduction.—A quasi-one dimensional (Q1D) geometry, as a model for a disordered wire, is of great interest in condensed matter theory. The electronic transport problem in weakly disordered Q1D systems can be solved analytically within some approximations (see, e.g., [1] for details). The Dorokhov-Mello-Pereyra-Kumar (DMPK) equation [2] and random matrix theory for the transfer matrix [3] are the two successful approaches which are generally applied to describe the behavior of conductance in a disordered wire. These two approaches give very similar solutions for the probability distribution of conductance in Q1D and predict some universal properties of electron transmission. They also give very similar expressions for the localization lengths (LL): $\xi_M \approx (M+1)l$ and $\xi_M \approx [\beta(M-1/2)+1]l$, respectively ($M$ is the number of the propagating channels, $l$ is the phenomenological mean free path, and $\beta = 1/2$ for orthogonal (unitary) symmetry class). In either approach, however, the phenomenological $l$ is viewed as a fixed parameter. The question how LL explicitly depends not only on energy $E$, but also on the coupling constants and the type of boundary conditions in Q1D disordered systems is left out in these analyses. What we are trying to point out is that in spite of the progress which has been made to towards a characterization of the localization in Q1D systems, microscopic analytic studies of LL as a quantum parameter of fundamental importance, has still not been achieved.

The first step in this direction was done by Dorokhov in Ref. [4], who calculated the LL of $M$ random tight-binding (TB) chains with random site-energies. The LL in a weak disordered regime was obtained by the author for a Q1D wire with $M$ channels, is independent of the number of channels $M$. This result was questioned by Heinrichs [5], where it was shown that for weak disorder and for coupled two- and three-chain systems ($M = 2, 3$) the inverse LL is proportional to $M$, in contrast to the result of Ref. [4]. However, this approach, adopted in [5] and based on a scattering matrix treatment of conductance, does not allow author to extend his studies of LL to Q1D systems with larger numbers of scattering channels $M$. Recently, progress has been made in taking into account an arbitrary number of channels in the calculation of LL. Römer and Schulz-Baldes [6] using a perturbative formula for the lowest Lyapunov exponent (the inverse LL) for Q1D TB Anderson strip model with PB conditions obtained LL’s dependence on energy $E$, propagating modes $M$ ($M$ is even) and disorder strength $W$. A non-perturbative analytical approach, based on the Green’s function formalism to solve the Dyson equation in Q1D and two-dimensional (2D) disordered systems without any restriction on the numbers of impurities and modes, was developed in Refs. [7,8]. For a TB Hamiltonian with several modes and on-site disorder the electron’s scattering matrix elements $T_{nm}$ (hence the wire conductance $G = \sum_{nm} T_{nm} T_{nm}^*$, in units of $e^2/h$) were analytically calculated for an arbitrary impurity profile without actually determining the eigenfunctions. In these papers only HW conditions were discussed, which correspond to arranging the parallel equidistant chains on a plane.

We have performed a careful numerical analysis and have derived the LL in a Q1D system with HW and PB conditions. In our numerical calculations we used Kubos formula for computing conductivity. The numerical results were compared with the existing analytical expressions of LL, calculated in Refs. [4,5]. Surprisingly, our numerical calculations show that none of these expressions for LL fit the numerical data well. Particularly, LLs calculated in Refs. [4,5,7,8] result in an incorrect dependence on $M$, while LLs calculated [6,8] correctly predicted the $M$ dependence, but failed to provide the exact magnitude of LL.

The discrepancy between the theory and our numerical results, as we will explain later on, is due to two main factors: (i) Since it is not easy to calculate the right-hand term of the equation (7) (see below), theoretical calculations assume that in the weak disordered regime the length $\langle \ln G \rangle$ can be replaced by length $\ln \langle G \rangle$ and by expanding to lowest order of the powers of the disorder and, after averaging over realizations one can get...
a closed analytical expression for LL in the Q1D system \((\langle \ldots \rangle \) denotes averaging over disorder realizations). However, because of not self-averaging the conductance \(G\), these lengths do not agree with each other and thus lead to a different answer for LL. Note that the same type of problem exists also in 1D disordered system where, in the weak disordered limit, LLs obtained numerically and analytically, differ by a factor of 2 (see e.g., Refs. \[10, 11]\).

(ii) As follows from the numerical analysis of the relationship between the different LLs in Q1D systems (see Eq. (1)), the right hand-side term is not zero. This is an essential piece of information, which allows us later on to introduce new LLs for different boundary conditions in the transverse direction, which fit the numerical data very well.

It is worth noting that while in 1D the relationships between the various lengths is well known (e.g., \(\langle \ln G \rangle = 4 \ln \langle G \rangle - \frac{4}{5} \ln \langle 1/G \rangle\), in Q1D, to the best of our knowledge, no such calculations have been previously reported. Our first goal consists in checking numerically what relationship exists for different lengths in the Q1D case. Once this is established, motivated by our doubts about the correctness of LLs results of Refs. \[4–9]\) and to overcome the difficulty of the discrepancy, we have reconsidered the calculation of LL for the Q1D TB anisotropic Anderson model, using the Greens function approach, developed in Refs. \[7–9]\). This is our second and main goal. The analytical results for LL with HW and PB conditions, Eqs. (9) and (11), are then compared with numerical results. Excellent agreement with analytical calculations can be achieved if one multiplies the expressions (9) and (11) by a factor 2 and shifts them up by \(\xi_1\) for HW and by \(\xi_1/2\) for PB conditions, respectively. \(\xi_1 = 96 \sin^2 k_1/W^2\) is the LL in 1D disordered system, calculated in the weak disordered regime \[12]\).

**Relationship between different lengths in Q1D systems.**— First we study the relationship between \(\langle \ln G \rangle\) and \(\ln \langle G \rangle\) in Q1D disordered systems. Our numerical calculations show, that these two lengths are connected through the relation

\[
\langle \ln G \rangle - 4 \ln \langle G \rangle = C. \tag{1}
\]

The constant \(C\) is different for HW and PB conditions and for each case is determined numerically. \(C\) tends to zero in the 1D case as expected. The length \(L\) dependence of \(\langle \ln G \rangle\) and \(4 \ln \langle G \rangle\) is plotted in Fig. 1 for \(M = 10\) and \(W = 1\). The slopes of the two lines are the same within error bars. For each value of \(W\) we used \(C\)'s that ensure that we are well inside the exponential decay (see Fig. 1).

Some technical details follow: to obtain the mean values \((\langle \ldots \rangle)\) we have used \(10^5\) independent realizations of the disordered strip. Assuming a Gaussian form (as we have checked) for the logarithm of the conductance, \(z = \ln G\), it is straightforward to show that the average of \(G\) is

\[
\langle G \rangle = \int_0^M G P(G) dG = \int_0^M P(\ln G) dG.
\]

Solving the last integral and combining it with the numerical results for \(\langle \ln G \rangle\) and its variance \(\sigma^2\) we get

\[
\langle G \rangle = \frac{1}{2} \exp(\langle \ln G \rangle + \sigma^2/2) \text{Erfc} \left( \frac{\langle \ln G \rangle + \sigma^2 - \ln M}{\sqrt{2}\sigma} \right), \tag{2}
\]

where Erfc is the complementary error function.

**Q1D TB anisotropic Anderson model.**— Let us discuss a Q1D disordered lattice of size \(L \times M\) described by the standard TB anisotropic Hamiltonian with nearest-neighbor transfers, \(t_x\) and \(t_y\) along the \(x\) and \(y\) directions, respectively

\[
\mathcal{H} = \sum_{j=1}^L \sum_{l=1}^M \epsilon_{j,l} |j,l\rangle \langle j,l| - \sum_{j,l} \sum_{\delta = \pm 1} |j,l\rangle t_x (j + \delta, l) |j,l\rangle t_y (j, l + \delta) \langle j, l + \delta|, \tag{3}
\]

where \(|j,l\rangle\) is the atomic orbital at site \((j,l)\) and \(\epsilon_{j,l}\) is the strength of the random potential at site \((j,l)\), assuming it to be uniformly distributed in the interval \((-W/2, W/2)\). The disordered region is connected to perfect leads on both ends, extended to \(\pm \infty\) in the \(x\) direction. \(L\) is the length of the system and \(M\) is the number of modes in the left and right leads. For simplicity we choose the lattice constant to be equal to 1. For further calculations we assume the existence of a confining potential \(V_c(y_l)\) in the discrete \(y\) direction \((y_l = l, l = 1, 2, ..., M)\) leading to a set of transverse modes, whose actual values depend, however, on BC conditions. For HW and PB conditions, the energy of the electron is given by the following di-
The appropriate eigenfunctions, \( \psi_n(y) \), of the 1D Schrödinger equation with periodic potential of the chain of atoms along the y direction with HW and PB conditions are (\( l = 1, 2, ..., M \))

\[
\psi_n(y) = \begin{cases} 
\sqrt{\frac{2}{M}} \sin \frac{\pi n y}{M+1} & \text{HW,} \\
\sqrt{2 - \delta_n} \exp \left[ i \frac{\pi n y}{M} \right] & \text{PB.}
\end{cases}
\]  

(5)

Next, closely following Refs. [7, 9], we evaluate the scattering matrix elements \( T_{nm} \), in the weak disordered regime. The result for the electron transmission amplitude \( T_{nm} \) is

\[
T_{nm} \approx e^{i k_m (L-1)} \times \begin{cases} 
1 - \frac{\sum_{l=1}^{M+1} \sum_{i,j=1}^{L} \epsilon_{ij} \psi_m \psi_n^\dagger \psi_n \psi_m^\dagger}{4DL \sin k_m} & \text{if } n = m, \\
- \frac{i \sum_{l=1}^{M+1} \sum_{i,j=1}^{L} \epsilon_{ij} \psi_m \psi_n^\dagger \psi_n \psi_m^\dagger}{2L \sin k_m \sin k_m} & \text{if } n \neq m,
\end{cases}
\]

(6)

where \( A_l = \frac{1}{L} \sum_{n=1}^{M} \frac{\sin^2(n \pi l / L)}{\sin k_n} \), \( \phi_j = (k_n - k_m)(j - 1) \) and \( D = 1 + i \sum_{l=1}^{M+1} \sum_{i,j=1}^{L} \epsilon_{ij} A_l \). The wave numbers \( k_n \) for the propagating modes are defined by Eq. (4), for HW and PB conditions, respectively. Similarly, \( L_t \) is equal to \( M + 1 \) or \( M \) depending on the BC.

The inverse LL \( \xi_M \) as a function of the system size \( L \) and modes \( M \) can be written as

\[
\frac{1}{\xi_M} = - \lim_{L \to \infty} \frac{1}{2ML} \left( \ln \sum_{n,m}^{M} |T_{nm}^{(N)}|^2 \right).
\]

(7)

Now, replacing \( \ln G \) by \( \langle \ln G \rangle \) and assuming that for weak disorder the transmission coefficients are close to 1 and thus the reflection coefficients are close to zero, we can expand the right-hand side of Eq. (7). Next, after ensemble averaging over the random potentials \( \epsilon_{ij} \) distributed uniformly according to the explicit expressions for \( T_{nm} \), Eq. (6) and keeping the terms to order \( W^2 \), we arrive at the following expression for the inverse LL

\[
\frac{1}{\xi_M} = \frac{W^2}{96M^2} \sum_{l=1}^{M} \left[ \sum_{n=1}^{M} \frac{\psi_n(y) \psi_n^\dagger(y)}{k_n} \right]^2,
\]

(8)

which is valid for both boundary conditions.

**Hard wall conditions.**—Using the explicit expressions for \( \psi_n(y) \) (see Eq. (5)) and (9) for the LL \( \xi_M \) with HW conditions, when the \( M \) channels are propagating, we obtain \( \xi_M \)

\[
\frac{1}{\xi_M^\text{HW}} = \frac{W^2}{192M^2(M+1)} \times \left[ \sum_{n=1}^{M} \frac{3 + \delta_{2n,M+1}}{\sin^2 k_n} \right] + 2 \sum_{n=1}^{M} \frac{2 + \delta_{n+p,M+1}}{\sin k_n \sin k_p}.
\]

(9)

\( k_n \) is the Fermi wave vector of the \( n \)-th subband (channel) and is determined by the energy dispersion relation (4). For \( M = 1 \) it reduces to the LL \( \xi_1 \) for a 1D chain. If there is no coupling to the second, third, etc, modes, all \( k_n \) are equal, and after the summation over the modes, we find from Eq. (9) \( \xi_M^\text{HW} = M \xi_1 \). This result is somewhat expected: it confirms the prediction of Thouless [12] that in the limit of weak coupling \( \xi_M^\text{HW} \) must be proportional to \( M \). Although one can get two correct limiting values \( \xi_1 \) and \( \xi_M \) from expression \( \xi_M^\text{HW} \), Eq. (9), it fails to give the exact value of LL for an arbitrary \( M \).

Our direct numerical computation of the LL for the Anderson model [8] shows that we can get an almost perfect agreement with the theoretical \( \chi_M^\text{HW} \), Eq. (9) for \( M \geq 2 \), if we multiply the latter by a factor 2 and shift it up by \( \xi_1 \), i.e., redefine new LL \( \chi_M^\text{HW} \)

\[
\chi_M^\text{HW} = \frac{\xi_M^\text{HW}}{2} + \xi_1, \quad M \geq 2.
\]

(10)

Figure 2 shows the \( M \) mode dependence of \( \chi_M^\text{HW} \). The solid lines have been computed from Eq. (10) and the dots denote the result of numerical calculations. The good agreement found fully supports the validity of the analytical expression for \( \chi_M^\text{HW} \). The comparison is free of any adjustable parameter. We have checked that the analytical expression, Eq. (10), agrees very well with the numerical data in the whole range of vertical hopping parameter \( 0 < t_y < 1 \) where the \( \chi_M^\text{HW} \) is a linear function with respect to \( M \). The non-linearity starts when \( t_y \geq 1 \) and for those \( t_y \) the numerical and analytical results start behaving differently due to the fact that the validity of formula (10) breaks down. For these \( t_y > 1 \) our data show that \( L/\chi_M^\text{HW} \approx 1 \), i.e. takes place at the crossover from a Q1D to 2D system.

**Periodic boundary conditions.**—The result for the LL reads

\[
\frac{1}{\xi_M^\text{PB}} = \frac{W^2}{96} \left[ \frac{1}{M^2} \sum_{l=0}^{M} \frac{2 - \delta_l - \delta_{l+M}}{\sin k_l} \right]^2 \text{, if } M \text{ even},
\]

(11)

\[
\frac{1}{\xi_M^\text{PB}} = \frac{W^2}{96} \left[ \frac{1}{(M-1)^2} \sum_{l=0}^{M-1} \frac{2 - \delta_l}{\sin k_l} \right]^2 \text{, if } M \text{ odd},
\]

where \( k_n \) must be defined from the dispersion relation (4).

The process of deriving the expression for even \( M \) is quite straightforward. Using the explicit form of the electron wave function \( \psi_n(y) \), (9) and Eq. (8) yields the desired result. The case for odd \( M \) requires special consideration. First, for the infinitely long periodic system
the conductance $G$ is an odd function of energy, which is in contrast to the symmetric behavior of $G$ with even $M$ modes. Second, the analysis of the conductance of the ideal TB model as a function of the energy (at fixed even $M$) shows that the change from one plateau value to the next one is 2 (in units of $e^2/h$), while in the case of even $M$, it is 1. Formally this means that $M$ must be replaced by $(M − 1)$ in the expression of LL with even number of $M$. This conjecture was numerically tested and supported by the direct numerical calculation of the LL (see Fig. 3). It is clear that the difference between $M$ and $(M − 1)$ is negligible for large $M$, but may not be negligible for small $M$.

As in the case of HW condition we get an excellent agreement with the theoretical $\xi_{M}^{PB}$, Eq. (11) for $M ≥ 2$, if we multiply the latter by a factor 2 and shift it up by $\xi_{1}/2$. The new LL $\chi_{M}^{PB}$ is

$$\chi_{M}^{PB} = \frac{\xi_{M}^{PB}}{2} + \frac{\xi_{1}}{2}, \quad M ≥ 2. \quad (12)$$

In Fig. 3 we have tested the prediction of the analytical theory against the numerical results where the $M$ mode dependence of $\chi_{M}^{PB}$, Eq. (12) is shown. Solid lines have been computed from Eq. (12) and dots denote result of numerical calculations. The good agreement between simulations (dots) with Eq. (12) is evident for a relatively large range of disorder $W$. In the right panel of Fig. 3 our numerical data for LL was compared with similar expression $\frac{1}{\xi} ≈ \frac{W}{8\pi M} \sum_{l,m=0}^{M-1} \frac{2-\delta_{l,m}}{\sin k_{l} \sin k_{m}}$ (dashed line) from Ref. 8. One can see that the slope of the dashed line agrees with numerical calculations, but certainly there is a problem with accurate numerical values of LL. To get a correct value for LL for an arbitrary $M$ one needs the dashed line to shift up by about 0.39$\xi_{1}$.

In summary, our numerical calculations indicate that in Q1D disordered systems the right-hand side term of Eq. (1) is not zero. This means that without a vertical shift it is impossible to explain the discrepancy between the theory and numerical data and get the correct analytical expression for LL in the framework of different approaches used in Refs. 4-9. Based on Eq. (1) we have presented the analytical expressions (10) and (12) for LL which are in excellent agreement with numerical calculations.

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