Scaling in Interaction-Assisted Coherent Transport

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The pair localization length $L_2$ of two interacting electrons in one-dimensional disordered systems is studied numerically. Using two direct approaches, we find $L_2 \approx L_1^\alpha$, where $L_1$ is the one-electron localization length and $\alpha \approx 1.65$. This demonstrates the enhancement effect proposed by Shepelyansky, but the value of $\alpha$ differs from previous estimates ($\alpha = 2$) in the disorder range considered. We explain this discrepancy using a scaling picture recently introduced by Imry and taking into account a more accurate distribution than previously assumed for the overlap of one-electron wavefunctions.

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Very recently, Shepelyansky considered the problem of two interacting electrons in a random potential, defined by the Schrödinger equation

$$
(E - V_{n_1,n_2})\psi_{n_1,n_2} = \psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}.
$$

(1)

Here, $V_{n_1,n_2} = V_{n_1} + V_{n_2} + U\delta_{n_1,n_2}$ characterizes the on-site interaction and $V_{n_1} \approx W/2 \times \text{random potential uniformly in the interval} [-W,W]$. The indices $n_1$ and $n_2$ denote the positions of the first and the second electron, respectively. Shepelyansky proposed that, as a consequence of the interaction $U$, certain eigenstates extend over a range $L_2$ much larger than the one-electron localization length $L_1 \propto W^{-2}$. A key quantity in the derivation of this spectacular result in one dimension is the matrix representation $U$ of the Hubbard interaction in the disordered diagonal basis of localized one-electron eigenstates. With $R_{n,i}$ the amplitude at site $n$ of the one-electron eigenstate with energy $E_i$ we have

$$
Q_{ij,lm} = \sum_n R_{n,j}R_{n,j}R_{n,i}R_{n,m}.
$$

(2)

The $Q_{ij,lm}$ vanish unless all four eigenstates are roughly localized within the same box of size $L_1$. Assuming that $R_{n,i} \propto a_n/\sqrt{L_1}$ inside the box, with $a_n$ a random number of order unity, and neglecting correlations among the $a_n$ at different sites $n$, one finds $Q \approx 1/L_1^{3/2}$ for a typical nonvanishing matrix element. In this, this estimate was adopted and used to reduce the original problem to a certain band matrix model, eventually giving $L_2 \propto L_1^{\alpha}$. Later, Imry employed the Thouless scaling block picture to reinforce, interpret and generalize this result. The key step in this approach involves the pair conductance $g_2 = (UQ/\delta_2)^2$, where $\delta_2$ is the two-particle level spacing in a block of size $L_1$ and $Q$ is evaluated between adjacent blocks. Using $Q \approx 1/L_1^{3/2}$, as before, Imry finds that $g_2 \approx 1$ on the scale $L_2 \propto L_1^{\alpha}$, in agreement with Shepelyansky. As a second important result both approaches predict that the effect does not depend on the sign of $U$.

In this letter, we confirm the enhancement effect by studying both the original model for finite size samples and an infinite “bag model” with medium–range interaction. However, we find $L_2 \propto L_1^\alpha$ with $\alpha \approx 1.65$ instead of $\alpha = 2$ in both cases. Moreover, the sign of $U$ is not entirely irrelevant. We suggest that the small value for $\alpha$ is due to a very peculiar distribution of the $Q_{ij,lm}$. Imry’s scaling approach, modified to take into account the correct $Q$–distribution, is shown to be more or less consistent with $\alpha \approx 1.65$ in one dimension.

Transfer matrix approach for finite size chains. Eq. (1) is formally identical to a single–electron Anderson model in two dimensions with symmetric (with respect to the diagonal $n_1 = n_2$) on-site disorder. The indices $n_1$ and $n_2$ can be interpreted as cartesian coordinates on a finite square lattice with $N^2$ sites. The $N^2$ eigenstates of the Hamiltonian are either symmetric or antisymmetric with respect to the interchange of $n_1$ and $n_2$. The interaction is relevant for the symmetric states only (corresponding to electrons with opposite spins). For the time being we disregard questions of symmetry and proceed in analogy to the 2d Anderson model. Imposing hard-wall boundary conditions in the $n_2$–direction, transfer in the $n_1$–direction is described by a product of $N$ matrices $M_p$. This amounts to calculating the transport of one electron along the 1d chain while the other one occupies some state (or “channel”) of the same chain. Note that only the energy $E$ of the pair of electrons is fixed. In numerical computations we are restricted to finite sizes, $M_p$ being a $N \times N$ matrix. This limitation is inessential for $L_2 < N$ and induces only minor finite–size corrections for the transfer matrix eigenvalues otherwise. We rewrite (1) in the form

$$
\begin{bmatrix}
  u_{N+1} \\
  u_N
\end{bmatrix} = \prod_{p=1}^{N} M_p \begin{bmatrix}
  u_1 \\
  u_0
\end{bmatrix},
$$

(3)

where $u_p$ is a vector with $N$ components $(\psi_{p,1}, \ldots, \psi_{p,N})$ and the transfer matrix $M_p$ is defined by:

$$
M_p = \begin{bmatrix}
  (E - V_p)1 - H_1 & -1 \\
  1 & 0
\end{bmatrix} - U \begin{bmatrix}
  \Delta_p & 0 \\
  0 & 0
\end{bmatrix}.
$$

(4)
Here, $H_1$ is the (transverse) single–particle Hamiltonian for the second electron on the disordered chain of $N$ sites with hard–wall boundary conditions, and $\Delta_p$ is a diagonal $N \times N$ matrix with $(\Delta_p)_{ii} = \delta_{ip}$.

Before we numerically evaluate the set of decay lengths characterizing this transfer matrix product, we insert a few qualitative remarks. With $R$ the orthogonal $N \times N$ matrix diagonalizing $H_1$ (i.e., $H_1 = R H_d R^T$, where $H_d$ is a diagonal matrix with entries $E_n$) we transform $M_p$ according to

$$M_p = \begin{bmatrix} R^T & 0 \\ 0 & R^T \end{bmatrix} M_p \begin{bmatrix} R & 0 \\ 0 & R \end{bmatrix}. \quad (5)$$

In the noninteracting case ($U = 0$) $\mathcal{M}(N) = \prod_{p=1}^N M_p$ reduces to $N$ decoupled products of $2 \times 2$ matrices and we deal with a system of $N$ decoupled chains, all described by the same Hamiltonian $H_1$. On each chain $\alpha$ the first electron propagates with energy $E_n - E_o$ while the second one occupies an eigenstate of $H_1$ with energy $E_o$. The transfer matrix $M_p$ defines $N$ localization lengths $\xi_n(E - E_o)$ related to $H_1$, eventually becoming a continuous density in the thermodynamic limit. In the interacting case ($U \neq 0$) we have to consider in addition the $N \times N$ matrix $U R^T \Delta_p R$ for each $M_p$, which gives rise to two modifications. First, this couples the $N$ chains by a hopping term $U R^T \alpha R \alpha \beta$ proportional to the overlap (at site $p$) of two eigenstates of $H_1$ with energies $E_n$ and $E_\beta$, respectively. We recover the central point of the present problem: the effect of the (local) interaction is determined by the spatial overlap of the eigenstates of $H_1$. If these states have random phases, the sign of $U$ will be irrelevant in the hopping terms. However, the second modification due to $U$, a shift of $V_p$ on chain $\alpha$ by $U R^T \alpha R \alpha \alpha$, will remain sensitive to this sign. In short, the interaction couples the 1d chains and modifies (smoothens or enhances) the fluctuations of $V_p$ at those sites where the eigenstates of $H_1$ are localized.

We have numerically studied $\langle M(N) \rangle = \prod_{p=1}^N M_p$ as a function of $U$ and $W$ at fixed $E$. We focus attention on the logarithms $\gamma_i(N) = 1/\xi_i(N)$ of the eigenvalues of $M^T(N) M(N)$ divided by $2N$. One expects this set of inverse decay lengths $1/\xi_i(N)$ to couple to a well–defined large–$N$ limit $\gamma_i$. We denote by $L_2 \equiv \xi_1$ the largest of these lengths to characterize the extension of the least localized quantum state of the electron pair. In Fig.1 we present the five smallest and five largest inverse decay lengths $\gamma_i(N)$ for a given sample of size $N = 100$ as a function of $U$. The curves exhibit large sample–dependent fluctuations, but having analyzed many different samples we can draw the following conclusions: (i) the largest lengths are increased by the interaction, confirming the effect discovered by Shepelyansky; (ii) as expected for local interactions, shorter decay lengths are less sensitive to $U$ since the electrons tend to be localized with small or vanishing overlap; (iii) on average the curves are symmetric around $U = 0$ at the band centre $E = 0$ (due to an exact symmetry of the ensemble of Hamiltonians), but this symmetry is broken for $E \neq 0$, and the sign of $U$ appears to be no longer irrelevant; (iv) the nearest–neighbour spacing distribution of the $1/\xi_i$ shows a crossover from Poisson statistics (for $U = 0$) to Wigner–Dyson statistics at finite $U$.

To determine the dependence of $L_2$ on $W$ we show in Fig.2 (note the log scale) the ensemble–average $L_2(N) = 1/(\gamma_1(N))$ as a function of $W$ for $N = 100, E = 0$, and $U = 1$. One gets $L_2 \propto W^{-2\alpha}$ with $2\alpha = 3.29$, a value which differs from the estimate of Shepelyansky $\frac{1}{2}$ and Imry $\frac{1}{2}$ ($\alpha = 2$). Although this qualitatively confirms the enhancement effect, a certain (weak) sensitivity of $L_2$ on the sign of $U$, and especially the value of $\alpha$, indicates that the approximations employed in $\frac{1}{2}, \frac{1}{2}$ were not accurate enough. We note that for the smallest disorder values considered ($W = 0.7, 0.8$) $L_1$ is of the order of the system size. Nevertheless a strong enhancement effect prevails. This interesting observation supports the claim $\frac{1}{2}$ that persistent currents (in metallic systems) are enhanced by interaction effects.

**Bag model with medium range interaction.** To further substantiate our results, we turn our attention to the “bag model” already mentioned in $\frac{1}{2}$. In the infinite square lattice in which each point $(n_1, n_2)$ corresponds to a wave function $\psi_{n_1, n_2}$ of the two–electron system, we consider now the transfer along the diagonal instead of the $n_1$–direction. We associate with each center–of–mass coordinate $n = n_1 + n_2$ a “transverse” vector $\phi_n$ containing $N_b$ two–particle configurations with fixed $n$, but increasing distance $|n_1 - n_2|$. In contrast to the previous study (where we have ignored the symmetry of the wave function) we assume $\psi_{n_1, n_2} = \psi_{n_2, n_1}$ and consider only points in the upper triangle of the scheme. The coupling between the $\phi_n$ can be written as

$$E \phi_{2n} = h_{2n} \phi_{2n} + t^{(e)} (\phi_{2n+1} + \phi_{2n-1}),$$
$$E \phi_{2n+1} = h_{2n+1} \phi_{2n+1} + t^{(o)} (\phi_{2n+2} + \phi_{n}). \quad (6)$$

The form of the matrices $h_i$ and $t^{(e,o)}$ follows directly from $\frac{1}{2}$ and we have to distinguish between $\phi_{2n}$ and $\phi_{2n+1}$ since only the former has an entry on the diagonal $n_1 = n_2$. The corresponding $2N_b \times 2N_b$ transfer matrices are given by

$$M^{(e,o)}_i = \begin{pmatrix} t^{(e,o)}_{i-1} (E - h_i) -1 \\ 1 \end{pmatrix}. \quad (7)$$

They have to be iterated on a set of $N_b$ different start vectors $\Omega^{(i)} = (\phi_1^{(i)}, \phi_2^{(i)})$ which have to be orthonormalized from time to time as the iteration progresses $\frac{1}{2}$. Summing up the logarithmic increases of the norms of these vectors one calculates the set of Lyapunov exponents $\gamma_i = 1/\xi_i$ of this transfer matrix. The start vectors $\psi^{(i)}$ tend to the stationary distribution of the eigenvectors of $M^T M$, where $M = \prod_{i=1}^\infty M_i^{(e)} M_i^{(o)}$. 
Unfortunately, the truncation of the transverse vectors $\phi_i$ in the bag model introduces an artificial, long–range interaction between the two electrons. They feel a hard wall whenever their relative separation $\Delta n$ reaches its maximum value $(\Delta n)_{\text{max}} = 2N_b$. A detailed analysis of the bag model therefore meets with two problems: (i) to determine the localization length $L_1$ for the noninteracting problem and (ii) to attribute any observed enhancement of $L_2 = \xi_1 > L_1$ either to the (unphysical) bag interaction or to the (physical) Hubbard interaction.

We have performed numerical calculations for $E = 0$ and $N_b = 100, 200, 300$ in the disorder range $0.7 \leq W \leq 2.0$. In our model the two electrons interact with $U = 1$ whenever their distance $\Delta n$ is smaller than a fixed value $(\Delta n)_{\text{int}}$. This modification of the Hubbard interaction is designed to enhance the physical effect as compared to the unphysical bag interaction. We have chosen $(\Delta n)_{\text{int}} = 20$ (to be compared with $(\Delta n)_{\text{max}} = 2N_b = 200, 400, 600$). In all cases the full Lyapunov spectrum and the corresponding modes (i.e. the average of the vectors $\phi_i$ over the full iteration process) have been calculated up to a statistical accuracy of at least 5 percent.

Modes with dominant weight at very small $\Delta n$ (maximal $\Delta n$) owe their existence to the physical Hubbard interaction (the bag interaction). Therefore Fig.3, where we show the modes corresponding to the two smallest Lyapunov exponents $\gamma_1$ and $\gamma_2$, demonstrates that the medium–range Hubbard–type interaction is slightly more effective in assisting coherent transport than the artificial bag interaction. The dependence of $L_2$ on the disorder parameter $W$ is determined, as for the previous case of finite systems, by plotting $\log L_2 = \log(1/\gamma_1)$ versus $\log W$. The corresponding curve for $N_b = 300$ is shown in Fig.2. We find $L_2 \propto W^{-2\alpha}$ with $2\alpha = 3.42$. This is in relatively good agreement with the previous model and confirms that $L_2$ does not scale as $L_1^{3/2}$.

Finally, we compare in the inset of Fig.3 the smallest 36 Lyapunov exponents (for $N_b = 100$) with and without the Hubbard–type interaction. Two points deserve to be mentioned: (i) The interaction selectively reduces the smallest Lyapunov exponents, demonstrating the profound effect on the localization properties of the system. (ii) The smallest exponents which are no longer appreciably influenced by the interaction can serve (via $L = 1/\gamma_1$) as a reasonably good estimate for the localization length $L_1$ of the noninteracting system. The corresponding modes are the first ones to propagate without taking advantage of interaction effects.

$Q$–statistics and scaling. To understand the discrepancy between our calculated and previously estimated exponents, we return to the overlap matrix element $[3]$. We have calculated the $Q$–distribution (see Fig.4) for a 1d system with $W = 1.0$ and $N = 200$ in the following way. Defining two adjacent boxes of size $L_1 \approx 25/W^2 = 25$ in the middle of the system, we selected all (noninteracting) eigenstates having their maximum in either of these blocks. Then the distribution was determined by considering all $Q_{ij,lm}$ involving two wavefunctions from each block, respectively. We find deviations from a Gaussian behavior in two respects. First, while the off–diagonal terms $Q_{ij,lm}$ ($i \neq j$ and/or $l \neq m$) are distributed symmetrically around zero, the diagonal elements $Q_{ii,jj}$ are always positive. These latter contributions describe simultaneous transitions of two electrons (with opposite spins) between state $i$ and state $j$. Therefore, they involve only two wavefunctions (and not four), are typically larger than the off–diagonal terms and preserve the sign of the interaction $U$. Second, both the symmetric off–diagonal and the asymmetric diagonal parts of the $Q$–distribution are very sharply peaked at zero and have small but very long tails. Fig. 4 suggests that the particular role of the diagonal elements and the strongly non–Gaussian character of the distributions might be responsible for the modified exponent $\alpha$. The form of $p(Q)$ affects both the arguments given by Shepelyansky and by Imry. The band matrix model assumes that all pairs of two–particle states localized within a distance $L_1$ are coupled with uncorrelated, uniformly distributed interaction matrix elements. The scaling block picture estimates the interblock coupling using essentially the same assumption. In reality, sizable coupling matrix elements are sparsely distributed (and most likely quite correlated) within $L_1$, so that the notion of a typical interblock coupling (or a well–defined bandwidth in the band matrix model) is not unproblematic.

We nevertheless make an attempt to improve previous estimates. Following Imry [3] we consider two blocks of size $L_1$, each containing $L_1^2$ two–particle states. We want to use the actual distribution $p(Q)$ and therefore have to reduce a variable with a highly non–trivial distribution to a “typical” value needed for the Thouless scaling block picture. For illustration, we consider two extreme cases. First we calculate a restricted average $\langle Q^2 \rangle_{\text{res}}$ of the overlap matrix elements $Q$ coupling a state in the first block and its nearest (in energy) neighbour in the second block. Such an average is unaffected by the particular distribution of the $Q_{ii,jj}$, which couple levels with spacings of the order of $1/L_1$ (instead of $1/L_1^2$), and turns out to be consistent with $L_2 \propto L_1^{2}$. Second, we calculate an unrestricted average over the full spectrum, including also large energy separations. We obtain $\langle Q^2 \rangle \propto L_1^{-3.30}$ which eventually gives $L_2 \propto L_1^{1.70}$ in good agreement with our independent transfer matrix studies. We believe that the second averaging procedure is more appropriate. For a noninteracting system divided into blocks of size $L_1$ the Thouless energy associated with a block is of the order of the one–particle level spacing $\delta_1$. The level uncertainty is therefore large compared to the two–particle spacing $\delta_2$ and should suffice to justify an unrestricted average [3].

In conclusion, we have found that the pair localization length $L_2$ scales with an exponent $\alpha \approx 1.65$, for a large range of system parameters and in contrast to
previous predictions. The deviation from the expected value could be traced back to the particular distribution of the overlap matrix elements $Q$, composed of a symmetric off–diagonal and a positive diagonal part, both sharply peaked with long tails. By means of Imry’s scaling picture the anomalous exponent, characterizing the interacting electrons, could be connected to properties of the noninteracting system. The relevance of the $Q_{ii,jj}$ raises some doubts concerning the independence of the effect on the sign of the interaction. Studying the $Q$–distribution for $d > 1$ might be a useful tool to investigate and understand the effect discovered by Shepelyansky also in higher-dimensional systems.

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FIG. 1. The five smallest and five largest inverse decay lengths $\gamma_{i}(N)$ for a given sample with $N = 100$, $W = 1$, and $E = 2$ as a function of the Hubbard interaction $U$.

FIG. 2. Log–log plot of the pair localization length $L_2$ as a function of the disorder $W$ for (i) the finite chain with $N = 100$ (solid) and (ii) the bag model with $N_b = 300$ (dotted). Both curves were calculated for $U = 1$ and $E = 0$. The exponent $2\alpha = 3.3$ and the behavior of $L_1$ are also indicated.

FIG. 3. The modes $\phi_{n}^{\alpha}$ corresponding to the two smallest Lyapunov exponents $\gamma_{1}$ (solid) and $\gamma_{2}$ (dashed) for the bag model with $N_b = 200$, $W = 1.5$, $U = 1$, and $E = 0$. Inset: The smallest 36 Lyapunov exponents for the same model, but $N_b = 100$ and (i) $U = 1$ (solid) and (ii) $U = 0$ (dotted).