Numerical results for two interacting particles in a random environment

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Abstract. Much evidence has been collected to date which shows that repulsive electron-electron interaction can lead to the formation of particle pairs in a one-dimensional random energy landscape. The localization length $\lambda_2$ of these pair states is finite, but larger than the localization length $\lambda_1$ of the individual particles. After a short review of previous work, we present numerical evidence for this effect based on an analysis of the interaction matrix elements and an application of the decimation method. The results based on the decimation method for a two-dimensional disordered medium support the localization-delocalization transition of pair states predicted recently.

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1 Introduction

Investigations into the interplay of disorder and many-body interactions continue to receive a lot of attention mainly due to the persistent current problem¹–³ and the experimental discovery of the two-dimensional (2D) metal-insulator-transition (MIT)⁴–⁶. In order to theoretically study this interplay, in principle with increasing system size one has to solve a problem with an exponentially growing number of states in the Hilbert space. At present, this can be achieved only for a few particles in 1D⁷,⁸ and very few particles in 2D⁹–¹². Shepelyansky¹³,¹⁴—following earlier work of Dhorokov¹⁵—proposed another approach looking at the properties of two interacting particles (TIP) in a random environment. The TIP Hamiltonian is

$$H = -t \sum_{n,m} (|n,m\rangle \langle n+1,m| + |n,m\rangle \langle n,m+1| + h.c.) + \sum_{n,m} |n,m\rangle (\epsilon_n + \epsilon_m + U\delta_{nm}) \langle n,m|$$ (1)

with positions $n$, $m$ of each particle on a chain of length $L$, hopping probability $t$ (which we use to define the energy scale, i.e., $t=1$), onsite interaction strength $U$, and random potentials $\epsilon_n \in [-W/2,W/2]$ for disorder $W$. Shepelyansky suggested that even for repulsive interactions the two particles would form pairs with larger localization length $\lambda_2$ than the two separate single particles (SP). Thus the interaction would enhance
the possibility of transport through the system.\textsuperscript{16} The perhaps even more surprising prediction was that at pair energy $E = 0$

$$\lambda_2 \propto U^2 \lambda_1^2,$$

where $\lambda_1$ is the SP localization length. Since $\lambda_1 \propto 105/W^2$ in 1D, this implies large values of $\lambda_2$ for small disorders $W$.

The first numerical studies devoted to the TIP problem used the transfer matrix method (TMM) to investigate the proposed enhancement of $\lambda_2$.\textsuperscript{13,17–24} Other direct numerical approaches to the TIP problem have been based on the time evolution of wave packets,\textsuperscript{13,25–28} exact diagonalization,\textsuperscript{29} variants of energy-level statistics\textsuperscript{30–32} and multifractal analysis,\textsuperscript{33,34} Green function approaches,\textsuperscript{35–38} perturbative methods\textsuperscript{39,40} and mappings to effective models.\textsuperscript{41–45} In these investigations usually (but not always\textsuperscript{17–24}) an enhancement of $\lambda_2$ compared to $\lambda_1$ has been found but the quantitative results tend to differ both from the analytical prediction in Eq. (2), and from each other. Furthermore, a check of the functional dependence of $\lambda_2$ on $\lambda_1$ is numerically very expensive since it requires very large system sizes $L \gg \lambda_2 \gg \lambda_1$. Extensions of the original arguments have been proposed for higher dimensions,\textsuperscript{16,41,26} TIP close to a Fermi sea\textsuperscript{46} and long-range interactions in 1D\textsuperscript{18,} and 2D.\textsuperscript{11}

In this paper, we present numerical results for the interaction matrix elements and show that a correct statistical description necessitates the use of the logarithmic instead of the commonly used arithmetic average. The resulting typical matrix element $u_{typ}$ has a different disorder dependence than the arithmetic mean $u_{abs}$. Following the arguments of Ref.,\textsuperscript{13,14} the use of $u_{typ}$ does not give rise to a power-law enhancement as in Eq. (2). However, taking into account the energy denominators, the power-law can be recovered but with a smaller power of, e.g., $1.4 \pm 0.2$ for $U = 1$. This value is in agreement with previous results in 1D.\textsuperscript{17,21–24,27,30,33–41,45,47} We further review results based on the application of the decimation method\textsuperscript{47–49} which allows for a direct computation of $\lambda_2(U)$. Augmenting the analysis with the finite-size-scaling (FSS) approach,\textsuperscript{50} we construct estimates $\xi_2(U)$ of the TIP localization length in the infinite system.\textsuperscript{47,49} For $U = 0$ they reproduce accurately the well-known dependence of $\lambda_1$ on disorder while for finite $U$, we find $\xi_2(U) \sim \xi_2(0)^{\beta(U)}$ with $\beta(U)$ varying between $\beta(0) = 1$ and $\beta(1) \approx 1.5$. Thus the enhancement persists, unlike for TMM,\textsuperscript{17–21,23,24} in the limit of large system size. Finally, we apply the decimation method in 2D. Again using FSS we find scaling functions for $0.5 \leq U \leq 2$ which exhibit two branches corresponding to localized and extended behavior for TIP in an infinite system, and we estimate the $U$ dependence of the critical disorder and the critical exponent at the transition.

Before presenting our data, we briefly review the analytical approach to TIP. The prediction of Shepelyansky is based upon looking at the interaction matrix element of a pair state $\psi_{kl} = \psi_k \psi_l$ with another pair state $\psi_{nm}$.\textsuperscript{13,14} Here $\psi_k$ denotes the SP eigenstate localized with $\lambda_1$ around site $k$ and we can restrict the states by $|k - l| \leq \lambda_1$, $|n - m| \leq \lambda_1$ and $|k - l| \leq \lambda_1$, $|k - m| \leq \lambda_1$. The interaction matrix elements are

$$u = \langle \psi_{kl}|U|\psi_{nm} \rangle = U \sum_{j=1}^{N} \psi_j^\dagger (j) \psi_j^\dagger (j) \psi_n (j) \psi_m (j),$$

}\textsuperscript{(3)
Fig. 1 Normalized distributions $P_o(u)$ of the off-diagonal coupling matrix elements $u$ for $\lambda_1 = 26$ ($W = 2$), $L = 200$, and $U = 1$. Thin solid, short-dashed, and long-dashed lines correspond to the TIP problem, the TIP problem with random interaction, and Eq. (4), respectively. The thick solid line denote TIP matrix elements for states with energy separation less than $\Delta E = 1/2$. Circles, diamonds, triangles, and squares mark the data for the 10 smallest $|u|$ in each case. The vertical lines above the inset indicate the respective values of $u_{\text{abs}} > u_{\text{typ}}$ as computed from the total distribution $P(u)$. Inset: same data on a linear scale.

where we used the Hubbard onsite interaction $U \sum_{\sigma} n_j^{\downarrow} n_j^{\uparrow}$ with the number operator $n_{j,\sigma}$ at site $j$ and spin $\sigma$. Assuming that the SP state is given as

$$\psi_k(j) \propto \frac{1}{\sqrt{\lambda_1}} \exp \left( - \frac{|j-k|}{\lambda_1} + i\theta_j \right)$$  \hspace{1cm} (4)

with $\theta_j$ a random phase, one finds\textsuperscript{13} that the average of $u$ has a magnitude of

$$u_{\text{abs}} \propto \lambda_1^{-3/2}. \hspace{1cm} (5)$$

Shepelyansky calculated the decay rate $\Gamma$ of a non-interacting eigenstate by means of Fermi’s golden rule $\Gamma \sim U^2/\lambda_1 t$\textsuperscript{13,14,39} Since the typical hopping distance is of the order of $\lambda_1$ the diffusion constant is $D \sim U^2 \lambda_1 / t$. Within a time $\tau$ the particle pair visits $N \sim U \lambda_1^{3/2} t^{-1/2} \tau^{1/2}$ states. Diffusion stops when the level spacing of the visited states is of the order of the frequency resolution $1/\tau$. This determines the cut-off time $\tau^*$ and $\lambda_2 \sim \sqrt{D \tau^*} \sim (U/t)^2 \lambda_1^2$ in agreement with Eq. (2). Applicability of Fermi’s golden rule requires $\Gamma \gg t/\lambda_1^2$ which is equivalent to $U^2 \lambda_1 / t^2 \gg 1$. This is exactly the condition for an enhancement of $\lambda_2$ compared to $\lambda_1$. Alternatively, similar results can be obtained by mapping the model onto a random-matrix model with entries chosen according to Eq. (5)\textsuperscript{13,43,44}. 


2 Numerical results for the interaction matrix elements

The qualitative arguments presented above should be checked for quantitative accuracy. Even before doing so for Eq. (2), it is already worthwhile to test the validity of (5) and the subsequent arguments. It was shown\textsuperscript{17} that the assumption of a Gaussian distribution of $u$ — necessary for taking the arithmetic or r.m.s. average — was oversimplified. We calculated\textsuperscript{51} the dependence of the averages on $\lambda_1$ and system size. To this end, we diagonalized the 1D Anderson model for given $L$ and $W$ and computed $u$ for all suitable states and many disorder configurations. In Fig. 1 we show the distribution of $u$ and the values of $u_{\text{typ}}$ and $u_{\text{abs}}$. Additionally, we include results for an interaction with randomly varying onsite term $U(j)$ and results for SP states with random phase as in Eq. (4). Based on these results, it was shown\textsuperscript{51} that due to the non-Gaussian distribution of $u$, one should use the logarithmic rather than the arithmetic average for $u$. However, whereas $u_{\text{abs}} \propto \lambda_1^{-1.5,34}$ the logarithmic average obeys $u_{\text{typ}} \propto \lambda_1^{-1.95}$ as shown in Fig. 2. Following the arguments above, this would imply $\lambda_2 \propto \lambda_1^{1.1}$. We emphasize that this does not mean that there is no enhancement of $\lambda_2$. Rather, the results\textsuperscript{51} indicate that the arguments of first-order perturbation theory\textsuperscript{13} capture the physics in a somewhat oversimplified form. Noting the possibly quite different energies of the pair states, it appears more suitable to average $u$ only over such states which differ in energy by $\Delta E \leq \pm |U|/2$. This leads to a different $\lambda_1$.
dependence with reduced exponent, e.g., \( u_{\text{typ}} \sim \lambda_1^{-1.8} \) for \( U = 1 \), cp. Fig. 2, implying

\[
\lambda_2 \propto \lambda_1^{1.4 \pm 0.2},
\]

in good agreement with previous data based on a wide variety of methods\(^{17,21–24,27,28,30,31,33–41,45,47}\) and also with the results of the next section.

### 3 Enhancement of the TIP localization length in 1D

The first numerical investigations\(^{13,17}\) of \( \lambda_2 \) used the TMM. Two of us studied the TIP problem by a different TMM\(^{18}\) at large \( L \) and found that (i) the enhancement \( \lambda_2/\lambda_1 \) decreases with increasing \( L \), (ii) the behavior of \( \lambda_2 \) for \( U = 0 \) is equal to \( \lambda_1 \) in the limit \( L \to \infty \) only, and (iii) for \( U \neq 0 \) the enhancement \( \lambda_2/\lambda_1 \) also vanishes completely in this limit. Therefore we concluded\(^{18–20}\) that the TMM applied to the TIP problem in 1D measures an enhancement which is due to the finiteness of the systems considered. It is now well understood\(^{37}\) that the main problem with the TMM approach is that the enhanced \( \lambda_2 \) is expected to appear along the diagonal sites of the TIP Hamiltonian, whereas the unsymmetrized TMMs\(^{17,18}\) proceed along an SP coordinate. Various new TMM techniques have been developed to take this into account,\(^{13,17,18,21,24}\) but still all TMMs share a common problem: in general the \( U = 0 \) result for \( \lambda_2 \) does not equal the value of \( \lambda_1/2 \) which is expected for non-interacting particles.\(^{47}\) Rather, they yield...
Fig. 4 Schematic view of two possible TIP decays in the 2D bar geometry.

\( \lambda_2(0) \approx \lambda_2(1) \) and thus \( \lambda_2(0) \gg \lambda_1/2 \). Therefore other methods appear to be more appropriate for the TIP problem.

Here we briefly review the results of another well-tested method of computing localization lengths for disordered systems, the decimation method where one replaces the full Hamiltonian (1) by an effective Hamiltonian for the doubly-occupied sites only. In accordance with the SP case, \( \lambda_2 \) is defined by the TIP Green function,

\[
\frac{1}{\lambda_2} = -\frac{1}{|L-1|} \ln |\langle 1 | G_2 | L \rangle|.
\]

(7)

We computed the Green function at \( E = 0 \) for 26 disorder values \( W \in [0.5, 9] \), for 24 system sizes \( L \in [51, 251] \), and 11 interaction strengths \( U = 0, 0.1, \ldots, 1.0 \). For each triplet of parameters \((W, L, U)\) we averaged \( 1/\lambda_2 \) over 1000 samples. By FSS of the \( \lambda_2(U) \) data we obtained the infinite-size localization lengths \( \xi_2(U) \) shown in Fig. 3.

We fitted our results by various suggested models. The best fit was obtained with

\[
\xi_2(U) \propto \xi_2(0)^{\beta(U)} \left[ 1 + \frac{c}{\xi_2(0)} \right].
\]

(8)

Such a \( U \)-dependent exponent for the enhancement \( \xi_2(U)/\xi_2(0) \) had been previously predicted with \( \beta \) up to 2 for \( U = 1 \). However, we find that \( \beta < 1.5 \) as shown in the inset of Fig. 3. Thus we do not see the quadratic behavior (2) when using the fit function of Ref.45. On the other hand, after scaling the data onto a single scaling curve and fitting

\[
\xi_2(U) - \xi_2(0) \propto \xi_2(0)^{\beta}
\]

(9)

as proposed with \( \beta = 2 \), we find indeed \( \beta = 2 \) for not too small disorder, e.g., \( W \geq 2.5 \) for \( U = 1 \), but observe a crossover to \( \beta = 3/2 \) for smaller \( W \).

For \( U \gtrsim 1.5 \) the enhancement decreases again; the position of the maximum depends upon \( W \). We thus find that the duality proposed for results at \( U \) and \( \sqrt{2}/U \) — which would imply a fixed maximum at \( U = 24^{1/4} \) — is approximately valid.

We remark that similar results are obtained when placing TIP in different potentials which is of relevance for a proposed experimental test of the TIP effect.
4 Localization-delocalization transition for TIP in 2D

Imry\textsuperscript{16,41} argued that two (onsite-)interacting particles in a 2D random potential show enhancement of $\lambda_2$ at $E = 0$ as

$$\lambda_2 \propto \lambda_1 \exp \left[ \frac{U^2 \lambda_1^2}{\xi^2} \right] \gg \lambda_1 \propto \exp \left[ \frac{t^2}{W^2} \right],$$

with $\lambda_1$ the SP localization length in 2D.\textsuperscript{50} Indeed, Ortuño and Cuevas\textsuperscript{54} numerically find a distinct enhancement in 2D for two particles with a short-ranged interaction. It is even so strong that an MIT occurs for $U = 1$ at $W_c = 9.3 \pm 0.2$ with critical exponent $\nu = 2.4 \pm 0.5$. Their result is based on the recursive Green function method previously employed for the 1D TIP case.\textsuperscript{35}

We applied the decimation method to the 2D TIP problem for rectangular bars of size $M \times L$ with $M < L$ at $E = 0$ for 36 disorders $W \in [3.5, 12]$, for system widths $M = 2, \ldots, 8$ at fixed $L = 51$, and 51 interactions strengths $U = 0, 0.04, \ldots, 2.0$ with hard wall boundary conditions. For the results presented here, we average the decay length of TIP states over every possible transmission path between coordinates $(1, 1)$ and various heights $y$ on the right hand side $(L, y)$ of the bar as shown in Fig. 4

$$\frac{1}{\lambda_2} = -\left\langle \frac{1}{M} \sum_{y=1}^{M} \ln \left| \langle 1, 1 | G_2 | L, y \rangle \right| \sqrt{(L - 1)^2 + (y - 1)^2} \right\rangle_W.$$ 

Here $\langle \cdot \rangle_W$ denotes the disorder average over 1500, 500, 250, 200, 100, 50 and 20 configurations for $M = 2, \ldots, 8$, respectively.\textsuperscript{55} To obtain a more accurate result the

\begin{figure}[h]
\centering
\includegraphics[width=0.9\textwidth]{Fig5.pdf}
\caption{FSS scaling curves (lines) and localization lengths $\lambda_2$ for TIP in 2D as a function of the scaling parameter $\xi_2$ for $U = 0$ (○), 1 (⊙), and 2 (∇).}
\end{figure}
value of $1/\lambda_2$ was actually obtained by fitting the slope of $\ln |\langle 1, 1 | G_2(x, y) \rangle |$ versus $\sqrt{(x-1)^2 + (y-1)^2}$ where $x \leq L$.

In Fig. 5, we show typical FSS results for three values of $U$. The quality of the scaling curves is not as good as in the 1D TIP analysis, due to the smaller samples and smaller number of configurations. The scaling curves for $U \lesssim 0.2$ can be described by a single branch corresponding to localized behavior. For $U \gtrsim 0.5$, the scaling curves have two branches indicating a transition of TIP states from localized to delocalized behavior. In the intermediate range $0.2 < U < 0.5$, FSS is less convincing and requires further investigations. We remark that the FSS results do not change appreciably within the accuracy of the data when we drop the data for $M = 2$ or 8.

In order to reliably extract the critical disorders $W_c$ and the correlation length exponents $\nu$ from the FSS data, we employed the FSS techniques of Refs. 50 and 56. In the lowest order approximation, the fit function is given as

$$\frac{\lambda_2}{M} = \Lambda_c + a M^{1/\nu} \left( \frac{W}{W_c} - 1 \right), \quad (12)$$

with fit parameters $\Lambda_c$, $a$, $W_c$ and $\nu$. We used a fit function containing up to the third power in $W/W_c$. In this way including deviations from the linear behavior in $W$ is important due to limited quality of the data. In Figs. 6 and 7, we show the resulting dependence of $W_c$ and $\nu$ on $U$. Note how the FSS gives unreliable results for $U < 0.5$, resulting in the incorrect prediction of $W_c(0) > 0$. As demonstrated in the inset of Fig. 6 the $W_c$ data can be approximated for $0.4 \leq U \leq 1$ by a power-law fit $W_c \propto U^{0.36 \pm 0.03}$. The critical exponent $\nu$ shows a slight decrease for $U \geq 0.5$ and
Fig. 7 Critical exponent $\nu$ according to Eq. (12). The data point (□) for $U = 1$ represents the result of Ref. $^{54}$. The error bars are obtained as in Fig. 6.

is in reasonable agreement with the value of $2.4 \pm 0.5$ obtained in Ref. $^{54}$ for $U = 1$. However, the (non-universal) value of $W_c = 8.1 \pm 0.1$ at $U = 1$ is somewhat different Ref. $^{54}$. We attribute this to our different definition (11) of $\lambda_2$. $^{55}$

5 Conclusions

In conclusion, we observe an enhancement of the TIP localization lengths due to onsite interaction both in 1D and 2D random potentials. This enhancement persists, unlike for TMM, $^{18,21,23}$ in the limit of large system size and after constructing infinite-sample-size estimates from the FSS curves. In the 2D case, it leads to numerical evidence for a localization-delocalization transition of the TIP states. We emphasize that this is not a metal-insulator transition in the standard sense since only the TIP states show the delocalization transition. The majority of non-paired states remains localized.

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