

Interaction-induced connectivity of disordered two-particle states

D. O. Krimer¹ and S. Flach^{2,3}

¹*Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/136, 1040 Vienna, Austria*

²*New Zealand Institute for Advanced Study, Centre for Theoretical Chemistry and Physics, Massey University, Auckland 0745, New Zealand*

³*IBS Center for Theoretical Physics of Complex Systems, 70 Yuseong-daero 1689-gil, Yuseong-gu, Daejeon, Korea*

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We study the interaction-induced connectivity in the Fock space of two particles in a disordered one-dimensional potential. Recent computational studies showed that the largest localization length ξ_2 of two interacting particles in a weakly random tight-binding chain is increasing unexpectedly slow relative to the single-particle localization length ξ_1 , questioning previous scaling estimates. We show this to be a consequence of the approximate restoring of momentum conservation of weakly localized single-particle eigenstates, and disorder-induced phase shifts for partially overlapping states. The leading resonant links appear among states which share the same energy and momentum. We substantiate our analytical approach by computational studies for up to $\xi_1 = 1000$. A potential nontrivial scaling regime sets in for $\xi_1 \approx 400$.

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Introduction. For decades, the interplay between Anderson localization [1] and many-body interactions [2,3] has been in the research focus of condensed matter. Most theoretical results are not rigorous, and rely on physical intuition, independent computational studies, and, of course, experimental data. The case of few interacting particles seems to be an exception, as computational approaches are expected to easily do the job here. For two interacting particles (TIPs) in a one-dimensional chain with weak diagonal disorder, a number of studies over the past 20 years produced interesting yet contradicting predictions on the scaling of the largest two-particle localization length $\xi_2 \sim \xi_1^\alpha$ with the single-particle localization length ξ_1 . These range from $\alpha = 2$ [4,5], $\alpha = 1.6$ [6], to $\alpha = 1$ [7,8], thus from the existence of a second length scale ($\alpha > 1$) to the nonexistence of such a scale ($\alpha = 1$). Recent computational studies of the TIP eigenstates [9] show that down to the weakest disorder values accessed by numerical diagonalizations [10–13], the largest TIP localization length is $\xi_2 \leq 2\xi_1$ [9]. Therefore, the above scaling predictions are not supported by published numerical results. In another recent study, a surprising TIP wave-packet subdiffusion on length scales $\xi_1 \ll l \ll \xi_2$ has been found for ξ_1 as large as $\xi_1 \approx 400$ [14], further fueling the quest to understand the TIP dynamics at weak disorder.

In this Rapid Communication, we address the intrinsic reasons for the listed discrepancies. We focus on the single-particle eigenstates (SPEs) and compute overlap integrals and connectivities in the Fock space of two-particle eigenstates (TPEs) at zero interaction. We show that, contrary to previous assumptions, the overlap integrals show a highly inhomogeneous distribution at weak disorder. SPEs gradually restore standing wave phase relations that occur in the tight-binding model without disorder, $W = 0$ [15], leading to approximate momentum conservation selection rules in the overlap integrals. At the same time, strongly connected TPEs have to satisfy approximate energy conservation. Large connectivities set in at previously unexpected low values of disorder, because of the combined action of momentum restoring and relative spatial shifts of the SPEs on the phase relations between interacting TPEs. We arrive at the surprising conclusion that the rigorous diagonalization of TIPs in the regime of strong

connectivity is a matter of future computations, as present CPUs are hardly capable of doing the job. Note that the model considered here can be experimentally realized in two-dimensional waveguide arrays [16–18].

Model. We consider the one-dimensional Hubbard Hamiltonian with disorder,

$$\hat{\mathcal{H}} \equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}, \quad (1)$$

$$\hat{\mathcal{H}}_0 = \sum_l [\epsilon_l \hat{a}_l^\dagger \hat{a}_l + \hat{a}_{l+1}^\dagger \hat{a}_l + \hat{a}_l^\dagger \hat{a}_{l+1}], \quad (2)$$

$$\hat{\mathcal{H}}_{\text{int}} = \sum_l \frac{U}{2} \hat{a}_l^\dagger \hat{a}_l^\dagger \hat{a}_l \hat{a}_l, \quad (3)$$

and two indistinguishable bosons. All energy scales are relative to the hopping strength in Eq. (2), which is equal to unity.

The Hamiltonian (1) consists of noninteracting and interacting parts, $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_{\text{int}}$, where \hat{a}_l^\dagger and \hat{a}_l are standard boson creation and annihilation operators on a lattice site l and U measures the interaction strength. The random uncorrelated on-site energies ϵ_l are chosen uniformly from the interval $[-W/2, W/2]$, with W denoting the disorder strength. The following results are not expected to change for other distributions with similarly finite moments.

One particle. In this case the interaction term does not contribute. Using the basis $|l\rangle \equiv a_l^\dagger |0\rangle$ with $l = 1, \dots, N$ (N is the number of lattice sites), the SPEs $|\nu\rangle = \sum_l^N A_l^{(\nu)} |l\rangle$ are defined through the localized eigenvectors $A_l^{(\nu)} \sim e^{-|l|/\xi_1^\nu}$ [1] of the eigenvalue problem

$$\lambda_\nu A_l^{(\nu)} = \epsilon_l A_l^{(\nu)} + A_{l+1}^{(\nu)} + A_{l-1}^{(\nu)}. \quad (4)$$

The eigenvalues $-2 - W/2 \leq \lambda \leq 2 + W/2$ fill a band with a width $\Delta_1 = 4 + W$. The most extended SPEs correspond to the band center $\lambda = 0$ with localization length

$$\xi_1(\lambda = 0, W) \approx 100/W^2, \quad (5)$$

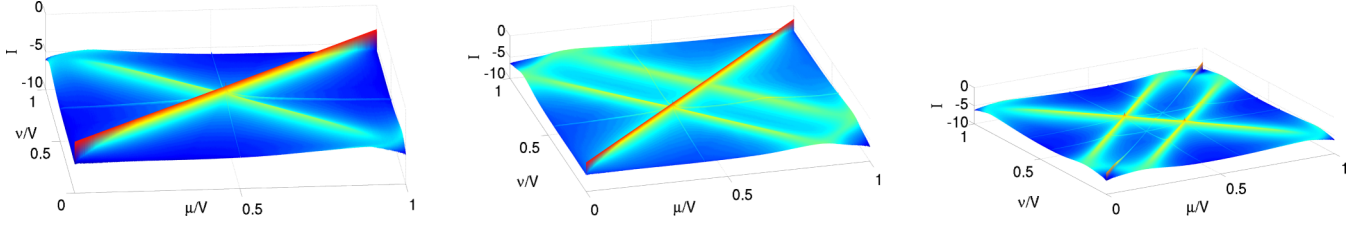


FIG. 1. (Color online) Averaged overlap integrals in log scale as a function of the Fock state $|v, \mu\rangle$ for the following reference Fock states, from left to right: $v_0 = \mu_0 = V/2$ (center), $v_0 = \mu_0 = 5/12 V$ (diagonal), $\mu_0 = 7/12 V$, $v_0 = 5/12 V$ (antidiagonal). $W = 0.5$.

in the limit of weak disorder $W \leq 4$ [19]. The average volume V which an SPE occupies is estimated to be about $V \approx 3\xi_1$ for weak disorder [6].

Two particles. For $U = 0$ we construct a complete basis of orthonormalized two-particle eigenstates which span a Fock space as product states of SPEs,

$$|\mu, v \geq \mu\rangle = \frac{|\mu\rangle \otimes |v\rangle}{\sqrt{1 + \delta_{\mu v}}}, \quad \hat{H}_0|\mu, v\rangle = (\lambda_\mu + \lambda_v)|\mu, v\rangle. \quad (6)$$

TIP eigenstates $|q\rangle$ of the interacting particle problem $\hat{H}|q\rangle = \lambda_q|q\rangle$ can be represented in Fock space as $|q\rangle = \sum_{v, \mu \leq v}^N \phi_{\mu v}^{(q)}|\mu, v\rangle$. The coefficients $\phi_{\mu v}^{(q)}$ satisfy the eigenvalue problem

$$\lambda_q \phi_{\mu_0 v_0}^{(q)} = \lambda_{\mu_0 v_0} \phi_{\mu_0 v_0}^{(q)} + \sum_{\mu, v} \frac{2U I_{\mu v}^{\mu_0 v_0} \phi_{\mu v}^{(q)}}{\sqrt{1 + \delta_{\mu_0 v_0}} \sqrt{1 + \delta_{\mu v}}}, \quad (7)$$

where

$$I_{\mu v}^{\mu_0 v_0} = \sum_l A_l^{(\mu_0)} A_l^{(v_0)} A_l^{(\mu)} A_l^{(v)} \quad (8)$$

are the overlap integrals. $\lambda_{\mu_0 v_0} \equiv \lambda_{\mu_0} + \lambda_{v_0}$ and therefore the noninteracting case $U = 0$ yields an eigenenergy band with width $\Delta_2 = 2\Delta_1$ [20].

It follows straight from Eq. (7) that two Fock states are strongly (nonperturbatively) coupled if

$$R_{\mu v}^{\mu_0 v_0} \equiv \left| \frac{\Delta \lambda_{\mu v}^{\mu_0 v_0}}{U I_{\mu v}^{\mu_0 v_0}} \right| < 1, \quad (9)$$

where the energy mismatch is given by

$$\Delta \lambda_{\mu v}^{\mu_0 v_0} = |\lambda_{\mu_0} + \lambda_{v_0} - \lambda_\mu - \lambda_v|. \quad (10)$$

For $U \gg 1$ the interaction separates two-particle bound states with double occupancy per site off a two-particle continuum of states with one particle per site [9,21,22]. In that case, the bound states localize in space even stronger than the single-particle states due to the energy separation cost to move one particle. The remaining states form a Hilbert space of two noninteracting spinless fermions and yield no increase in the localization length as well (as compared to the single-particle case). Therefore, the strongest effect the interaction can have on increasing the localization length is for $U \approx 1$, which we will assume from here on.

It follows from (9) that a strong link is realized when the energy mismatch $\Delta \lambda$ is small (ideally zero) and the overlap integral I is sufficiently large. The amount of possible strong (resonant) links from a given reference Fock state $|\mu_0, v_0\rangle$ is finite. Overlap integrals are exponentially small unless all four single-particle states which define one integral I are

sufficiently close to each other in real space. Thus, a given reference Fock state has at most approximately V^2 other basis states which form an interaction network, from which a resonant subset can be chosen.

Overlap integrals and energy mismatch. We first numerically diagonalize the single-particle problem (4). We choose a single-particle reference state with energy close to zero, and determine the subset of all neighboring SPEs in the same localization volume V . We order them with increasing energy corresponding to increasing indices v, μ . The corresponding momentum can be well approximated as $p_v = \pi v/V$. The obtained two-dimensional momentum space is used to construct interacting Fock states. Next we choose a reference Fock state with v_0, μ_0 for $W = 0.5$ and perform a disorder averaging of the overlap integrals I with Fock states with some given v, μ . The result is shown in Fig. 1 for the reference state being at the center, the diagonal, and the antidiagonal of the two-dimensional momentum space.

We find that the overlap integrals are predominantly nonzero along certain straight lines. These lines follow simple momentum conservation rules for two interacting particles in the absence of disorder in a box of size V [23]. This happens because in one dimension the localization length is of the order of the mean free path [19], and for weak disorder the quasimomenta become good quantum numbers. The eigenstate will therefore be similar to a standing wave with exponentially decaying tails.

These findings underpin that v is a momentum index for weak disorder. This is one of the reasons why previous attempts to estimate averages of overlap integrals over the whole momentum space were not useful [4,5].

Let us minimize the energy mismatch (10). Neglecting disorder except for its trapping of particles, the single-particle energy in a box can be estimated as $-2 \cos(p) = -2 \cos \pi \frac{v}{V}$. Therefore, the energy mismatch is exactly zero if the condition

$$\cos \pi \frac{v_0}{V} + \cos \pi \frac{\mu_0}{V} = \cos \pi \frac{v}{V} + \cos \pi \frac{\mu}{V} \quad (11)$$

is satisfied. It defines some curved line in $\{v, \mu\}$ space. The notable exception is the antidiagonal straight line in Fig. 1 (left and right plots) which does conserve both the energy and the momentum. Note that this coincidence of momentum and energy conservation for pairs of two-particle Fock states along the antidiagonal is the result of the restoring of a particle-hole symmetry of the considered model in the limit of vanishing disorder. The tight-binding model is a member of a family of models with hopping over odd distances in real space only, which allows the introduction of bipartite AB

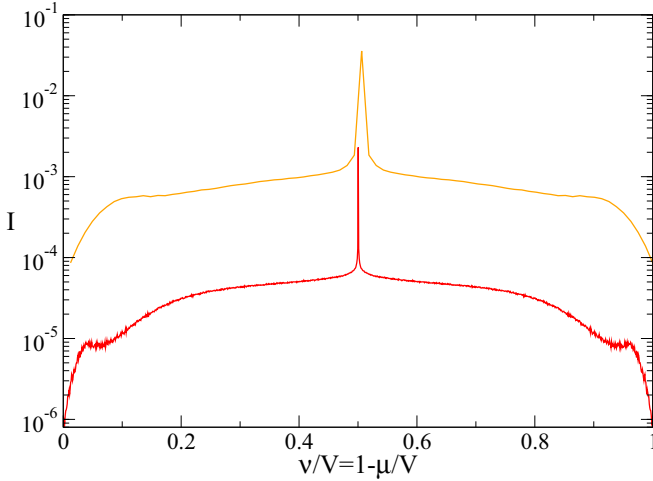


FIG. 2. (Color online) Averaged overlap integrals along the anti-diagonal for $W = 2$ (upper curve) and $W = 0.5$ (lower curve). The reference Fock state is at the center $v_0 = \mu_0 = V/2$.

sublattices, and results (for $W = 0$) in the eigenvector property $A_l(\lambda) = (-1)^l A_l(-\lambda)$ [15].

We focus on the subset of Fock states along the anti-diagonal only with $v_0 = \mu_0 = V/2$ (center) and $v + \mu = v_0 + \mu_0$. It is this tiny subset which is capable of setting up the strongest resonant network and substantially delocalize two interacting particles, as compared to one. We plot the variation of the overlap integrals along the anti-diagonal for $W = 2$ and $W = 0.5$ in Fig. 2. We observe a peak at the center which corresponds to $\langle I_{v_0 v_0}^{v_0 v_0} \rangle$. Its value can be estimated using normalization properties of SPEs as $\langle I_{v_0 v_0}^{v_0 v_0} \rangle \approx 1/V$. For $W = 2$ this yields 0.013 and for $W = 0.5$ it yields 0.0008, which are reasonably close to the numerical data 0.03 and 0.002. In particular, their ratio is 16 from the estimate and 15 from numerics, showing that we correctly determine the scaling. Off the peak we find a plateau at significantly reduced values $\sim 10^{-3}$ ($W = 2$) and $\sim 10^{-5}$ ($W = 0.5$). This reduction is due to relative shifts of SPEs in real space. For weak disorder, assume that each SPE is given by $A_l^{(v)} = \frac{1}{\sqrt{V}} e^{2\pi i(l-l_v)v/V}$ for $l_v \leq l \leq l_v + V$, where l_v encodes the spatial position of the SPE. The average of the overlap integral along the anti-diagonal is equivalent to averaging $I_{v, V-v}^{V/2, V/2}$ over v and over all possible values of l_v, l_μ . This yields $\langle I_{ad} \rangle = \frac{3}{4V^2}$. The numerical prefactor $3/4$ originates from the relative shift of flat and constant distributions along the lattice. The scaling $1/V^2$, however, is due to the phase mismatch of SPEs shifted relatively to each other. (A similar calculation for SPEs which are not shifted relative to each other will give $\langle I_{ad} \rangle = 1/V$.) This scaling is much weaker than the $V^{-3/2}$ law predicted in Refs. [4,5] because the standing wave phase correlations were neglected. The distributions of the energy mismatch $\Delta\lambda$ along the anti-diagonal follow approximately a normal distribution with the characteristic energy scale Δ_1 [24], due to the central limit theorem already at work. A quick estimate of the probability of resonance (9) yields a number independent of V . Therefore, fluctuations of the overlap integral values, and their correlations to the energy mismatch, might be of decisive importance.

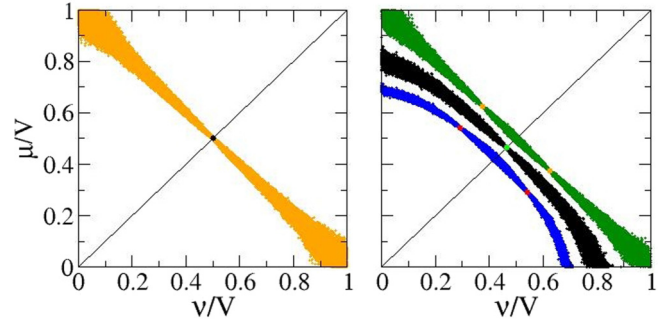


FIG. 3. (Color online) Points represent those pairs of μ, ν which satisfy the resonance condition $R_{\mu\nu}^{\mu_0\nu_0} \leq 1$ with the reference modes μ_0, ν_0 . Calculations are performed for $W = 0.5$ and different pairs of μ_0, ν_0 (shown by solid circles) located at the center (left panel) and at anti-diagonal, diagonal, and arbitrary location of μ_0, ν_0 (right panel).

Let us turn to numerical data. In Fig. 3 we show the observed locations of all resonant partner Fock states ($R < 1$) for different reference Fock states. For a reference state $v_0 = \mu_0 = V/2$ we nicely observe the grouping of all network partners along the anti-diagonal (Fig. 3, left plot). For another reference state $v_0 = 0.4V, \mu_0 = 0.6V$ on the anti-diagonal, the network partners still belong to the anti-diagonal neighborhood, and simply their number decreases (Fig. 3, right plot). For reference states off the anti-diagonal (Fig. 3, right plot) the network partners are located close to curved lines which are a manifestation of the single-particle dispersion [energy conservation—see Eq. (11)], with even smaller partner numbers. Therefore, we confirm that resonances are defined by momentum and energy conservation.

Connectivity. A central property of any network is the connectivity K —the number of links from a given reference state to other partners. Values of $\langle K \rangle \leq 2$ do not lead to any substantial increase of the localization length, as there is a high probability to terminate the path after one or two connections. For a given pair μ_0 and ν_0 , the connectivity K to all pairs of modes μ and ν residing the same localization volume is defined as the number of connections for which R fulfills the condition (9) (if any). We evaluated its average $\langle K \rangle$ for $v_0 = \mu_0 = V/2$: $\langle K \rangle(W = 2) = 1.1$, $\langle K \rangle(W = 0.75) = 5.4$, $\langle K \rangle(W = 0.5) = 12$, $\langle K \rangle(W = 0.35) = 25$. Therefore, the potentially interesting regime of sufficiently large connectivity is accessed only for $W < 1$. Previous diagonalization studies were exploring $1 < W < 4$. Despite the fact that $V(W = 4) \approx 20$ and $V(W = 1) \approx 300$, the numerically accessed parameter interval turns out to be irrelevant for the study of a possible dramatic increase in ξ_2 . The reason is the above discussed smallness in the overlap integrals which originates from the relative shifts of SPEs with standing wave phase relations. We note that the connectivity increase for $W < 1$ happens also for other choices of μ_0, ν_0 . For instance, for $v_0 = V/4, \mu_0 = 3V/4$ we find $\langle K \rangle(W = 0.5) = 7.5$. Still, it is much weaker than the numbers obtained for the anti-diagonal, as shown in Figs. 4(a) and 4(b). In Fig. 4(c) we show the distribution of K for $W = 0.35$ and two reference Fock states—for the center and the diagonal similar to those shown in Fig. 1.

Larger values of $\langle K \rangle$ do not necessarily lead to an enhancement of the localization length, since there can be

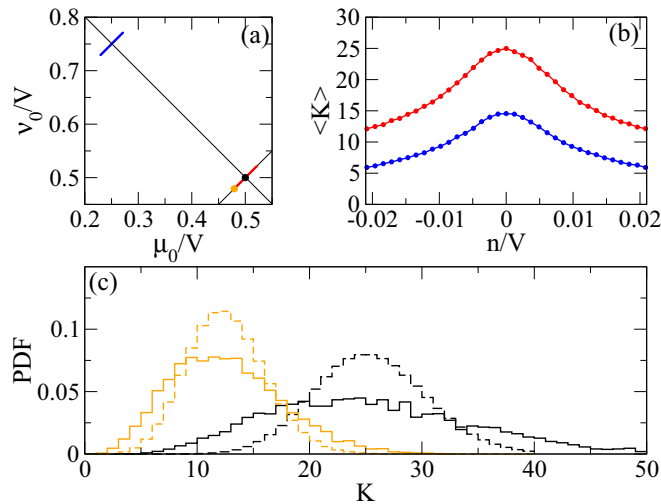


FIG. 4. (Color online) Statistical properties of the coordination number K . (a) The colored line segments perpendicular to the antidiagonal represent the pairs of μ_0, ν_0 taken in the calculations. (b) Average coordination number $\langle K \rangle$ (solid lines with symbols) for the reference modes from the line segments in (a) (the same coloring is kept). Here n/V measures the deviation along the line segments from the antidiagonal. (c) PDFs $\mathcal{W}(K)$ for two pairs of μ_0 and ν_0 . Dashed lines: Corresponding binomial distributions with the same average coordination number $\langle K \rangle$ as obtained from $\mathcal{W}(K)$. The strength of disorder $W = 0.35$.

closed loops in the resonant network in Fock space, whose length simply increases. The existence of loops is enforcing a certain degree of correlations between the resonant links. Assume the opposite, i.e., that the actual values of $R < 1$, which define a set of links from a given reference state to other Fock states, are not correlated. Then, the connectivity K must be binomially distributed because K would be nothing more than a number of successful events $R < 1$ in a sequence of L independent tossings each of which yields success $R < 1$ with probability p . Thus one expects

$$\mathcal{W}(K) = \frac{L!}{k!(L-k)!} p^k (1-p)^{L-k}. \quad (12)$$

Note that the average coordination number $\langle K \rangle$ for the binomial distribution is related to p as $\langle K \rangle = Lp$. On the

other hand, we know $\langle K \rangle$ from the numerical simulations and therefore can easily calculate the success probability p . We test this hypothesis. Results of the comparison of the numerically obtained $\mathcal{W}(K)$ and corresponding binomial distributions are shown in Fig. 4(c). We observe a strong deviation of numerical PDFs from the binomial distributions, concluding that resonances are not completely independent events. This might be a hint that resonant loops in Fock space are formed, which could act against delocalization.

Conclusions. We have shown that, contrary to previous assumptions, a possible substantial increase in the localization length of two interacting particles in a random potential sets in at unexpectedly weak disorder values. This is due to a gradual restoring of momentum conservation in single-particle eigenstates in the limit of vanishing disorder. That, in turn, enforces a highly inhomogeneous resonance network of matrix elements. The scaling of the overlap integrals along the resonant network is much weaker than predicted in previous papers because phase correlations and relative position shifts of eigenstates have to be taken into account. Resonant links between Fock states follow the resonance network. The connectivity in Fock space grows substantially with weak disorder, indicating the possibility of the emergence of a different localization length scale for two interacting particles. Because this potential regime is setting in at anomalously weak disorder strength, previous numerical scaling tests are not conclusive (too strong disorder). But even more, with current computers and exact diagonalization methods, it is highly nontrivial to enter the desired potential scaling regime which starts at $W = 0.5$ and should extend at least down to $W = 0.05$ to estimate exponents. Therefore, we are in need of different computational methods. We also conjecture that a breaking of particle-hole symmetry by adding next-to-nearest neighbor hoppings will lead to a further suppression of the delocalization trend by interactions. We finally note that our results could be of interest for the recent interest in many-body localization [25] with numerical [26] and experimental [27] efforts to illuminate the dynamics in high-dimensional Fock spaces, which is largely controlled by the properties of the overlap integrals discussed in this work.

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