Interaction-induced connectivity of disordered two-particle states

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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 $\xi_2$ of two interacting particles in a weakly random tight binding chain is increasing unexpectedly slow relative to the single particle localization length $\xi_1$, 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 $\xi_1 \approx 1000$. A potential nontrivial scaling regime sets in for $\xi_1 \approx 400$, way beyond all previous numerical attacks.

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**Introduction.** — The interplay between Anderson localization $^1$ and many body interactions $^2$ $^3$ has been for decades 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 (TIP) in a one-dimensional chain with weak diagonal disorder a number of studies over the past twenty years produced interesting yet contradicting predictions on the scaling of the largest two-particle localization length $\xi_2 \sim \xi_l^1$ with the single particle localization length $\xi_1$. 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 $^{10}$ $^{12}$, 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 wavepacket subdiffusion on length scales $\xi_1 \ll l \ll \xi_2$ has been found for $\xi_1$ as large as $\xi_1 \approx 400$ $^14$, further fueling the request to understand the TIP dynamics at weak disorder.

In this work we address the intrinsic reasons for the listed discrepancies. We focus on the single particle eigenstates (SPE) and compute overlap integrals and connectivities in the Fock space of two particle eigenstates (TPE) at zero interaction. We show, that contrary to previous assumptions, the overlap integrals show a highly inhomogeneous distribution at weak disorder. SPE 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 TPE 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 SPE on the phase relations between interacting TPE. We arrive at the surprising conclusion that the rigorous diagonalization of TIP in the regime of strong connectivity is a matter of future computations, as present CPUs are hardly capable of doing the job.

**Model.** — We consider the Hubbard Hamiltonian with disorder

\[ \hat{H} \equiv \hat{H}_0 + \hat{H}_{\text{int}}, \]

\[ \hat{H}_0 = \sum_i [\epsilon_i \hat{a}^+_i \hat{a}_i + \hat{a}^+_i \hat{a}_i], \]

\[ \hat{H}_{\text{int}} = \frac{U}{2} \sum_i [\hat{a}^+_i \hat{a}_{i+1} \hat{a}_{i+1}], \]

and two indistinguishable bosons. Note that the results are not changing when considering two distinguishable particles, e.g. two fermions with opposite spins.

The Hamiltonian $^1$ consists of non-interacting and interacting parts, $\hat{H}_0$ and $\hat{H}_{\text{int}}$, where $\hat{a}^+_i$ and $\hat{a}_i$ are standard boson creation and annihilation operators on a lattice site $l$ and $U$ measures the interaction strength. The random uncorrelated on-site energies $\varepsilon_i$ are chosen uniformly from the interval $[-W/2, W/2]$, with $W$ denoting the disorder strength.

**One particle.** — In this case the interaction term does not contribute. Using the basis $|l\rangle \equiv a^+_l |0\rangle$ with $l = 1, \ldots, N$ ($N$ is the number of lattice sites), the SPE $|\nu\rangle = \sum_l A_{l}^{(\nu)} |l\rangle$ are defined through the localized eigenvectors $A_{l}^{(\nu)} \sim e^{-i|l|/\xi^\nu_l}$ $^1$ of the eigenvalue problem

\[ \lambda_{\nu} A_{l}^{(\nu)} = \epsilon_i A_{l+1}^{(\nu)} + (A_{l+1}^{(\nu)} + A_{l-1}^{(\nu)}). \]

The eigenvalues $-2 - W/2 \leq \lambda \leq 2 + W/2$ fill a band with a width $\Delta_1 = 4 + W$. The most extended SPE...
correspond to the band center $\lambda = 0$ with localization length
\[ \xi_1(\lambda = 0, W) \approx 100/W^2, \tag{5} \]
in the limit of weak disorder $W \leq 4$ \cite{4}. The average volume $V$ which an SPE occupies is estimated to be about $V \approx 3\xi_1$ for weak disorder \cite{4}.

Two particles.— For $U = 0$ we construct a complete basis of orthonormalized two-particle eigenstates which span a Fock space as product states of SPE
\[ |\mu, \nu \geq \mu\rangle = \frac{|\mu\rangle \otimes |\nu\rangle}{\sqrt{1 + \delta_{\mu, \nu}}}, \quad \tilde{\mathcal{H}}_0|\mu, \nu\rangle = (\lambda_\mu + \lambda_\nu)|\mu, \nu\rangle. \tag{6} \]
TIP eigenstates $|q\rangle$ of the interacting particle problem $\hat{\mathcal{H}}(q) = \lambda_\mu(q)$ can be represented in Fock space as $|q\rangle = \sum_{\nu, \mu \leq \nu} \phi_{\mu \nu}(q)|\mu, \nu\rangle$. The coefficients $\phi_{\mu \nu}(q)$ satisfy the eigenvalue problem
\[ \lambda_q \phi_{\mu \nu}(q) = \lambda_{\mu \nu}(q) \phi_{\mu \nu}(q) + \sum_{\mu, \nu} \frac{2U I_{\mu \nu}^0 \phi_{\mu \nu}(q)}{\sqrt{1 + \delta_{\mu, \nu}^0}} \sqrt{1 + \delta_{\mu, \nu}^0}, \tag{7} \]
where
\[ I_{\mu \nu} = \sum_{l} A_{l}^{(\mu)} A_{l}^{(\nu)} A_{l}^{(\mu)} A_{l}^{(\nu)} \tag{8} \]
are the overlap integrals. $\lambda_{\mu \nu} = \lambda_{\mu 0} + \lambda_{\nu 0}$ and therefore the noninteracting case $U = 0$ yields an eigenergy band with width $\Delta_2 = 2\Delta_1$ \cite{17}.

It follows straight from Eq.(7) that two Fock states are strongly (nonperturbatively) coupled if
\[ R_{\mu \nu}^{00} = \left| \frac{\Delta \lambda_{\mu \nu}^{00}}{U I_{\mu \nu}^{00}} \right| < 1 \tag{9} \]
where the energy mismatch is given by
\[ \Delta \lambda_{\mu \nu}^{00} = |\lambda_{\mu 0} + \lambda_{\nu 0} - \lambda_\mu - \lambda_\nu| \tag{10} \]
For $U \gg 1$ the interaction separates two particle bound states with double occupancy per site off a continuum of states with one particle per site \cite{9} \cite{18} \cite{19}. 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 \cite{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 $|\mu_0, \nu_0\rangle$ 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.

\textbf{Overlap integrals and energy mismatch}.— We first numerically diagonalize the single particle problem \cite{4}. We choose a single particle reference state with energy close to zero, and determine the subset of all neighbouring SPE in the same localization volume $V$. We order them with increasing energy corresponding to increasing indices $\nu, \mu$. The corresponding momentum can be well approximated as $p_\nu = \pi \nu / V$. The obtained two-dimensional momentum space is used to construct interacting Fock states. Next we choose a reference Fock state with $\nu_0, \mu_0$ for $W = 0.5$ and perform a disorder averaging of the overlap integrals $I$ with Fock states with some given $\nu, \mu$. 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 a box of size $V$ \cite{20}, underpinning therefore that $\nu$ 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 \cite{14} \cite{15}.

Let us minimize the energy mismatch \cite{10}. The single particle energy can be estimated as $-2 \cos(p) = -2 \cos \pi \nu / V$. Therefore the energy mismatch is exactly ze-
roed if the condition
\[ \cos \frac{\pi \nu_0}{V} + \cos \frac{\pi \mu_0}{V} = \cos \frac{\pi \nu}{V} + \cos \frac{\pi \mu}{V} \]  
(11)
is satisfied. It defines some curved line in \( \{ \nu, \mu \} \) 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 allowed 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 AB sublattices, and results (for \( W = 0 \)) in the eigenvector property
\[ A_i(\lambda) = (-1)^i A_i(-\lambda) \]
[15].

We focus on the subset of Fock states along the antidiagonal only with \( \nu_0 = \mu_0 = V/2 \) (center) and \( \nu + \mu = \nu_0 + \mu_0 \). It is this tiny subset which is capable to set 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 antidiagonal for \( W = 2 \) and \( W = 0.5 \) in Fig.2. We observe a peak at the center which corresponds to \( \langle I^{\nu_0}_{\mu_0+i} \rangle \). Its value can be estimated using normalization properties of SPE as \( \langle I^{\nu_0}_{\mu_0+i} \rangle \approx 1/V \). For \( W = 2 \) this yields 0.013 and for \( W = 0.5 \) respectively 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 SPE in real space.

For weak disorder, assume that each SPE is given by
\[ A_i(\nu) = \frac{1}{\sqrt{V}} e^{2\pi i (l - l_\nu) \nu / V} \]  
for \( l_\nu \leq l \leq l_\nu + V \), where \( l_\nu \) encodes the spatial position of the SPE. The average of the overlap integral along the antidiagonal is equivalent to averaging \( l^{V/2} \) over \( \nu \) and over all possible values of \( l_\nu, l_\mu \). This yields \( \langle I_{\text{ad}} \rangle = \frac{3}{4} \). 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 SPE shifted relatively to each other [21]. This scaling is much weaker than the \( V^{-3/2} \) law predicted in [22, 20] because the standing wave phase correlations were neglected. The distributions of the energy mismatch \( \Delta \lambda \) along the antidiagonal follow approximately a normal distribution with the characteristic energy scale \( \Delta \lambda \), due to the central limit theorem already at work. A quick estimate of the probability of resonance [0] 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.

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 \( \nu_0 = \mu_0 = V/2 \) we nicely observe the grouping of all network partners along the antidiagonal (Fig.3 left plot). For another reference state \( \nu_0 = 0.4V \), \( \mu_0 = 0.6V \) on the antidiagonal the network partners still belong to the antidiagonal neighborhood, simply their number decreases (Fig.3 right plot). For reference states off the antidiagonal (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 \( \mu_0 \) and \( \nu_0 \) the

Fig. 2: Averaged overlap integrals along the antidiagonal for \( W = 2 \) (upper curve) and \( W = 0.5 \) (lower curve). The reference Fock state is at the center \( \nu_0 = \mu_0 = V/2 \).

Fig. 3: Points represent those pairs of \( \mu, \nu \) which satisfy the resonance condition \( R^{\mu \nu}_{\mu_0 \nu_0} \leq 1 \) with the reference modes \( \mu_0, \nu_0 \). Calculations are performed for \( W = 0.5 \) and different pairs of \( \mu_0, \nu_0 \) (shown by filled circles) located at the centre (left panel) and at antidiagonal, diagonal and arbitrary location of \( \mu_0, \nu_0 \) (right panel).
Fig. 4: Statistical properties of the coordination number \( K \).
(a) The colored line segments perpendicular to the antidiagonal represent the pairs of \( \mu_0, \nu_0 \) 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 \( W(K) \) for two pairs of \( \mu_0 \) and \( \nu_0 \). Dashed lines: corresponding Binomial distributions with the same average coordination number \( \langle K \rangle \). The strength of disorder \( W = 0.35 \).

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 new localization length scale for two interacting particles. Because this potential regime is setting in at anomalously weak disorder strengths, 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 new computational methods. We also conjecture that a breaking of particle-hole symmetry by adding next-to-nearest neighbour hoppings will lead to a further suppression of the delocalization trend by interactions.
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