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Non monotonic influence of Hubbard interaction on the Anderson localization of two-electron wavepackets

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HIGHLIGHTS

- We show a non monotonic behavior of the Anderson localization phenomenon.
- This behavior is associated with interaction between electrons.
- We show such non-monotonic behavior is consistent with some many-body calculations.

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ABSTRACT

We show that the Hubbard-like interaction between two electrons moving in a random one-dimensional potential landscape has a non monotonic influence on the Anderson localization phenomenon. Within a tight-binding approach, we follow the time-evolution of initially localized two-electron wavepackets and compute the participation number of all two-particles eigenstates. We evidence that the coupling between bounded and unbounded two-particles states leads to an overall weakening of Anderson localization of the predominant unbounded states. However, such coupling becomes ineffective in the regime of large interaction strengths on which the energy bands corresponding to these two classes of eigenstates become quite detached. We unveil that these two competing effects are at the origin of the non monotonic influence of the inter-particle interaction on Anderson localization.

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1. Introduction

Disorder and electron–electron interaction play important roles in the understanding of several solid state properties. These two ingredients are responsible by the insulating character of certain systems, known respectively as Anderson [1] and Mott [2] insulators. In general, Anderson localization can be understood as originated on the destructive interference of electronic waves scattered by a random potential that may lead to its exponential localization. On the other hand, Mott Q3 insulators arise due to the high energetic cost of atomic double occupancy that inhibits the electronic hopping.

For non-interacting particles, Anderson localization can be considered well understood and it has been indeed experimentally verified [1,3,4]. However, even though systems with coexisting electron–electron interaction and disorder have been investigated intensively [1,5], full understanding of the interplay between these two ingredients is still distant. Particularly interesting is the weakening of Anderson localization promoted by electron–electron interaction. A great interest in this field has been stimulated by the possible metallic behavior in two-dimensional disordered systems with strongly correlated electrons [6], contrasting with the prediction of the scaling theory of Anderson localization. Initially observed

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as persistent currents in mesoscopic rings [7,8], this phenomenon suggests that the localization degree can be reduced by the Coulomb interaction. In particular, it was observed that the persistent current in the presence of Coulomb interaction becomes larger than that observed for non-interacting electrons [7–9].

Other many-body systems such as fermions in optical lattices [10], ultra-cold condensates [11,12], Anderson–Hubbard models in 1D [13–17], 2D and 3D [18], and 2D Coulomb glasses [19] also exhibit a similar phenomenology, suggesting some degree of competition between disorder and interaction. The interaction promotes a reduction in the degree of localization only for systems at weak and intermediate values of interaction. This feature is signaled by the non monotonic dependence of the localization length as a function of the interaction strength in Anderson–Hubbard systems [13,15,18] and in persistent currents [8,9]. The phase diagrams for correlated fermions in optical lattices [10] and ultra-cold bosons in disordered traps [12] also indicate this behavior. Further, the DC conductance as a function of the interaction strength in 2D Coulomb glasses shows that a weak Coulomb interaction can enhance the conductivity of strongly disordered samples, while it reduces the conductance in the case of weak disorder [19]. These systems in 1D reveal a non monotonic dependence of DC conductance as a function of the interaction strength [14].

However, even within the framework of an on-site Coulomb interaction, numerical studies of many body systems represent a challenging task due to the fact that the number of electronic configurations grows exponentially with the system size. Adding disorder the problem becomes even more difficult, since most of the measures of localization used in the study of non-interacting systems are not easily applicable to many-body states [20]. Thus, many efforts have been driven to study models with a low electronic density that are able to recover some physical aspects present in many body systems. Within this context, we study a model consisting of two interacting electrons in a disordered chain aiming to closely analyze the interplay of disorder and inter-particle interaction on the localization of electronic waves [20–28]. This class of models has been approached by using several techniques such as transfer-matrix method [23], time evolution of wavepackets [21,24,25], exact diagonalization [26] and Green's function [27]. Here, by solving the time-dependent Schroedinger equation, we will show the existence of two regimes: one in which a weak interaction promotes an increase of the localization length, and a second regime in which a strong interaction reinforces Anderson localization. Therefore the maximum weakening of Anderson localization is achieved at an intermediate value of the inter-particle coupling. An exact diagonalization of the Hamiltonian matrix will be used to unveil the underlying physical mechanism responsible for this non monotonic influence of the inter-particle interaction on the wavepacket spreading.

2. Model and formalism

In what follows, we will restrict our analysis to the case of electrons with opposite spins. The Anderson–Hubbard tight-binding equation for two interacting electrons in a 1D system with uncorrelated disorder is given by [24,29]

$$H = \sum_n \sum_s J(c^\dagger_{n+1,s}c_{n,s} + c^\dagger_{n,s}c_{n+1,s}) + \sum_n \sum_s \epsilon_n c^\dagger_{n,s}c_{n,s} + \sum_n U c^\dagger_{n,\uparrow}c_{n,\uparrow}c^\dagger_{n,\downarrow}c_{n,\downarrow}, \tag{1}$$

where $c_{n,s}$ and $c^\dagger_{n,s}$ are the annihilation and creation operators for the electron at site n with spin s, J is the hopping amplitude, ϵ_n is the potential at site n, considered as a random variable with a uniform distribution in the interval $[-W/2, W/2]$, and U is an on-site Hubbard interaction.

In order to follow the time evolution of wavepackets, we solved the time dependent Schroedinger equation by expanding the wavefunction in the Wannier representation $|\Phi(t)\rangle = \sum_{n_1,n_2} f_{n_1,n_2}(t)|n_1, s_1; n_2, s_2\rangle$ where the ket $|n_1, s_1; n_2, s_2\rangle$ represents a state with one electron with spin s_1 at site n_1 and the other electron with spin s_2 at site n_2. Once the initial state is prepared as a direct product of states, the electrons will always be distinguishable by their spins since the Hamiltonian does not involve spin exchange interactions. The temporal evolution of the wavefunction components in the Wannier representation is governed by the time-dependent Schroedinger equation

$$\mathrm{i}\frac{\mathrm{d}f_{n_1,n_2}(t)}{\mathrm{d}t} = f_{n_1+1,n_2}(t) + f_{n_1-1,n_2}(t) + f_{n_1,n_2+1}(t) + f_{n_1,n_2-1}(t) + \left[\epsilon_{n_1} + \epsilon_{n_2} + \delta_{n_1,n_2}U\right]f_{n_1,n_2}(t), \tag{2}$$

where we used units of $\hbar = J = 1$. The above set of equations was solved numerically using a high-order method based on Taylor's expansion of the evolution operator $\Gamma(\Delta t)$,

$$\Gamma(\Delta t) = \mathrm{e}^{-\mathrm{i}H\Delta t} = 1 + \sum_{l=1}^{l_0} \frac{(-\mathrm{i}H\Delta t)^l}{l!}, \tag{3}$$

where H is the Hamiltonian. The wavefunction at time Δt is given by $|\Phi(\Delta t)\rangle = \Gamma(\Delta t)|\Phi(t=0)\rangle$, which is used recursively to obtain the wavefunction at time t. The following results were taken by using $\Delta t = 0.07$ and the sum was truncated at $l_0 = 20$. This cutoff was sufficient to keep the wavefunction norm conservation along the entire time interval considered. Aiming to characterize the dynamic behavior of the wavepacket, we computed typical quantities that can bring information about its spacial extension, as it will be detailed below. Additionally, to characterize the nature of two-electrons eigenstates, we numerically diagonalized the complete Hamiltonian to obtain all eigenvectors $|\Phi\rangle = \sum_{n_1,n_2} f_{n_1,n_2}|n_1, s_1; n_2, s_2\rangle$ and eigenvalues E.

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