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The role of on-site and nearest-neighbor interactions in the correlated two-particles quantum walk

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ABSTRACT

We study the influence of the on-site and nearest-neighbor interactions on the eigenstates and dynamics of two-particles restricted to move in a one-dimensional optical lattice. An effective tight-binding approach with non-local interactions is employed in order to consider the non-perfect screening of the coulomb interaction between two-particles. Numerical and analytical results unveil the emergence of a new sub-band of bound states due to the nearest-neighbor interaction, besides a broadening of the usual sub-band associated with the hubbard-like on-site coupling. Furthermore, we solve the time-dependent schrodinger equation to follow the time evolution of an initially localized two-particles state. While the on-site interaction is responsible for a correlated dynamics in which particles occupy predominantly the same site, nearest-neighbor interactions is shown to be able to induce a quantum walk on which the particles remain predominantly in neighboring sites.

1. Introduction

The advancements of techniques in cooling and manipulating ultracold atoms in optical lattices have promoted remarkable progress in condensed-matter physics. For example, one can use a non-interacting Bose–Einstein condensate to study Anderson localization, [1,2] observe persistent Bloch oscillations of weak-interacting bosonic Sr atoms [3] or use an ultracold fermionic atoms to implement the Haldane model and characterize its topological band structure [4]. In particular, the control of the interactions using Feshbach [5,6] resonance technique and the control of kinetic energy via lattice depth in ultracold atoms have provided a route to explore the physics of Hubbard models [7–10]. These advancements in experimental techniques are an important step in the research and understanding of quantum many-body states.

Recently, Bose–Einstein condensate of ^{87}Rb atoms in a cubic 3D optical lattice exemplified the correspondence between the Hubbard model and ultracold atoms in optical lattices [11]. A two-atom bound state was observed that exhibit long lifetimes and arises from the lattice band structure and repulsion between particles. Pairing of particles can be produced in an analogous manner in Fermionic atoms [12] and Bose–Fermi mixtures [13]. In general lines, it is believed that the stability of bound particles could be the basis of an abundance of new quantum many-body states or phases. For example, the coherence of Cooper-pair tunneling in Josephson-junction systems has been extensively studied due to their great potential in both quantum computation and nanotechnology [14]. In a seminal paper Shepelyansky [15] found that bound states of two interacting particles are responsible by weakening of Anderson localization. This behavior has been seen in other works, both theoretical [16,17] as well as experimental bosonic [18] and fermionic [19] systems. Bound states of two interacting particles are also responsible for inducing the coherent phenomenon of frequency doubling of Bloch oscillations [20,22–24]. Predicted for two interacting particles subjected to an external electric field and restricted to move in a linear chain [20,22,23], its experimental observation was recently reported in ultracold atoms of bosonic ^{87}Rb [24]. An equivalent photonic setup, where two particles in 1D are mapped to a 2D array of waveguide, has been proposed [25] and experimentally achieved in waveguide lattices [26]. Besides, few interacting bosons in a one-dimensional lattice with dc bias displays fractional Bloch periods which are inversely proportional to the number of bosons clustered into a bound state [27]. An experimental setup to create anyons in one-dimensional lattices with fully tuneable exchange statistics is proposed by Keilmann and collaborators [28]. The experiment proposes features such as the full control and tuneability of the particles' exchange statistics. More recent studies displays a scheme for realizing the anyon Hubbard model. The scheme allows for controllable effective interactions for an exact two-body hard-core constraint [29].

In this work, we will show that two interacting electrons allocated in an optical lattice can produce the emergence of a two

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sub-band of bound states. Described in the framework of the tight-binding Hubbard model hamiltonian wherein there is on-site and nearest-neighbor interactions between particles, we examine the eigenstates and the time dependence of wavepackets. Numerical and analytical results unveil the emergence of a new sub-band of bound states due to the nearest-neighbor interaction, besides a broadening of the usual sub-band associated with the Hubbard-like on-site coupling [30,20]. By following the time evolution of wavepackets, we will show that while the on-site interaction is responsible for a correlated dynamics in which particles occupy predominantly the same site, nearest-neighbor interaction is shown to be able to induce a quantum walk on which the particles remain predominantly in neighboring sites.

2. Model and formalism

In order to describe two-interacting electrons with opposite spins placed in an optical lattice, while there is on-site and nearest-neighbor interactions between them, we consider a tight-binding Hubbard model hamiltonian as

$$\mathcal{H} = J\sum_{\langle lm\rangle}\sum_{\sigma} c^{\dagger}_{l,\sigma}c_{m,\sigma} + U\sum_{l}\hat{n}_{l,1}\hat{n}_{l,2} + V\sum_{\langle lm\rangle}\sum_{\sigma,\sigma'}\hat{n}_{l,\sigma}\hat{n}_{m,\sigma'} + \sum_{l}\epsilon_l\hat{n}_{l,\sigma}. \quad (1)$$

Here $c^{\dagger}_{l,\sigma}$ and $c_{l,\sigma}$ are the creation and annihilation operators for the particle at site l with spin state σ. $\langle lm\rangle$ denotes nearest-neighbor and $\hat{n}_{l,\sigma} = c^{\dagger}_{l,\sigma}c_{l,\sigma}$. J is the nearest-neighbor hopping, ϵ_l the on-site energies, U and V the on-site and the nearest-neighbor interaction strength respectively. The screened Coulomb potential contains an exponential damping factor associated with the inverse screening length [21]. As the nearest-neighbor interaction V is added in order to mimic the non-perfect screening of particles, we assume that the screening length is very small and we will focus on values $V \leq U/3$.

The central object of interest is to identify the role of the non-local on-site Hubbard interaction between particles on the eigenstates and the dynamic behavior of wavepackets. Therefore, initially we will apply a numerical diagonalization procedure of the Hamiltonian in order to obtain all eigenvectors $|\Phi\rangle = \sum_{l,m}\phi(l,m)|l,\sigma;m,\sigma'\rangle$ and eigenvalues E. On the other hand, in order to follow the time evolution of wavepackets, we solve the time-dependent Schrödinger equation by expanding the wavefunction in Wannier representation

$$|\Phi(t)\rangle = \sum_{l,m}\phi_{l,m}(t)|l,\sigma;m,\sigma'\rangle, \quad (2)$$

where the ket $|l,\sigma;m,\sigma'\rangle$ represents a state with one particle with spin σ at site l, and the other particle with spin σ' at site m. In this model we consider the particle as being distinguishable by their spin state since the Hamiltonian does not involve spin exchange interactions. Thus, the time evolution of the wavefunction in the Wannier representation becomes

$$J[\phi_{l-1,m}(t)+\phi_{l+1,m}(t)+\phi_{l,m-1}(t)+\phi_{l,m+1}(t)] + V(\delta_{l+1,m}+\delta_{l-1,m})\phi_{l,m}(t)+\delta_{l,m}U\phi_{l,m}(t) = i\frac{d\phi_{l,m}(t)}{dt}, \quad (3)$$

where we used the on-site energies ϵ_l as the reference energy ($\epsilon_l = 0$) without any loss of generality, besides using units of $\hbar = J = 1$.

The above set of equations was solved numerically using a high-order method based on the Taylor expansion of the evolution operator $\Gamma(\Delta t)$,

$$\Gamma(\Delta t) = e^{-iH\Delta t} = 1 + \sum_{n=1}^{n_f}\frac{(-iH\Delta t)^s n}{n!} \quad (4)$$

where H is the Hamiltonian. The wavefunction at time Δt is given by $|\Phi(\Delta t)\rangle = \Gamma(\Delta t)|\Phi(t=0)\rangle$, 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 $n_f = 20$. This cutoff was sufficient to keep the wavefunction norm conservation along the entire time interval considered. We followed the time evolution of an initially Gaussian wavepacket with width ρ

$$\langle l,\sigma;m,\sigma'|\Phi(t=0)\rangle = \frac{1}{A(\rho)}\exp\left[-\frac{(l-l_0)^2}{4\rho^2}\right] \times\exp\left[-\frac{(m-m_0)^2}{4\rho^2}\right], \quad (5)$$

where the initial positions (l_0, m_0) were considered to be centered at $(N/2-d_0, N/2+d_0)$. Through the above-described approach, we computed typical quantities that can bring information about the eigenstates and wavepacket time-evolution, as will be detailed below.

3. Results

3.1. Eigenstates: numerical and analytical analysis

We firstly examine the two-particles eigenstates by applying a numerical diagonalization procedure of the complete Hamiltonian to an open chain with $N=200$ sites. In Fig. 1 we show results for the normalized density of states defined as

$$DOS(E) = \frac{1}{N}\sum_{l}\delta(E-E_l), \quad (6)$$

versus energy E for $U = 4, 8$ and 12, without nearest-neighbor interaction $V=0$ (see brown filled curve) and with nearest-neighbor interaction $V = U/3$ (see unfilled curve). Insets show amplifications of the density of states, highlighting different aspects between $V=0$ and $V \neq 0$. For $U=4$ the DOS exhibits the

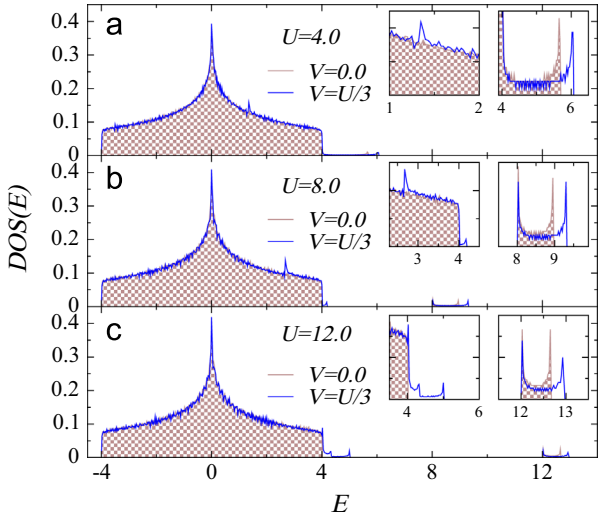

Fig. 1. Normalized density of states (DOS) versus energy (E) for $U = 4, 8$ and 12, computed for open crystalline chains ($\epsilon_l = 0$ for all n) with $N=200$ sites. The presence of the nearest-neighbor interaction (here $V = U/3$) gives rise to a new sub-band of bound states, besides increasing the width of the "on-site" sub-band (see unfilled curve). The insets show amplifications of the density of states around the sub-bands.