Unidirectional quantum walk of two correlated particles: Separating bound-pair and unbound wavepacket components

A. R. C. Buarque and W. S. Dias

Instituto de Física, Universidade Federal de Alagoas, 57072-970 Maceió, AL, Brazil

We study the unidirectional transport of two-particle quantum wavepackets in a regular one-dimensional lattice. We show that the bound-pair state component behaves differently from unbound states when subjected to an external pulsed electric field. Thus, strongly entangled particles exhibit a quite distinct dynamics when compared to a single particle system. With respect to centroid motion, our numerical results are corroborated with an analytical expression obtained using a semiclassical approach. The wavefunction profile reveals that the particle-particle interaction induces the splitting of the initial wavepacket into two branches that propagate with specific directions and drift velocities. With a proper external field tunning, the wavepacket components can perform an unidirectional transport on the same or opposite directions. The amplitude of each mode is related to the degree of entanglement between particles, which presents a non-monotonic dependence on the interaction strength.

PACS numbers: 03.65.Ud, 03.75.Lm, 67.85.-d, 05.60.Gg, 37.10.Jk

I. INTRODUCTION

Unlike a classic random walker, a quantum walk can be in a coherent superposition of several positions and exploring multiple trajectories over an n-dimensional graph. In periodic systems, for example, the quantum particle propagates much faster (ballistic propagation) than its classical counterpart (diffusive propagation) [1]. Quantum walkers have been widely studied in a variety of different settings such as in the development of quantum algorithms [2,4], efficient energy transfer in proteins complex [5], classical optics [6,7], waveguide lattices [8,9], nuclear magnetic resonance [10], quantum dots [11], trapped atoms in optical lattices [12,13], disorder [14,15], interacting particles [16,17] and bacteria behavior in biological systems [18].

Despite the recent progress, many investigations on quantum walks are related to a single walker, primarily in the experimental scope. On the other hand, quantum effects are considerably enhanced in systems with more than one walker. In such cases, generalizations that consider many interacting walkers can provide useful information regarding to universal and efficient quantum computation [19]. Interaction between walkers typically results in the appearance of entanglement and have been shown to improve certain aspects, such as in the graph isomorphism problem [20]. Quantum walks of interacting and non-interacting quantum particles are fundamentally different in the context of solving the computational problem of graph isomorphism. In this case, it was reported that two interacting bosons are more powerful than single particles and two non-interacting particles for distinguishing non-isomorphic strongly regular graphs [21]. Quantum walks of two identical photons revealed quantum correlations that depended critically on the input state of the quantum walk [3]. Fundamental effects such as the emergence of correlations in two-particle quantum walks were recently reported for interacting atoms in an optical lattice [13]. The control over the interacting atoms in the regime where the dynamics is dominated by interparticle interactions made it possible to observe the frequency doubling of Bloch oscillations, predicted for electron systems [22] and recently simulated with photons in a waveguide array [23].

Within the studies involving quantum dynamics under the influence of external fields, the unidirectional transport of wavepackets promoted by superposed static and harmonic fields has been greatly explored [24–29]. A weakly interacting Bose-Einstein condensate of Cs atoms in a tilted lattice potential was used to demonstrate that harmonic driving can lead to matter-wave transport over macroscopic distances [26]. This directed motion is promoted when the frequency of the AC field is a multiple of the frequency of the usual Bloch oscillations. Furthermore, the average velocity displayed by the wavepacket depends on the magnitudes of the AC and DC field components and on the initial phase of the AC field. Super Bloch oscillations and breathing take place with an amplitude that diverges as the resonance condition is approached [27]. For initially localized and uncorrelated two-particle quantum wavepackets evolving in a 1D discrete lattice, it has been reported that the particles become strongly entangled when directed by a harmonic AC field which is resonant with frequency-doubled Bloch oscillations promoted by a static DC field [28]. These theoretical and experimental works have shown the possibility of using external fields to manipulate entangled matter-states.

The aim of this paper is to propose a new protocol for manipulating quantum matter-states of two correlated particles in a regular one-dimensional (1D) lattice. More specifically, we consider two interacting particles placed in a linear discrete lattice under the effect of a Gaussian time-dependent electric field. Pulsed external fields (including Gaussian-Pulses) have been used in different scientific contexts [30,31], making the experimental implementation feasible. In the framework of the tight-
binding Hubbard model Hamiltonian with on-site inter-particle interaction, we will follow the time evolution of wavepackets and compute typical physical quantities to characterize the wavepacket dynamics along the chain. In particular, we will show that a proper tuning of the pulsed electric field can control the migration of a pair of strongly entangled particles. Our numerical results are corroborated with an analytical expression obtained using a semi-classical approach. Since the external field acts in a different way on bound-pair and unbound states, we will show that the initial wavepacket splits into two branches which propagates in specific directions and drift velocities. The amplitude of each mode will be related to the degree of entanglement of the two particles, which exhibits a non-monotonic dependence on the interaction between particles. As such, we explore the possibility of controlling the direction and drift velocity of two distinct wavepacket components.

II. MODEL AND FORMALISM

The system under consideration contains two interacting particles placed in a one-dimensional discrete lattice of spacing $a$ under the action of an external field. In the framework of the tight-binding Hubbard model, the Hamiltonian can be described as

$$H = \sum_n \sum_{s=1,2} J (c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s}) + \sum_n \sum_{s=1,2} [\epsilon_n c_{n,s}^\dagger c_{n,s} - eF(t)n_a] + \sum_n U c_{n,1}^\dagger c_{n,1} c_{n,2}^\dagger c_{n,2},$$

(1)

where $c_{n,s}$ and $c_{n,s}^\dagger$ are the annihilation and creation operators for particles of charge $e$ at site $n$ with spin $s$, $J$ is the nearest-neighbor hopping amplitude, $\epsilon_n$ is the potential at site $n$ and $U$ is the on-site Hubbard interaction. A possible physical realization of the present model consists of two bosonic atoms in an optical lattice under a tilting pulse. It has been recently shown experimentally that two interacting bosons in a tilted optical lattice [13] has similar features of two interacting charged particles under an external uniform field [22]. Here, the external field consists of a Gaussian-pulse applied parallel to the chain length, which can be expressed as

$$F(t) = B(\rho) e^{\rho^2 [(t-\tau)^2]} ,$$

(2)

where $\rho$ controls the duration of each pulse and $\tau$ is the time of reference. For very small values of $\rho$, $F(t)$ represents a delta-like pulse at $t \approx \tau$. Pulsed external fields (including Gaussian-Pulses) have been reported in different settings such as reorientation of nematic liquid crystals [30], the experimental realization of a quantum $\delta$-kicked rotor in ultracold sodium atoms trapped in a 1D potential [31], analysis of the transient membrane response for cells [32], deceleration and bunching of cold molecules [33] and wave-packet manipulation using pulses with a smooth envelope [35].

In the following, we will consider the case $U > 0$, corresponding to Hubbard repulsion. In order to follow the time evolution of wavepackets, we solved the time dependent Schrödinger equation by expanding the wavefunction in the Wannier representation $|\Phi(t)\rangle = \sum_{n_1,n_2} f_{n_1,n_2}(t)|n_1;1,n_2;2\rangle$ where the ket $|n_1;1,n_2;2\rangle$ represents a state with one particle with spin 1 at site $n_1$ and the other particle with spin 2 at site $n_2$. We consider the particles distinguishable by their spin state. Once the initial state is prepared as a direct product of states, the particles 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 Schrödinger equation

$$i \frac{df_{n_1,n_2}(t)}{dt} = f_{n_1+1,n_2}(t) + f_{n_1-1,n_2}(t) + f_{n_1,n_2+1}(t) + f_{n_1,n_2-1}(t) + [\epsilon_{n_1} + \epsilon_{n_2} - F(t)(n_1 + n_2) + \delta_{n_1,n_2} U] f_{n_1,n_2}(t),$$

(3)

where the on-site energies $\epsilon_n$ were taken as the reference energy ($\epsilon_0 = 0$) and we used units of $\hbar = J = e = a = 1$. The above set of equations were solved numerically by using fourth order Runge-Kutta method with step size about $10^{-4}$ in order to keep the wavefunction norm conservation along the entire time interval considered. We followed the time evolution of an initially Gaussian wavepacket with width $\sigma$:

$$\langle n_1,1;n_2,2|\Phi(t=0)\rangle = \frac{1}{A(\sigma)} e^{-\frac{(n_1-n_01)^2}{4\sigma^2}} e^{-\frac{(n_2-n_02)^2}{4\sigma^2}},$$

(4)

where the initial positions $(n_01, n_02)$ 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 wavepacket time-evolution, as it will be detailed below.

III. RESULTS AND DISCUSSION

We start following the time evolution of the wavepacket centroid associated with each particle defined as

$$\bar{n}_i(t) = \sum_{n_1,n_2} (n_i)|f_{n_1,n_2}(t)|^2, \quad i = 1,2.$$

(5)

Due to the symmetry of the initial state and interaction Hamiltonian, one has that $\bar{n}_1(t) = \bar{n}_2(t)$. In fig.[1] we plot the centroid evolution for an initial wave-packet width $\sigma = 1.0$, $d_0 = 0$ and (a) $U = 0.0$ and (b) $U = 4.0$. We adjusted the value of $B(\rho) = 1$ in order to apply an electric pulse at time $\tau = 10$ whose impulse $\int_0^\infty F(t)dt$
In order to better characterize the wavepacket dynamics, we collected the centroid after different electric pulse settings. With these data, we computed the average center-of-mass velocity of wave-packet. However, the dynamic behavior displayed by particles with interaction strength \( U = 4.0 \) is clearly distinct from that provided by non-interacting particles (\( U = 0 \)).

Thus, keeping in mind the energy dispersion of the single particle problem and its relationship with the group velocity of wave-packets, we have

\[
k = k_0 + \frac{e}{\hbar} \int_{t_1}^{t_f} F(t) dt. \tag{6}
\]

FIG. 1: Time evolution of the average position of particle 1 for four settings of electric field pulses applied at \( \tau = 10 \) time units. The resulting impulses of the electric pulses are \( I = 3\pi/2, 5\pi/4, 3\pi/4, \pi/2 \). The dynamic behavior displayed by particles with interaction strength \( U = 4.0 \) is clearly distinct from that provided by non-interacting particles (\( U = 0 \)).

FIG. 2: Impulse dependence of the centroid velocity for (a) \( U = 0.0 \), (b) \( U = 4.0 \) and (c) \( U = 10.0 \) and two distinct initial wave packets \( \sigma = 1.0, 4.0 \). For \( U = 0.0 \) the sine-like behavior is in good agreement with the semi-classical prediction for non-interacting particles. On the other hand, for an intermediate interaction strength, the bound states seems to play a predominant role on the dynamics of particles. The solid line corresponds to the semi-classical dependence for particles performing coherent hoppings.

Thus, keeping in mind the energy dispersion of the single particle problem and its relationship with the group velocity of wave-packet centered around some \( k' \) state, the sine-like behavior displayed in fig. 2a, is easily recovered. By increasing of the initial wavepacket width, the dynamics converges to semiclassical prediction, with limits \( \pm 2Ja/\hbar \). For a narrow initial wavepacket (\( \sigma = 1.0 \)) and intermediate interaction strength \( U = 4.0 \) (see fig. 2b), \( \langle v(t) \rangle \) displays a distinct dependence on the field impulse. Now, besides the pure (bound) states covering the range \(-4J \leq E \leq 4J\), there is a band of bound-pair states covering the range \( U \leq E \leq \sqrt{U^2 + 16J^2} \). These bound-pair states play a predominant role in the wavepacket dynamics. By assuming a transformation to the center-of-mass coordinate \( f(n_1, n_2) = e^{ik(n_1+n_2)}\chi(n_1-n_2) \) it is possible to show (more technical details are found in ref. \[37\]) that in the absence of interaction \( U \) we have

\[
E = 4J\cos(ka)\cos(za). \tag{7}
\]

Here, \( k \) is the center of mass momentum and \( z \) is the
FIG. 3: Time evolution of the one-particle wavefunction profile in the absence of interaction \((U = 0.0)\), intermediate \((U = 4.0)\) and strong particle-particle interaction \((U = 10.0)\). Electric pulse applied at \(\tau = 10\) time units whose resulting impulse are: top panels \(I = 5\pi/4\) and bottom panels \(I = \pi/3\). While \(U = 0.0\) results in a behavior consistent with the single-particle formalism, the interaction induces a competition of bound-pair and unbound states, which associated with the electric pulse, splits the wavepacket in two parts. Both components (bound-pair and unbound states) perform an unidirectional transport, but may propagate along (a-c) opposite or (d-f) the same direction.

In order to exemplify the competitive character presented above it is shown in fig. 3 the time evolution of the one-particle wavefunction profile in the absence of interaction \((U = 0.0)\), intermediate \((U = 4.0)\) and strong particle-particle interaction \((U = 10.0)\). The electric pulse was applied at \(\tau = 10\) time units, whose resulting impulse are: top panels \(I = 5\pi/4\) and bottom panels \(I = \pi/3\). For both electric field configurations, \(U = 0.0\) shows that the entire wavepacket is driven to perform a unidirectional transport along the chain, consistent with the single-particle formalism. On the other hand, the electric pulse on the system with the interaction between particles turned on induces the splitting of the wavepacket in two wavefronts. One is associated to unbound states, while the other is governed by bound-pair states. A similar behavior was reported for correlated bosons in optical lattices in the presence of doubly modulated AC-fields \cite{29}. The on-site interaction and the lattice shaking displays independent modulating frequencies, that when properly adjusted can offer a bifurcating quantum motion of pair correlated particles propagating in opposite directions. However, we show that both components (bound-pair and unbound components) performs an unidirectional transport, but can propagate in the opposite [see fig. 3(a–c)] as well as the same [see fig. 3(d–f)].
FIG. 4: (a) Purity function computed after 100 time units \(\langle P_{12}(t_f)\rangle\) versus interaction \(U\) for distinct applied electric pulses. The degree of entanglement displays a non-monotonic dependence on \(U\) and is greater for electric pulses which promote higher velocities of the unbound branch. (b) For an intermediary interaction strength the time evolution of quantum purity function indicates that the wavepacket develops a continuously increasing degree of quantum entanglement when the electric pulse promote higher velocity of the unbound branch. However, this behavior is not monotonic. After an intermediate interaction strength, the degree of entanglement is reduced. This non-monotonic behavior is related to the competitive character described above, where the interaction favors the coherent hopping associated with bound states while the wavepacket widening decreases the double occupancy probability. We also note that the degree of entanglement is larger for electric pulses that promote larger velocities at the unbound branch. Fig. 4 displays the time evolution of the purity function for \(U = 0, 2, 10\) and electric field impulses \(I = 7\pi/4, \pi/2\). While the two particles are not entangled for \(U = 0\), for \(U = 2\) and \(I = \pi/2\) the purity function continuously decreases in time. This feature indicates that the wavepacket develops quantum entanglement over a continuously growing chain segment. In this configuration the electric pulse promotes the largest velocity of the unbound branch. In contrast, for other settings, the degree of entanglement quickly saturates, reinforcing the fact that unbounded states plays a more significative role in the wavepacket dynamics in the regime of very strong interactions.

IV. SUMMARY AND CONCLUSIONS

In summary, we introduced a scheme to generate and manipulate spatially entangled two-particle states by driving them using a pulsed electric field. More specifically, our results showed that bound-pair and unbound states of an initially entanglement wavepacket can be controlled separately. This allows to split the wavepacket into two fractions that develops unidirectional transport, with speed and direction of each branch externally controlled by the pulsed field. The electric field can be adjusted in order to make these two components (bound-pair and unbound states) propagate either in the same or opposite directions. The amplitude of each mode is related to the degree of entanglement of the two particles, which presents a non-monotonic dependence with the interaction between particles. This behavior comes from the competitive character between bound-pair and unbound states. This competition leads to an optimal range of couplings to obtain a strongly correlated dynamics of the two interacting particles. Our analysis is based on observables that can be experimentally verified, such as the wavepacket profile \[13\] and quantum purity \[40\]. Thus, these recent experimental achievements strongly indicate that the scheme proposed here is feasible in systems of ultracold atoms trapped on one-dimensional optical lattices under a tilting pulse. We hope that our work may impel further investigations aiming the manipulation of entangled particles in low-dimensional systems.

V. ACKNOWLEDGMENTS

We would like to thank M. L. Lyra for critical comments and suggestions. This work was partially sup-
ported by FAPEAL (Fundaçâo de Apoio à Pesquisa do Estado de Alagoas).

References

[1] J. Kempe, Contemp. Phys. 44, 307 (2003).
[2] N. Shenvi, J. Kempe, and K. Birgitta Whaley, Phys. Rev. A 67, 052307 (2003).
[3] S. Chakraborty, L. Novo, A. Ambainis, Y. Omar, Phys. Rev. Lett. 116, 100501 (2016).
[4] Portugal R., Quantum Walks and Search Algorithms (New York: Springer) (2013).
[5] M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik, The Journal of Chem. Phys. 129, 174106 (2008).
[6] A. Schreiber, et al., Phys. Rev. Lett. 104, 050502 (2010).
[7] M. Gräfe, et al., Sci. Rep. 2, 562 (2012).
[8] Hagai B. Perets, et al., Phys. Rev. Lett. 100, 170506 (2008).
[9] A. Peruzzo, et al, Science 329, 1500 (2010).
[10] Jiangfeng Du, et al., Phys. Rev. A 67, 042316 (2003).
[11] K. Manouchehri and J. B. Wang, J. of Phys. A: Math. and Theor. 41, (2008) 6.
[12] M. Karski, et al, Science 325, 174 (2009).
[13] P. M. Preiss, et al, Science 347, 1229 (2015).
[14] Yue Yin, D. E. Katsanos, and S. N. Evangelou, Phys. Rev. A 77, (2008) 022302.
[15] S. R. Jackson, T. J. Khoo, and F. W. Strauch, Phys. Rev. A 86, 022335 (2012).
[16] L. Wang, Li Wang, and Y. Zhang, Phys. Rev. A 90, 063618 (2014).
[17] A.S. Peixoto, W.S. Dias, Solid State Commun. 242, 68 (2016).
[18] Seth Lloyd, J. Phys. Conf. Ser 302, 012037 (2011).
[19] A. M. Childs, D. Gosset, Z. Webb, Science 339, 791 (2013).
[20] S. D. Berry and J. B. Wang, Phys. Rev. A 83, 042317 (2011).
[21] J. K. Gamble, M. Friesen, D. Zhou, R. Joynt, S. N. Coppersmith, Phys. Rev. A 81, 052313 (2010).
[22] W. S. Dias, E. M. Nascimento, M. L. Lyra, and F.A.B.F. de Moura, Phys. Rev. B 76, 155124 (2007).
[23] G. Corrielli, et al., Nature Communications 4, 1555 (2013).
[24] Q. Thommen, J. C. Garreau, and V. Zehne, Phys. Rev. A 65, 053406 (2002).
[25] V. V. Ivanov, A. Alberti, M. Schioppo, G. Ferrari, M. Artoni, M. L. Chiofalo, G. M. Tino, Phys. Rev. Lett. 100, 043602 (2008).
[26] E. Haller, R. Hart, M. J. Mark, J. G. Danzl, L. Reichsollner, H. C. Nagerl, Phys. Rev. Lett. 104, 200403 (2010).
[27] R. A. Caetano and M. L. Lyra, Phys. Lett. A 375, 2770 (2011).
[28] W. S. Dias, F. A. B. F. de Moura, and M. L. Lyra, Phys. Rev. A 93, 023623 (2016).
[29] Yi Zheng and Shi-Jie Yang, New J. Phys. 18, 013005 (2016).
[30] Taeko I. Urano, Hiro-o Hamaguchi, Chem. Phys. Lett. 195, 287 (1992).
[31] F. L. Moore, J. C. Robinson, C. F. Bharucha, B. Sundaram, M. G. Raizen, Phys. Rev. Lett. 75, 4598 (1995).
[32] Q. Hu, et al, Phys. Rev. E 71, 031914 (2005).
[33] G. Dong, W. Lu, and P. F. Barker, Phys Rev. A 69, 013409 (2004).
[34] S. J. Beebe and Karl H. Schoenbach, Journal of Biomed. and Biot. 2005, 297 (2005).
[35] S. Arlinghaus and M. Holthaus, Phys. Rev. A 84, 063617 (2011).
[36] A. R. C. B. da Silva, F. A. B. F. de Moura, W. S. Dias, Solid State Comm. 236, 12 (2016).
[37] J. F. Weisz and F. Claro, J. Phys.: Condens. Matter 15, 3213 (2003).
[38] D. L. Shepelyansky, Physical Review Letters 73, 2607 (1994).
[39] W.S. Dias and M.L. Lyra, Physica A 411, 35 (2014).
[40] Rajibul Islam, et al, Nature 528, 77 (2015).