

Frequency doubling of Bloch oscillations for interacting electrons in a static electric field

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We study numerically the effect of the on-site Hubbard interaction U on the dynamics of two electrons subjected to an external electric field and restricted to move in a linear chain with open boundaries. We solve the time-dependent Schrödinger equation to follow the time evolution of an initially localized two-electron state. For electrons initially far apart, the wave packet develops Bloch oscillations whose characteristic frequency is in agreement with a semiclassical calculation. For initially close electrons in a singlet state, a frequency doubling sets up, which is more pronounced for intermediate couplings. We discuss this effect by revealing the opposite trends the electron-electron coupling produces on the wave-packet components corresponding to bounded and unbounded states.

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I. INTRODUCTION

The nature of one-electron eigenstates has a significant influence on the electronic properties of solids. In pure periodic systems, the one-electron eigenstates are Bloch waves which are translational invariant and delocalized in the thermodynamic limit. In the absence of scattering or electron-electron interaction, the system behaves as a perfect conductor whenever the Fermi energy falls into the conduction band. This picture can be drastically changed in the presence of disorder, interaction, or a dc external electric field.

In disordered systems, the one-electron eigenstates are obtained using the well-known Anderson formalism.¹⁻³ For weak disorder, the electronic states in three-dimensional geometries display a localization-delocalization transition (LDT). It is well known that the LDT is absent for low-dimensional systems with time-reversal symmetry at any disorder strength.¹ Some years ago, it was reported that the presence of short-range⁴⁻⁷ or long-range correlations⁸⁻¹⁷ in disorder induces the appearance of truly delocalized states in low dimensions. On the other hand, when the on-site electron-electron interaction is turned on, the electronic system can display a correlation-driven transition from a paramagnetic metal to a paramagnetic insulator.¹⁸⁻²² This transition is called Mott transition, and its basic features can be studied by employing the Hubbard model for electrons interacting with each other through an extremely short-ranged repulsive Coulomb interaction.¹⁸⁻²² The electronic states are also influenced by the presence of a dc electric field. Under this constraint, the electronic wave packet becomes localized in a finite fraction of the lattice, an effect usually called dynamical localization. The electron wave packet displays the so-called Bloch oscillations,²³⁻²⁵ whose amplitude is proportional to the bandwidth of electronic states. Electronic Bloch oscillations were observed for the first time in semiconductor superlattices²⁶ (for an overview, see Ref. 27). A similar phenomenon of sustained oscillations of the electromagnetic field, named photon Bloch oscillations, was also reported in two-dimensional waveguide arrays and optical superlattices based on porous silicon.²⁸

A key problem in condensed matter physics is to understand the electronic transport when the above ingredients

(disorder, interaction, and electric field) are simultaneously present. The interplay between disorder and dynamical localization due to an electric field was recently studied in Refs. 29 and 30. It was numerically proven that coherent Bloch oscillations can appear whenever the disorder distribution displays appropriated long-range correlations in both one-dimensional²⁹ and two-dimensional³⁰ systems. The problem involving disorder and electron-electron interaction has been a subject of great interest due to their competitive role.³¹⁻⁴⁴ It has been shown that on-site Coulomb interactions weaken the Anderson localization induced by disorder. Shepelyansky³¹ pioneered the study of two interacting electrons moving in a disordered one-dimensional (1D) system, and obtained an enhanced propagation effect of an interacting electron pair over distances larger than the single-particle localization length, as indeed predicted in disordered mesoscopic rings threaded by a magnetic flux.³³

Recently, the interplay between dynamical localization and electron-electron interaction was reported in Refs. 45-48. By using numerical and analytical calculations, the problem involving N interacting electrons moving along a chain and subject to an external electric field was studied in Ref. 45. It was shown that the N -particle problem is identical to that of a single particle moving in an N -dimensional lattice, with defect surfaces dividing the space in symmetric domains. The authors have shown that in the limit of weak hopping integral, the electron-electron interaction induces an additional oscillation of the eigenstate drift velocity. The period of this oscillation was found to be determined solely by the range and strength of the electron-electron interaction.⁴⁵ The spectral properties of the Bose-Hubbard Hamiltonian under the additional action of a static field were studied in Ref. 46. It was shown that for intermediate strengths of the static field, a rapid decay of the Bloch oscillations of the mean atomic momentum arises. It was also shown that the time scale of this decay provides a direct measure for the decay of particle-particle coherence across the lattice.⁴⁶ By using an extended dynamical mean-field theory,⁴⁷ the effect on a large electric field on interacting electrons was studied, numerically demonstrating that the Bloch oscillations decay due to electron correlations.

In this paper, we provide a detailed analysis of the phenomenon of electronic Bloch oscillations in low-dimensional

systems with two interacting electrons. To this end, we focus on the electric-field-biased wave-packet dynamics of two electrons moving in a 1D pure chain. We use numerical methods to solve the Schrödinger equation and compute the density of states, the stationary eigenstates, and the time evolution of the two-electron wave packet. Starting from an initial Gaussian wave packet, we show that the electric field promotes sustained Bloch oscillations, whose predominant mode displays a frequency doubling depending on the relative contributions coming from bounded and unbounded states. The values for the characteristic frequency and amplitude of the Bloch oscillations will be discussed under the light of a semiclassical approach.

II. MODEL AND FORMALISM

The Anderson-Hubbard tight-binding equation for two interacting electrons in the presence of a static uniform electric field F is given by^{43,44}

$$H = \sum_n \sum_s W(c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s}) + \sum_n \sum_s [\epsilon_n + eF\mathbf{an}] c_{n,s}^\dagger c_{n,s} + \sum_n U c_{n,\uparrow}^\dagger c_{n,\uparrow} c_{n,\downarrow}^\dagger c_{n,\downarrow}, \quad (1)$$

where $c_{n,s}$ and $c_{n,s}^\dagger$ are the annihilation and creation operators for the electron at site n with spin s , \mathbf{n} is the position operator, W is the hopping amplitude, and e is the electron charge. As we will be mainly interested in the dynamical localization induced by the external electric field applied parallel to the chain length, we will consider open chains as the more appropriate boundary condition. However, the actual boundary condition has no significant influence on the numerical results concerning the dynamical localization induced by the external field because the wave packet becomes trapped in a segment much smaller than the chain length. In order to follow the time evolution of wave packets, we solve the time-dependent Schrödinger equation by expanding the wave function in the Wannier representation

$$|\Phi(t)\rangle = \sum_{n_1, n_2} f_{n_1, n_2}(t) |n_1 s_1, n_2 s_2\rangle, \quad (2)$$

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 . In order to allow for double occupancy of the on-site orbital, we will consider in the following that the electrons are in distinct spin states (singlet state). 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 time evolution of the wave function in the Wannier representation becomes

$$i \frac{df_{n_1, n_2}(t)}{dt} = f_{n_1+1, n_2}(t) + f_{n_1-1, n_2}(t) + f_{n_1, n_2+1}(t) + f_{n_1, n_2-1}(t) + [F(n_1 + n_2) + \delta_{n_1, n_2} U] f_{n_1, n_2}(t), \quad (3)$$

where we used units of $\hbar = W = e = a = 1$. The on-site energies ϵ_n were taken as the reference energy ($\epsilon_n = 0$) without any

loss of generality. The above set of equations was solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $V(\Delta t)$:

$$V(\Delta t) = \exp(iH\Delta t) = 1 + \sum_{l=1}^{n_o} \frac{(iH\Delta t)^l}{l!}, \quad (4)$$

where H is the Hamiltonian. The wave function at time Δt is given by $|\Phi(\Delta t)\rangle = V(\Delta t)|\Phi(t=0)\rangle$. The method can be used recursively to obtain the wave function at time t . The following results were taken by using $\Delta t = 0.05$, and the sum was truncated at $n_o = 20$. This cutoff was sufficient to keep the wave-function norm conservation along the entire time interval considered. We followed the time evolution of an initially Gaussian wave packet with width σ :

$$\langle n_1 s_1, n_2 s_2 | \Phi(t=0) \rangle = \frac{1}{A(\sigma)} \exp\left[-\frac{(n_1 - n_1^0)^2}{4\sigma^2}\right] \times \exp\left[-\frac{(n_2 - n_2^0)^2}{4\sigma^2}\right] \quad (5)$$

and computed the centroid of both electrons defined as

$$\langle n_i(t) \rangle = \sum_{n_1, n_2} (n_i - n_i^0) |f_{n_1, n_2}(t)|^2, \quad i = 1 \text{ and } 2. \quad (6)$$

The initial positions (n_1^0, n_2^0) will be considered to be centered at $(L/2 - d_0, L/2 + d_0)$. In addition, we will apply a numerical diagonalization procedure of the complete Hamiltonian in the absence of electric field to obtain all eigenvectors $|\Phi^j\rangle = \sum_{n_1, n_2} f_{n_1, n_2}^j |n_1 s_1, n_2 s_2\rangle$ and eigenvalues E_j . Further, we will compute the normalized density of states (density of states per particle) defined as

$$\text{DOS}(E) = \frac{1}{L^2} \sum_j \delta(E - E_j), \quad (7)$$

and the average distance $d(E_j)$ between the two electrons

$$d(E_j) = \sum_{n_1, n_2} |n_2 - n_1| |f_{n_1, n_2}^j|^2. \quad (8)$$

The average distance brings information regarding the correlation between the electrons so that a small $d(E_j)$ signals a bounded two-electron eigenstate.

III. RESULTS

We apply our numerical diagonalization to an open chain with $L = 100$ sites. In Fig. 1, we show results for the normalized DOS versus energy E for $U = 0, 2, 4$, and 6 . For $U = 0$, the DOS is exactly the same as that obtained for the tight-binding 2D Anderson Hamiltonian for one electron in a square lattice geometry. For $U > 0$, we observe the emergence of a new subband. For $U \ll 4W$, the new subband is merged with the two-dimensional DOS. For $U \approx 4W$, the subband fully separates from the main band. According to previous analytical calculations,⁴⁵ this new subband shall correspond to bound states and cover the energy range $U \leq E \leq \sqrt{U^2 + 16W^2}$, which is corroborated by our numerical

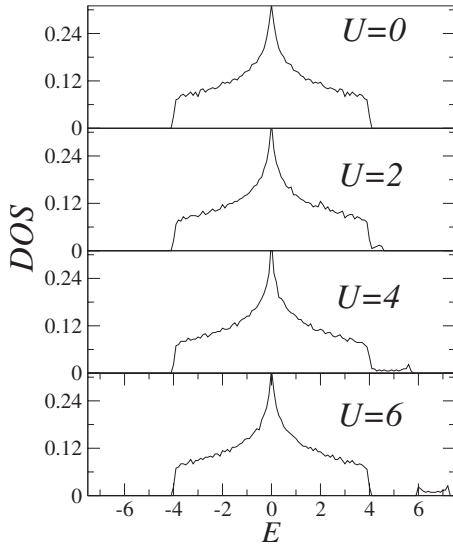


FIG. 1. Normalized density of states (DOS) versus energy E for $U=0, 2, 4,$ and 6 , computed for an open chain ($\epsilon_n=0$ for all n) with $L=100$ sites. For $U=0$, the density of states is exactly the same as that obtained from the tight-binding two-dimensional Anderson Hamiltonian for one electron in a square lattice geometry. A subband of bounded states is clearly seen for large U .

result. In Fig. 2, we show the average distance $d(E_j)$ between the two electrons versus energy E_j for $U=0, 2, 4,$ and 6 . For $U=0$, the electrons are noninteracting and the average distance is $L/3$. The structure seen in Fig. 2 reflects finite-size and boundary effects. For $U>0$, the eigenstates within the subband display small average distances $d(E_j)$ (amplified in the insets). Therefore, the eigenstates within the subband are indeed bounded (pairing) eigenstates.

The time evolution of the centroid $\langle n_i(t) \rangle$ is shown in the left panel of Fig. 3. We show results for a chain with $L=120$ sites, wave-packet width $\sigma=1$, $d_0=10$, and (a) $F=0.5$, $U=0$; (b) $F=0.5$, $U=4$; (c) $F=0.75$, $U=0$; and (d) $F=0.75$, $U=4$. The centroid displays an oscillatory pattern. The Fourier transform (see right panel) $\langle n_i(\omega) \rangle$ clearly shows that the predominant oscillation frequency is close to previous predictions using semiclassical arguments $\omega=F$.²³⁻²⁵ For such large initial electron-electron distances $d_0 \gg \sigma$, the Bloch oscillations do not depend on the Coulomb interaction U once the wave packet remains trapped by the electrical field around its initial position, for which the double occupancy probability is vanishingly small.

In Fig. 4, we show results for the centroid $\langle n_i(t) \rangle$ computed using a chain with $L=120$ sites, $\sigma=1$, $d_0=0$ (initially close electrons), $F=0.5$, and (a) $U=0$, (b) $U=4$, and (c) $U=10$. For $U=0$, the centroid displays an oscillatory pattern with frequency close to $\omega=F$. For $U=4$, the Fourier transform $\langle n_i(\omega) \rangle$ clearly shows that the centroid displays an oscillatory pattern with a predominant frequency close to $\omega=2F$. For much stronger interactions, the $\omega=F$ frequency is reamplified. The modulation in the oscillation pattern observed at finite U is mainly related to the small splitting of the peak at $\omega=F$. Such splitting is of the order of W^2/U for large U . It is due to the electron-electron interaction, which is also responsible for the emergence of an additional

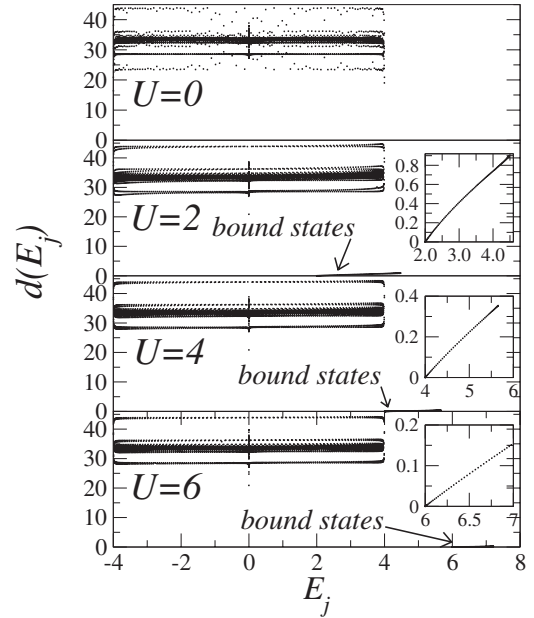


FIG. 2. The average distance $d(E_j)$ between the two electrons versus energy E for $U=0, 2, 4,$ and 6 , computed in a chain ($\epsilon_n=0$ for all n) with $L=100$ sites and open boundaries. The average distance between noninteracting Bloch-like electrons is $L/3$. The structure is due to finite-size and boundary effects. For $U>0$, the eigenstates within the subband have small distances $d(E_j)$, reflecting the bounded nature of these states. The insets show amplifications of the average electron-electron distance within the band of bounded states.

oscillation frequency of the drift velocity of bounded eigenstates.⁴⁵

In order to understand the role played by the electron-electron interaction in the emergence of the above described frequency doubling process for intermediate interactions, we computed the long-time average of the double occupancy probability $P_2 = \sum_{j=1}^L \langle |f_{j,j}(t)|^2 \rangle$ as a function of the Coulomb interaction U for several initial wave-packet widths $\sigma=0, 1,$

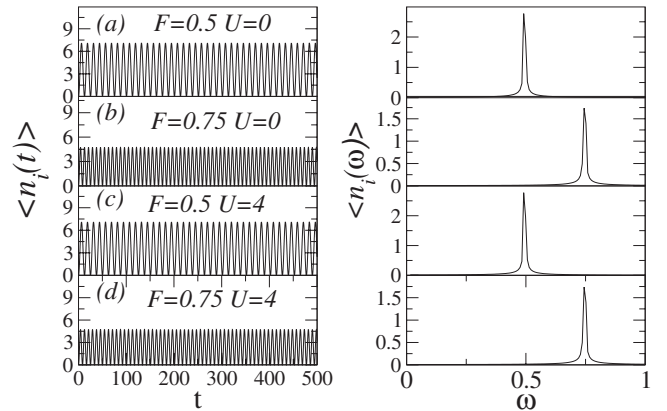


FIG. 3. Left panel: Centroid $\langle n_i(t) \rangle$ computed using a chain with $L=120$ sites, wave-packet width $\sigma=1$, $d_0=10$, and electric field strengths (a) $F=0.5$, $U=0$; (b) $F=0.75$, $U=0$; (c) $F=0.5$, $U=4$; and (d) $F=0.75$, $U=4$. The Fourier transform (see right panel) $\langle n_i(\omega) \rangle$ clearly shows that the centroid displays an oscillatory pattern with frequency close to $\omega=F$.

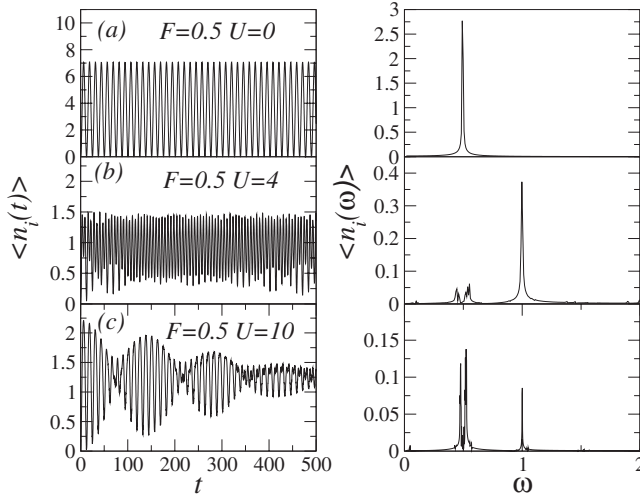


FIG. 4. Left panel: Centroid $\langle n_i(t) \rangle$ computed using a chain with $L=120$ sites, wave-packet width $\sigma=1$, initial electron-electron distance $d_0=0$, electric field strength $F=0.5$, and distinct Hubbard interactions: (a) $U=0$, (b) $U=4$, and (c) $U=10$. For $U=0$, the centroid displays an oscillatory pattern with frequency close to $\omega=F$. For $U=4$, the Fourier transform $\langle n_i(\omega) \rangle$ clearly shows that the centroid displays an oscillatory pattern with a predominant frequency close to $\omega=2F$.

2, 3, and 4, as reported in Fig. 5. For $\sigma=0$, both electrons are initially placed at the central site in such a way that the initial double occupancy is $P_2(t=0)=1$. Whenever $U=0$, the electron wave packets spread independently, although remaining trapped over a finite segment due to the presence of the external field. Therefore, the long-time double occupancy probability becomes small (of the order of the inverse asymptotic wave-packet width). As the interaction is turned on, the emergence of bounded states correlates the two-electron dynamics. For large interaction strengths, the initial state is mostly superposed to bound states and, therefore, the double occupancy remains close to unity. This means that the elec-

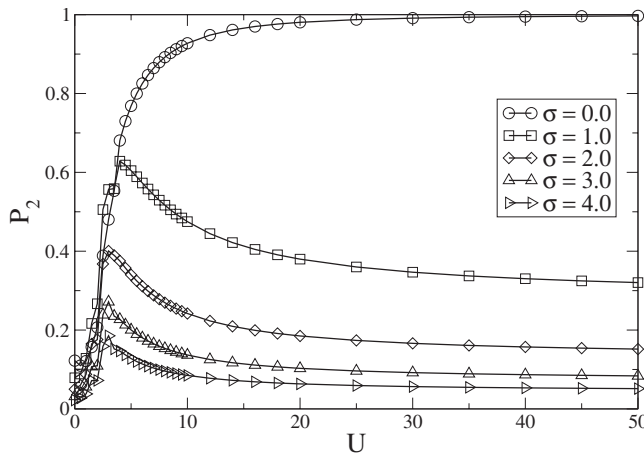


FIG. 5. The asymptotic time-averaged double occupation probability $P_2 = \sum_{j=1}^L \langle |f_{j,j}(t)|^2 \rangle$ versus U for initial wave-packet widths $\sigma=0, 1, 2, 3$, and 4. For finite wave-packet widths, P_2 develops a maximum signaling the coupling strength that favors the frequency doubling of the Bloch oscillations.

trons behave as a single particle executing coherent hoppings.

In the cases for which the initial wave packet has a finite width, the initial double occupancy probability is smaller than 1. At finite interaction strengths U , the contributions coming from the wave-packet superposition with bounded and unbounded states have opposite trends. While the interaction favors the coherent hopping associated with bounded states, its repulsive character enhances the wave-packet width. Such enhanced spread decreases the double occupancy probability coming from the superposition with unbounded states. This competition results in a nonmonotonic dependence of P_2 on the Coulomb interaction U obtained in Fig. 5 for finite initial wave-packet widths. The interaction potential U corresponding to the maximum of the long-time double occupancy probability represents also the physical situation of maximal coherence between the two-electron hopping. This maximum double occupancy probability as well as the characteristic Coulomb interaction are decreasing functions of the initial wave-packet width.

According to the above analysis, the wave-packet component corresponding to bounded states will have a dynamical evolution typical of a single particle composed of the electron pair. As such, the effective local electrical potential felt by this composed particle will be $2eFan$, thus explaining the observed frequency doubling. This effect becomes more pronounced for intermediate couplings that produce maximal double occupancy. Another signature of the competition between bounded and unbounded states is also clearly seen in the own time evolution of the one-particle centroid. According to the semiclassical prediction, the amplitude of the centroid oscillations shall be proportional to the bandwidth. In Fig. 4, one sees that the relation between the oscillation amplitudes for $U=0$ (unbounded states) and $U=4$ (predominance of bounded states) reflects the ratio between the width of the bounded and unbounded energy bands.

IV. SUMMARY AND CONCLUSIONS

In summary, we studied the one-dimensional dynamics of two interacting electrons with opposite spins under the influence of a static uniform electrical field F . When the electrons are far apart, they develop Bloch oscillations induced by the applied field whose characteristic frequency is given by $\omega = eFa/\hbar$ according to a semiclassical approach,²⁹ where e is the electron charge and a the lattice spacing. For electrons whose initial wave packets present a significant spatial superposition with each other, the Bloch oscillations develop a frequency doubled component which is more pronounced at intermediate couplings. Such frequency doubling is associated with the emergence of bounded states of two electrons in a singlet configuration. For electrons with parallel spins (triplet state), the local Coulomb interaction is ineffective and no frequency doubling shall appear. By computing the asymptotic double occupancy probability, we revealed two opposite trends that the electron-electron interaction produces on the wave-packet dynamics. For the components associated with bounded states, the Coulomb interaction keeps the electrons paired and produces coherent hoppings. For the

unbounded components, the repulsive character of the interaction enhances the wave-packet width, thus diminishing the double occupancy probability. The competition between these two effects leads to an optimal coupling to obtain a coherent dynamics of the two-electron system. The coupled electrons effectively behave as a single particle with charge $2e$, thus explaining the frequency doubling of the Bloch oscillations. The frequency doubling induced by the two-particle interaction reported here seems to be quite a general phenomenon, and can possibly be found in other systems with bounded states, such as interacting spin waves and phonons. This result will also be relevant to the analysis of the interplay between interaction and disorder to the localization theory of interacting electrons. Experimental testing

of the interaction-induced frequency doubling of Bloch oscillations would require systems with high densities of conducting electrons in order to achieve the optimal coupling condition. However, one shall keep in mind that additional electron-electron correlations may need to be taken into account to properly analyze such a regime of strongly correlated many-electron systems.

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