Field-assisted doublon manipulation in the Hubbard model: A quantum doublon ratchet

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Abstract – For the fermionic Hubbard model at strong coupling, we demonstrate that directional transport of localized doublons (repulsively bound pairs of two particles occupying the same site of the crystal lattice) can be achieved by applying an unbiased ac field of time-asymmetric (sawtooth-like) shape. The mechanism involves a transition to intermediate states of virtually zero double occupation which are reached by splitting the doublon by fields of the order of the Hubbard interaction. The process is discussed on the basis of numerically exact calculations for small clusters, and we apply it to more complex states to manipulate the charge order pattern of one-dimensional systems.

To control and tune macroscopic properties by directly manipulating processes on the atomic scale is an ultimate goal in condensed-matter physics. For example, one can selectively excite definite phonon modes [1] and thus create long-lived transients which exhibit interesting properties like superconductivity [2]. The design of suitable mechanisms that support such objectives requires to understand the underlying interplay of strong fields and many-particle interactions, which, nowadays, can be simulated and studied for more and more diverse situations by experiments with ultracold atoms [3–5]. The unprecedented control over the parameters in those systems allows one to explore the crossover between few- and many-particle physics [6] and to probe or manipulate systems with single-site resolution [7]. This makes cold atoms well suited to analyze field-induced processes all the way from addressing single particles to complex many-particle states. In extended systems, the impact of an electric field on the correlated particle motion is already nontrivial at weak to moderate interactions (leading, e.g., to damping of Bloch oscillations [8,9] or nonlinear transport [10]). However, it becomes even more subtle if both the interactions and the field are comparable to or larger than the bandwidth. In this regime, electric fields can lead to a breakdown of a Mott insulator [11–13] (which is the many-body analog of the Zener breakdown in band insulators), and when the field and the interaction are resonant, the coupling of many degenerate states can lead to the emergence of phases which are described in terms of effective spin models [14–16].

In this letter, we investigate a controlled manipulation of few-particle states based on the interplay of a local repulsive interaction and an external field. More precisely, we develop a protocol by which a time-asymmetric alternating (ac) field is used to translate a repulsively bound “doublon” [17] in the Hubbard model along a chain in a directional motion, reminiscent of a (nondissipative) ratchet [18]. In the case of a single particle on a tight binding chain, an unbiased time-periodic driving cannot lead to a finite current or set an initially localized particle into motion, not even when the driving is asymmetric in time and thus breaks time-reversal symmetry [19,20]. By contrast, the rectification effect in our protocol relies on the interaction between the two particles that form the doublon, which will also allow us to use the protocol for a controlled transmutation of more complex states. In the context of semiconductor heterostructures, the mechanism can be viewed as a generalization of an optimal control problem which has been discussed for a double quantum dot system, where gate voltage variations on the gigahertz scale allow for specific manipulations of the electronic structure [21,22]. On the other hand, the protocol is in line with charge transfer effects in molecules exposed to asymmetric laser fields [23] and, thus, seems widely applicable.
Further split into a Wannier-Stark ladder [25] with states spaced by approximately $F_0$ (for the lower band) or $2F_0$ (for the upper band). For sufficiently strong fields, the Stark effect thus leads to essential mixing of states of high and low double occupation. For $J = 0$, the crossing occurs at characteristic field strengths $|F_0| = U/n$ with integer $n \geq 1$, when the doublon on site $i$ is resonant with two separated particles on sites $i$ and $i + n$ (for $F_0 > 0$) or on sites $i$ and $i - n$ (for $F_0 < 0$). For $J \neq 0$, these resonant levels hybridize and turn into avoided crossings.

In the following, we consider the states labeled $|a\rangle$ to $|g\rangle$ in fig. 1(a) ($F_0$ finite). Both states $|a\rangle$ and $|b\rangle$ describe a doublon $|D_3\rangle = |↑↓\rangle$ which is localized by the field on the central site $3$ of the chain, see figs. 1(b) and (c). The states $|c\rangle$ to $|f\rangle$ are very close in energy, become fully degenerate for $|F_0| \rightarrow \infty$ and have low double occupancy. The energetically lowest and highest states in this manifold correspond to the anti-symmetric and symmetric superpositions $\frac{1}{\sqrt{2}}(|↑↓\rangle + |↓↑\rangle)$ and $\frac{1}{\sqrt{2}}(|↑↓\rangle - |↓↑\rangle)$, respectively (see $|f\rangle$ in fig. 1(d)). In between we find states of the form $\frac{1}{\sqrt{2}}(|↑↓\rangle \pm |↓↑\rangle)$ which pass straight through the avoided level crossing at $|F_0| = 10J$. Finally, $|g\rangle$ is the superposition $|S_{35}\rangle = \frac{1}{\sqrt{2}}(|↑↓\rangle + |↓↑\rangle)$, see fig. 1(e), which, like $|f\rangle$, has practically zero double occupancy.

Now let us suppose we prepare the system in the doublon state $|a\rangle$ at a weak field $F_0$. If the field is then ramped up to $|F_0| \gg U$ on a fast time scale, the local doublon is preserved, and the system is diabatically transferred into state $|b\rangle$. Contrarily, if the field is turned on smoothly, different final states can be reached depending on which avoided crossing is followed adiabatically. For example, if we quickly pass the crossings at $|F_0| = U/n$ for $n > 1$ and then slowly switch through the resonance at $|F_0| = 10J$ we will end up in state $|S_{35}\rangle$. Similarly we can transfer the system into state $|S_{34}\rangle$ by switching adiabatically around the $n = 2$ crossing at $|F_0| = 5J$ (note that the much narrower crossing requires an essentially slower field tuning in this case).

Including positive and negative fields, a repeated swap between states of the form $|D_i\rangle$ and $|S_j\rangle$ can now be exploited to manipulate doublons in a time-dependent fashion: The field cycle indicated by the green arrows in fig. 2(a), e.g., moves a doublon on site 3 (label $|\alpha_3\rangle$) by one lattice spacing to the right (label $|\alpha_4\rangle$). As a definite realization of the cycle we choose a time-dependent field $F(t) = F(t)e_{x}$ of the form

$$F(t) = \begin{cases} \frac{F_1 + \gamma(t - t_0)}{2}, & t_0 < t \leq t_0', \\ \frac{-F_2 + \gamma(t - t_0)}{2}, & t_0 < t \leq t_0'', \\ F_0, & \text{otherwise}, \end{cases}$$

with $\gamma = (F_2 - F_1)/\Delta t$ and $t_0'' = t_0 + \Delta t$ (fig. 2(b)). First, irrelevant level crossings are passed by the sudden change of the electric field from $F_0$ to $F_1$, and the field is ramped linearly (within a time interval $\Delta t$) from $F_1$ to $F_2$ through the $n = 1$ resonance to split the doublon. Thereafter the field is suddenly reversed (leaving the state invariant), and
In eq. (2), we set \( F \) reverse the transport direction. Finally, we note that an adequate slowly (\( \Delta t \approx 10J^{-1} \)) to generate the displaced doublon with high fidelity. The oscillations in the fidelity can be explained by Bloch oscillations of the intermediate unpaired state \( |S_{43}\rangle \) at frequency \( \omega_B(t) = |F(t)| \), which are also visible in fig. 2(b). Furthermore, fig. 3(a) proves that it is possible, by applying multiple cycles of the form (2), to successively move the doublon site by site through the whole lattice without destroying the spatio-temporal coherence. Because \( F(t) \) has zero time average, any motion of the doublon corresponds to a ratchet-like rectification of the field, where changing the sign of the field cycle will reverse the transport direction. Finally, we note that an external trapping potential \( V_{\text{trap}} \) would not impede the realization of the protocol with cold atoms. This is because the local trapping field \( -\nabla V_{\text{trap}} \) is typically smaller than \( J \) or \( U \) and thus smaller than the external field at its turning points \( F_1 \) and \( F_2 \) in the protocol (2), while the fidelity of the final state does not sensitively depend on \( F_1 \) and \( F_2 \) as long as they are far from the resonance \( F = U \).

Fig. 3: (Color online) (a) Field-assisted directional transport of an initially localized doublon through a one-dimensional chain with ten sites at \( U = 10J \) by one site per field cycle; the field parameters are as in fig. 2(b). (b) Same as fig. 2(b) but for the translation of the doublon by two sites at a time (\( F_0 = J, \ F_1 = 4.25J, F_2 = 10J \) and \( \Delta t = 59.98J^{-1} \)). (c) Field-assisted doublon transport by two sites per field cycle (field parameters as in fig. 3(c)). After seven (three) cycles, the total double occupation is decreased from 0.96 to 0.87 (0.62) in panel (a) (panel (c)).

An interesting question is whether the doublon manipulation protocol can be generalized to higher dimensions. If the field is applied along a principal axis of the lattice, the protocol will not work because particles can delocalize in directions perpendicular to the field. Although the doublon moves only with a reduced hopping \( J^2/U \), the intermediate state of two separated particles can delocalize on a time scale \( 1/J \) which does not depend on \( U \) and is not small compared to the traverse of the level crossing. On the other hand, if the field is applied along the lattice diagonal, the transverse doublon and single-particle decay are strongly suppressed, because to place a particle perpendicular to \( \mathbf{F}_0 \) requires two hopping processes against field gradients of \( \pm|\mathbf{F}_0| \), t.e., via an off-resonant intermediate

\(^1\)In order to time evolve the many-body state according to \( |\Psi(t)\rangle = U(t,0)|\Psi_0\rangle \), with \( U(t',t) = T \exp (-iJ^{-1}\int dsH(s)) \) and time-ordering operator \( T \), we use an “exact diagonalization” approach based on the Krylov time-propagation technique.

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state. Figure 4 shows the time evolution during two successive field cycles for a doublon which is initially prepared on the site \( r = (2, 2) \) of a 5 \( \times \) 5 square lattice (the parameters \( F_{0,1,2} \) are as in fig. 2(b) and \( \Delta t = 3.7 J^{-1} \)). Obviously, the first cycle, which is centered at \( t=10J^{-1} \), splits the doublon into two equal parts which become localized on the next-nearest-neighbor sites \((2,3)\) and \((3,2)\). According to this observation, we might expect that additional field cycles lead to further transverse fragmentation, such that the doublon dynamics resembles the classical diffusion dynamics on a Galton board (quinconx) [26] which results in a binomial distribution \( B_n(r_\perp) \) with \( n \geq 0 \). However, fig. 4 reveals that this picture is not applicable, and quantum interference effects are important: After the second cycle (for \( t \geq 35J^{-1} \)) we recover a single doublon which is well localized on site \((3,3)\), cf. the blue line. Furthermore, close to 50% of the doublon are lost during the first cycle, while the second cycle almost preserves the total doublon weight.

To better understand the very different nature of the first and second cycle, we separately study the time evolution of states that are present at half the field cycle at times \( t = 10J^{-1} \) and \( 30J^{-1} \), i.e., when the field has just switched sign. Ideally, these states have zero double occupancy and form a triangle \( abc \) on the lattice which is either facing into the direction \( F(t) \) (triangle \( a \) in fig. 5(a), intermediate state during the first cycle) or into the opposite direction (triangle \( b \) in fig. 5(b), intermediate state during the second cycle). At the avoided crossing \( F(t) = -U \), a state with two particles on triangle \( a \) becomes resonantly coupled by two hoppings with states where particles reside outside the triangle (a particle can move from site \( b \) to sites \( 2 \) or \( 3 \) via a resonant doublon state on sites \( a \) and \( c \), respectively). A state on triangle \( b \), on the other hand, is only coupled resonantly to states within the triangle, i.e., the doublon on site \( b \). Hence there is an additional channel for coherence loss when state \( |\Psi_3\rangle \) is moved through the crossing, which is always as dominant as the main process of forming the doublon and can thus not be avoided. As seen from fig. 4(a), the coherence loss in the first cycle is accompanied by scattering of particles from site \((3,2)\) to site \((3,1)\) and equally from \((2,3)\) to \((1,3)\) (see the arrow). To further illustrate the effect, we can prepare wave functions \(|\Psi_3\rangle = \frac{1}{\sqrt{6}} \sum_{\sigma} |\uparrow, \downarrow, \downarrow\rangle_{\sigma} \), where \( \mathcal{P} \) denotes all permutations of the sites \( a, b, c \). The ket-state is encoded as \(|a, b, c\rangle\).

During the negative part of the field cycle \( F(t) \), the states \(|\Psi_3\rangle \) and \(|\Psi_4\rangle \) evolve as shown in fig. 5(c). In particular, we find a difference of a factor of two in the total double occupancies \( d_a(t) \) and \( d_c(t) \) for times \( t > 4J^{-1} \) which goes along with an early increase of the density \( n_{\sigma \alpha} = \sum_{\beta} \langle n_{\beta \sigma} \rangle_\alpha \) at \( t \approx 2J^{-1} \) in contrast to \( n_{\sigma \alpha} \) for times \( t \geq 2J^{-1} \).

In fig. 4(b), we extend the analysis of fig. 4(a) and monitor the transverse charge distribution \( \langle n_{\sigma} \rangle_r \) (colored solid lines) over more than two field cycles; note that the distributions are time-averaged over a period of \( 10J^{-1} \) and have been normalized to 1. As discussed above, the diagonal doublon transport occurs in two stages. In the course of the field cycle the doublon is split into two equal parts and becomes resonantly coupled to states within the triangle. These states are alternately prepared on the site \( r_0 = (2, 2) \) and \( r = (2, 3) \) in the negative part of the field cycle (black solid line); the calculations have been performed for an \( 8 \times 8 \) cluster with the initial states \( \Psi_{\beta, a} \) prepared in its center. The field parameters \( F_{0,1,2} \) are as in fig. 4, \( U = 10J \) and \( \Delta t = 3.75J^{-1} \).

Fig. 5: (Color online) (a) and (b): illustration of the states \(|\Psi_2\rangle \) and \(|\Psi_3\rangle \) as defined in the text. (c) Time evolution of \( d_{a, c}(t) \) and \( n_{a, c}(t) \) in the negative part of the field cycle \( F(t) \) (black solid line); the calculations have been performed for an \( 8 \times 8 \) cluster with the initial states \( \Psi_{\beta, a} \) prepared in its center. The field parameters \( F_{0,1,2} \) are as in fig. 4, \( U = 10J \) and \( \Delta t = 3.75J^{-1} \).
Field-assisted doublon manipulation in the Hubbard model

![Diagram 1](image1.png)

![Diagram 2](image2.png)

![Diagram 3](image3.png)

![Diagram 4](image4.png)

![Diagram 5](image5.png)

![Diagram 6](image6.png)

![Diagram 7](image7.png)

![Diagram 8](image8.png)

![Diagram 9](image9.png)

![Diagram 10](image10.png)

Fig. 6: (Color online) Field-assisted manipulation of charge order on an eight-site Hubbard chain at $U = 20J$ and half-filling; the number of up and down spins is $N = \sum_i n_{i\sigma} = 4$. (a) Time evolution of the densities $\langle n_{i\sigma} \rangle$ (top panel) and of the total double occupation $d_i$ (center panel) for the system initially prepared in the “band insulating” state $|22220000\rangle$. The bottom panel shows the time evolution of the doublon-doublon correlation function $c_l$ as defined in the text. Panels (b)–(f) show the local density $\langle n_{i\sigma} \rangle$ and the double occupation $d_i$ for times $t/J^{-1} = 0, 40, 60, 80$ and 100. The field parameters are $F_0 = J, F_1 = 12.5J, F_2 = 36J$ and $\Delta t = 10J^{-1}$. The time dependence of the field is indicated by the black solid line in the center panel of (a).

of this, $\langle n_{i\sigma} \rangle$ broadens (during odd cycles) and gets compressed (during even cycles). In particular, we find that the degree of compression is such that the transverse decay of the two-particle wave function is smaller than the broadening of a binomial distribution $B_{n-1}(F_L)$, cf. fig. 4(c). This again elucidates the quantum nature of the ratchet-like motion.

Because the protocol relies on many-particle interactions, it can potentially be used to transform more complex states among each other. In the final part of this letter, we use the protocol to transfer a “band-insulating cluster” into a charge-ordered configuration. To this end, we start from a one-dimensional band insulator modeled by a half-filled eight-site Hubbard chain at $U = 20J$ which is initially in the Stark eigenstate $|\Psi_0\rangle = |22220000\rangle$ for $F_0 = J$, i.e., the first 4 sites are doubly occupied and the remaining sites are empty; the initial double occupation is $d(0) = \sum_i d_i(0) = 4$. In figs. 6(a)–(f), we plot the time evolution of the system following four field cycles $F(t) = F(t)e_i$ of the asymmetric form (2), with similar field parameters as before. As one can see, the first cycle displaces only the doublon which is closest to the spatial charge discontinuity whereas all other carriers inside the insulating region (sites 1 to 3) remain Pauli blocked. Therefore, site 4 is almost empty at the onset of the second cycle at time $t = 40J^{-1}$ (fig. 6(c)), and subsequently two doublons can be moved simultaneously by the field, leaving behind two holes on sites 3 and 5 at $t = 60J^{-1}$ (fig. 6(d)). Consistently the total double occupancy drops temporarily by $\Delta d \approx 2$ during the second cycle. Assisted by the third cycle the initial isolating state is then further transferred into one with alternating charge density but still high double occupancy, see the arrow in fig. 6(a). Aside from some minor loss of coherence the state at $t = 80J^{-1}$ is well described by the charge-ordered configuration $|02020202\rangle$, compare with fig. 6(e). Finally, the next cycle shifts the whole charge-ordered configuration by one site to $|02020202\rangle$ (fig. 6(f)), where more than 75% of the initial double occupancy is preserved for the chosen field parameters; for optimal control parameters and an extended system (where finite-size effects become negligible) we expect to observe an even more pronounced signature of this inversion. To further characterize the many-body state we computed the connected correlation function $C_l = \frac{1}{N} \sum_{[i,j]=l} \langle (d_i d_j) - \langle d_i \rangle \langle d_j \rangle \rangle$ for $d_i = n_{i\uparrow} n_{i\downarrow}$, which measures the correlation between two doubly occupied sites at a distance $l$ averaged over the entire Hubbard chain. The target state $|02020202\rangle$ is a product state with very weak correlations, and accordingly we find that $C_l$ is rather featureless in the state prepared by the protocol where $|C_{l=0}\rangle$ does not exceed a value of 0.07 during the simulation. The time evolution of the unconnected parts $c_l = \frac{1}{N} \sum_{[i,j]=l} \langle d_i d_j \rangle$ is shown as additional information in the bottom panel of fig. 6(a) and underline that the coherence loss is due to the delocalization of doublons (shift of weight in $c_l$ from even to odd $l$ for $t > 70J^{-1}$).

From fig. 6 it is obvious that the fidelity with which the charge-ordered product state can be prepared is lower than for the transfer of a single doublon in fig. 2, and it is thus interesting to note an ultimate limiting factor in the limit of large system sizes $L$: For large $L$, the transition between the two states $\ldots|2020|2020\ldots$ and $\ldots|1111|1111\ldots$ is related to a quantum phase transition [16], which implies that the gap at the level anti-crossing vanishes for $L \to \infty$, making it increasingly difficult for larger systems to shift the charge-density-wave configuration in a finite time without exciting the system.

In summary, we have studied a quantum ratchet effect in which doublons in the Hubbard model are moved by unbiased but time-asymmetric electric fields. The effect exploits an adiabatic switching through avoided level crossings in the Stark spectrum (for $U/J \gg 1$) and involves a complete but temporary fragmentation of the doublon at intermediate times. Though adiabaticity is required to avoid dephasing, the mechanism is extremely fast, taking place on time scales comparable to the inverse hopping. The process allows for a directional transport of many doublons simultaneously, and it may be applied to manipulate more complex many-body states. As such, the protocol is interesting from the theoretical perspective.
because it is associated with fast dynamical transitions between states of spatially homogeneous and inhomogeneous charge densities. Moreover, it shows that the use of avoided crossings in the Stark spectrum can be a rather general guiding principle to design charge transfer protocols, e.g., for electrons in molecules, while in detail optimal control theory could be used to further improve upon their fidelity. Although the Hubbard model certainly does not describe the spectrum of a molecule, there is extensive literature on reduced descriptions using one-dimensional model atoms, e.g., [27–30]. At specific bond lengths the corresponding Stark-spectrum can look very similar to that of the Hubbard model investigated in the present letter, i.e., there exists an avoided energy level crossing between the spatially symmetric ground state of a diatomic molecule and the eigenstate (at small field) where both electrons are either situated mainly at the right or the left nucleus (being equivalent of a right or left doublon). The investigation of charge transfer processes based on adiabatic and anti-adiabatic level crossings in these systems thus is an interesting future study. Furthermore, fields of the order $U$ can easily be realized for ultracold atoms in optical lattices [31] such that the proposed manipulation scheme may be a good test ground for experimental setups with single-site resolution. In condensed-matter systems, fields corresponding to $F \sim U$ would be extremely large, but related protocols might still play a role for the manipulation of complex states. For example, the shift of the [20202020] configuration which we have demonstrated may be reflected in the rectification of time-asymmetric laser pulses in a charge-ordered medium.

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