Optical suppression of electron motion in low-dimensional correlated electron system

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Suppression of electron motion under an alternating current (AC) electric field is examined in a one-dimensional Hubbard model. Utilizing three complementary calculation methods, it is found unambiguously that magnitudes of the kinetic-energy suppressions are influenced sensitively by the Coulomb interaction as well as the electron density. The phase and frequency in the AC field do not bring about major effects. The results are interpreted as a combined effect of the Coulomb interaction and the AC field, and provide a guiding principle for the photocontrol of correlated electron motion.

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The ultrafast control of electronic states using light has been a challenging and exciting topic in the field of condensed matter physics for the past several decades [1-3]. Recent significant progress in ultrafast optical techniques, x-ray laser facilities, and computational algorithms has accelerated developments concerning fundamental research into electron dynamics. One of the attractive topics in this research field is the exploration of photoinduced hidden states [4-9]. Several transient electronic and structural hidden states, which do not appear under conditions of thermal equilibrium, have been discovered in correlated electron materials owing to their complex degrees of freedom.

Another vital and desirable target in this field is establishment of methods to control the electronic parameters of a solid. Once such methods are settled, a core procedure for manipulating the electronic states of matter and their functionalities using light will be obtained. The theoretical proposals of the photoinduced sign changes in the electronic interactions and the magnetic exchange interactions [10] may yield new routes towards optical manipulation of magnetism and superconductivity.

The suppression of the electron motion induced by an intense alternating current (AC) field is a prototypical example of the light-control of electronic parameters. The so-called “dynamical localization” (DL) phenomenon was predicted for the non-interacting charged particle systems, where the hopping integral is multiplied by the zeroth-order Bessel function [12-14]. The sign and magnitude of the effective $t$ are expected to be adjusted by varying the light parameters. This approach has been recognized as a successful strategy for controlling correlated electron materials; competitions and cooperations between the kinetic-energy suppression and the Coulomb interaction energy provide the phase instabilities and the novel photoinduced phenomena [15-21]. However, despite recent intensive researches, the kinetic-energy suppression phenomenon itself has been addressed within the original framework of the non-interacting electron system.

In this Letter, we perform a semi-qualitative investigation of the manner in which the electron correlation effect influences the photoinduced electron motion suppression in a correlated electron system. As a prototypical correlated electron model, we analyze a one-dimensional Hubbard model under an AC electric field. Unambiguous results are obtained by using three complementary methods: the infinite time-evolving block decimation (iTEBD) algorithm, the Floquet theory combined with the exact diagonalization (ED) method, termed “Floquet+ED”, and the perturbation method. The kinetic energy is obtained for wide parameter regions of the on-site Coulomb interaction $U$, the electron density $n$, and the amplitude $A_0$, frequency $\omega$, and phase $\phi$ of the AC field. The kinetic-energy suppressions vary sensitively in response to both $n$ and $U/\omega$. Typical examples of the normalized time-averaged kinetic energy are presented in Fig. 1(a). The present results indicate that the Coulomb interaction does not only induce the system instabilities in cooperation with the photoinduced kinetic-energy suppression, but also influences the suppression phenomenon itself.

The Hubbard model in the one-dimensional lattice analyzed in the present paper is defined as

$$\mathcal{H} = - \sum_{i,\sigma} \left( tc_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{H.c.} \right) + U \sum_{i} \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right),$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the creation (annihilation) operator for an electron at site $i$ with spin $\sigma$, $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator, $t$ is the hopping integral between the nearest neighboring sites, and $U$ is the on-site Coulomb interaction. The first and second terms are denoted as $\mathcal{H}_{\text{kin}}$ and $\mathcal{H}_{\text{int}}$, respectively. The time-dependent external field is introduced in $\mathcal{H}_{\text{kin}}$ as the Peierls phase as $t \rightarrow t e^{-iA(\tau)}$ where $A(\tau)$ is the vector potential at time $\tau$. The Hubbard Hamiltonian in which $A(\tau)$ is introduced is denoted as $\mathcal{H}_A$. The light velocity, lattice constant, elementary charge, and Planck constant are set to one, and the Coulomb gauge is adopted. The semi-infinite AC field is applied along the chain, having the form

$$A(\tau) = \begin{cases} (A_0/\omega)e^{-\tau^2/(2\tau_n^2)} \sin(\omega \tau) & (\tau < 0), \\ (A_0/\omega) \sin(\omega \tau) & (\tau \geq 0), \end{cases}$$

where we chose $\tau_n = 1/t$ for the numerical calculations. The electron density is $n = N/L$, where $N$ and $L$ are the electron number and the system size. The light velocity, lattice constant, elementary charge, and Planck constant are set to one, and the Coulomb gauge is adopted.
and site numbers, respectively, and \( n = 1 \) corresponds to the half filling.

The electronic states under the AC field are analyzed by utilizing three complementary methods. First, we introduce the results obtained using the iTEBD method \([21, 24]\), which are known as an efficient simulation algorithm for quantum many-body systems in the thermodynamic limit. The wave function is represented in the matrix-product form \([21, 24]\) with the matrix dimension \( \chi \). The ground state \( |0\rangle \) is calculated by using the infinite density-matrix renormalization group method \([25]\). The time-evolved states are obtained from \( |\Psi(\tau)\rangle \propto \prod \exp(-i\delta \tau \mathcal{H})|0\rangle \), with a small time difference \( \delta \tau \). For most of the numerical calculations presented in this paper, we choose \( \chi = 100 \) and \( \delta \tau = 0.01/t \). Note that the truncation error in the ground state at \( U/t = 8 \), \( n = 0.945 \), and \( \chi = 100 \) is less than \( 10^{-5} \). The deviations of \( n \) in the time evolved-state are less than \( 10^{-4} \) until \( \tau = 50/t \).

Typical time profiles of \( A(\tau) \) and the normalized kinetic energy \( K(\tau)/K_0 \) are shown in Fig. 1(b). We define \( K(\tau) = \langle \Psi(\tau)|\mathcal{H}_{\text{kin}}|\Psi(\tau)\rangle \), which is measurable as the total weight of the optical spectra, and \( K_0 \) is the kinetic energy without the external field. As the AC field is introduced at approximately \( \tau = 0 \), \( K(\tau)/K_0 \) responds rapidly, and the system moves into a steady state smoothly. The differences between the calculated results for \( \chi = 50 \) and 100 are less than 0.2\% [see the bold and dotted lines in Fig. 1(b)]. We note that both \( K(\tau) \) and \( K_0 \) are negative, and \( K(\tau)/K_0 \) measures the absolute value of the kinetic energy. The time-averaged kinetic energy \( \bar{K} \) is calculated from \( K(\tau) \) in the stationary state indicated in Fig. 1(b).

The reduction of \( \bar{K}/K_0 \) is termed the kinetic-energy suppression in the present paper. In a similar manner, the time-averaged double occupancy \( \bar{D}/D_0 \) is deduced from the time profiles of \( D(\tau) = \langle \Psi(\tau)|\sum_i n_{i\uparrow} n_{i\downarrow}|\Psi(\tau)\rangle \).

The results of \( \bar{K}/K_0 \) at \( n = 0.6854 \) and 0.945 for \( U/t = 8 \) are presented in Fig. 1(a). Each data set for several \( \omega \) is scaled on a single curve as a function of \( A_0/\omega \), and the data within \( A_0/\omega \leq 0.3 \) are well fit by the zeroth-order Bessel function defined as

\[
\bar{K}/K_0 = J_0 (c_K A_0/\omega). \tag{3}
\]

Here, a numerical factor \( c_K \), termed the “suppression factor”, measures the suppression magnitude and \( c_K = 1 \) is expected from the conventional DL theory in a non-interacting...
Here, we focus on systems far from the half filling ($n \lesssim 0.8$). Instead of the $A(\tau)$ given in Eq. (2), $A(\tau) = (A_0/\omega) \sin \omega \tau$ for all time is introduced in the Hubbard Hamiltonian. The eigen-value equations for the Floquet states [26, 27] are given by

$$\sum_m H_{nm}^\omega |\phi_m^\alpha\rangle = \varepsilon_\alpha |\phi_m^\alpha\rangle,$$

with the Floquet Hamiltonian being expressed as

$$H_{nm}^\omega = H_{n-m} - m \omega \delta_{mn}.$$  \hspace{1cm} (4)

We define that $H_m$ and $|\phi_m^\alpha\rangle$ are the $m$-th Fourier components of the time-dependent Hamiltonian $H_A$ and the $\alpha$-th Floquet state $|\phi_\alpha(\tau)\rangle$, respectively, and $\varepsilon_\alpha$ is the $\alpha$-th Floquet quasi-energy. The wave function at time $\tau$ is given by $|\Psi(\tau)\rangle = \sum_\alpha c_\alpha e^{-i\varepsilon_\alpha \tau} |\phi_\alpha(\tau)\rangle$ with $c_\alpha = (\phi_\alpha^{n=0}|0\rangle$, where $|0\rangle$ is the ground state of $H$. Equation (4) is solved in $L$-site clusters, where the number of the Fourier components is truncated to $2N_{ph} + 1$. The quasi-energies $\varepsilon_\alpha$ and the corresponding weights $|c_\alpha|^2$ are shown in Fig. 3(a). For $A_0/\omega < 0.5$, one Floquet state is dominant with the weights for the other states being less than $10^{-3}$. In the calculations of $|\Psi(\tau)\rangle$, all Floquet states are considered when the Floquet+ED method is employed, and the dominant state is considered when the perturbation method is employed. Convergences of the results with respect to $N_{ph}$ are confirmed.

The suppression coefficients obtained using the Floquet+ED methods are plotted in Fig. 2(b) (open symbols). The $U/\tau$ dependence of $c_K$ reproduces the results yielded by the iTEBD methods semi-qualitatively. The numerical data are smoothly connected from the weak to strong coupling regimes, and approach $c_K = 1$ at $U/\tau = 0$. As can be seen from the logarithmic plots shown in Fig. 3(b), $c_K$ varies with $(U/t)^2$ and $(U/t)^{-1}$ in the weak and strong coupling limits, respectively. This method is also advantageous as it can elucidate the detailed $\omega$ dependence of $c_K$ [see in Fig. 3(c)]. The data for a wide frequency range ($0.2 \leq \omega/t \leq 0.6$) are well scaled by a single curve. That is, the $c_K - U/t$ curve does not depend on $\omega$ within these data sets, in which the frequency limits, $\omega \ll U, t$ and $\omega \gg U, t$, are incorporated. A dip structure at approximately $U/t = 8$ for $\omega/t = 6$ is most likely due to the resonant transitions.

The physical interpretations of the results presented above are obtained using the perturbation method with respect to the AC field. The Floquet Hamiltonian in Eq. (5) is separated into two components, such that $H_{nm}^\omega = (V_0)^{nm} + (V_A)^{nm}$, where $(V_0)^{nm}$ is defined as $H_{nm}$ with $A_0 = 0$, and $(V_A)^{nm}$ is the remaining component which is treated as the perturbational term. The explicit form of $c_K$ calculated up to the second-order perturbation is given in the Supplemental Material (SM) [28], and is evaluated numerically using the ED method in finite size clusters. As shown in Fig. 3(d), which also shows the data obtained using the Floquet+ED method, the results yielded by the two methods almost coincide with each other, although some differences exist in the results for
(N, L) = (4, 8). The good agreement between the two different methods can also be seen in the results for $\mathcal{D}$ (not shown).

It is confirmed numerically that, of the several terms in Eq. (S.9) in SM, the second term is dominant, as

$$c^2_K \sim 1 + 2 \sum_{i \neq 0} \frac{\langle i | H_{\text{kin}} | 0 \rangle^2}{K_0 (E_0 - E_i)}.$$  \hspace{1cm} (6)

where $| i \rangle$ is eigen state of $\mathcal{H}$ with energy $E_i$. This equation implies that $c_K$ is greater than one within the present approximation. We note that $\langle i | H_{\text{kin}} | 0 \rangle = 0$ in the non-interacting system, as $| i \rangle$ and $| 0 \rangle$ are the eigen states of $H_{\text{kin}}$. The direct calculations performed using the ED method demonstrate that the numerator (denominator) in the second term in Eq. (6) governs the $U/t$ dependence of $c_K$ in the region of $U/t \lesssim 5$ ($U/t \gtrsim 5$). The deviation of $c_K$ from one is interpreted as being attributable to the electron scattering near the Fermi level, whereas that in the strong coupling regime is due to the scattering between the remnants of the lower and upper Hubbard bands with the energy differences of the order of $U$. In other word, the electron redistribution to the higher energy states due to the Coulomb interaction promotes the photoinduced kinetic-energy suppression.

We show the effects of the phase in the AC field. The phase degree of freedom $\phi$ is introduced in the vector potential as $A_\phi(\tau) = \theta(\tau) (A_0/\omega) \sin (\omega \tau + \phi) - \sin \phi$. When $\phi = 0$, $A_\phi(\tau)$ reduces to Eq. (2) with $\tau_0 = 0$, and the oscillation in $A_\phi(\tau)$ is symmetric with respect to the origin, as shown in Fig. 4(a). On the other hand, when $\phi = \pi/2$, the oscillation in $A_\phi(\tau)$ is asymmetric, but that in the electric field is symmetric. In the non-interacting system, we have an exact expression, i.e., $\mathcal{K}/K_0 = J_0(A_0/\omega) \cos (A_0/\omega) \sin \phi$, where an apparent cosine factor appears as a result of the phase. The phase effect introduced in the Hubbard Hamiltonian is examined using the iTEBD method. The results obtained for $U/t = 8$ and $n = 0.685$ are presented in Fig. 4(b); $\mathcal{K}$ at $\phi = 0$ and $\pi/2$ are well fit by $J_0(c_K A_0/\omega)$ and $J_0(c_K A_0/\omega) \cos (A_0/\omega)$, respectively, where $c_K = 1.11$ in both cases. It is concluded that the deviation of $c_K$ from one does not depend on the choice of phase, but it is attributable to the intrinsic effects.

Thus far, we have primarily focused on the results for systems far from the half filling ($n \ll 0.8$). This is because the analysis accuracy of this case for the Floquet+ED and perturbation methods is limited. The short-range magnetic interaction of the order of $t^2/U$ provides an additional energy scale near the half filling, and may play a role in the suppression of $c_K$ under the AC field. Although the results yielded by the iTEBD method shown in Fig. 4 are reliable even near the half filling, further analyses are required as future research questions. It is likely that the size effect on the ED method, the Floquet states that are neglected during implementation of the perturbation methods, and the higher-order perturbations are considered in that case.

The present study reports several invaluable findings for experimental observations of the electron motion suppression under an AC field. First, for wide $U/t$ range from the weak to strong coupling regimes, and electron density, the reduction of $\mathcal{K}/K_0$ is well scaled by the modified zeroth-order Bessel function for small $A_0/\omega$ at least. Second, the suppression is most remarkable at approximately $n = 0.8$ and $U/t = 10$, and is reduced in the vicinity of the half-filled state. This finding aids appropriate selection of target materials for experimental observations. Third, the phase of the AC field does not play an essential role in the suppression; this finding provides valuable information for setting up the light pulse in experiment. Theoretical calculations for higher dimensional systems are required for direct comparison with experiment, although the present results via the perturbation method are obtained without assumptions regarding the system dimensions.

In summary, the correlated electron dynamics under an AC field is examined for a one-dimensional Hubbard model. Through the analyses using the three complementary methods, it is found that the photoinduced kinetic-energy suppression itself is influenced sensitively by the on-site Coulomb interaction as well as the electron density. The results are interpreted as a combination effect of the electron redistribution via the Coulomb interaction and the AC field. The present results will be checked directly through systematic experiments involving a series of low-dimensional conducting organic solids as well as cold-atom systems.

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Supplemental Material for

“Optical suppression of electron motion in low-dimensional correlated electron system”

In this Supplemental Material, we derive the analytical expression of the “suppression factor” $c_K$ shown in Eq. (6) in the main text by using the perturbation method. In the case of the small $A = A_0/\omega$, this is defined as a coefficient in the time-averaged kinetic energy given as

$$
\bar{K}/K_0 = J_0(c_K A) \sim 1 - \frac{1}{4}(c_K A)^2 + O(A^3),
$$

(S.1)

We adopt the Hubbard model $H$ in a one-dimensional chain in the main text, although the following formulae are given in a $d$-dimensional lattice.

In the Floquet theory, the $m$th-order Fourier component of the time-dependent Hamiltonian is given by

$$
H_m = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} d\tau e^{im\omega \tau} H_A
$$

$$
= \delta_{m,0} H_{\text{int}} + \left\{ \mathcal{J}_m(A) H_{\text{kin}} + \mathcal{J}_m(A)(-iJ) \right\} (m: \text{even}),
$$

(S.2)

where $H_A$ is the Hubbard Hamiltonian where $A(\tau)$ is taken into account as the Peierls phase. We introduce $J = \sum_{k\sigma} \sum_{\nu=1}^d (2t \sin k_{\nu} c_{k\sigma}^\dagger \bar{c}_{k\sigma})$ with the Fourier component of the fermion operators $c_{k\sigma} = L^{-d/2} \sum_j e^{-i\mathbf{k} \cdot \mathbf{R}_j} c_{j\sigma}$. The Floquet eigen-value equation is given by

$$
H^\omega |\phi_\alpha\rangle = \varepsilon_\alpha |\phi_\alpha\rangle,
$$

(S.3)

which corresponds to Eq. (4) in the main text. We introduce a vector space $\{|n\rangle\}_{n \in \mathbb{Z}}$ so that $|\phi_\alpha^0\rangle$ and $H^\omega_{nm}$ in Eq. (4) are represented as $|\phi_\alpha^0\rangle = |n\rangle|\phi_\alpha\rangle$ and $H^\omega_{nm} = \langle n|H^\omega|m\rangle$, respectively. The AC field is applied to the system in the ground state $|0\rangle$ of $H$ at $\tau = 0$. An expectation value of an operator $O(\tau)$ at time $\tau$ is given by

$$
\langle \Psi(\tau)|O(\tau)|\Psi(\tau)\rangle = \sum_{\alpha\beta} \sum_{mn} c_\alpha^m c_\beta e^{-i(\varepsilon_\beta - \varepsilon_\alpha)\tau} \times e^{-i(n-m)\omega \tau} \langle \phi^m_\alpha|O(\tau)|\phi^n_\beta\rangle,
$$

(S.4)

where $\Psi(\tau)$ is the wave function at $\tau$, and $c_\alpha = \langle \phi^0_\alpha|0\rangle$.

Equation (S.4) is evaluated by the perturbation theory. The Floquet Hamiltonian $H^\omega$ in Eq. (S.3) is separated into the unperturbed and perturbed components as

$$
H^\omega = V_0 + V_A,
$$

(S.5)

where $V_0$ is defined as $H^\omega$ at $A = 0$, and $V_A$ is the remaining part of $H^\omega$. The quasienergy and the wave function in the $j$th-order perturbation are given by $\varepsilon_\alpha^{(j)}$ and $|\phi_\alpha^{(j)}\rangle$, respectively. For the non-degenerate eigenstate of $V_0$, the eigenstate of $H^\omega$ is obtained up to the first order of $V_A$ as

$$
|\phi_\alpha\rangle = |\phi_\alpha^{(1)}\rangle + \mathcal{N}|\phi_\alpha^{(0)}\rangle + O(V_A^2)
$$

$$
\approx \sum_{\beta(\neq \alpha)} |\phi_\beta^{(0)}\rangle \frac{|\phi_{\beta}^{(0)}^\dagger V_A |\phi_\alpha^{(0)}\rangle}{\varepsilon_\alpha^{(0)} - \varepsilon_\beta^{(0)}} + \mathcal{N}|\phi_\alpha^{(0)}\rangle,
$$

(S.6)

where a constant $\mathcal{N}$ is determined by the normalization. Since the unperturbed Hamiltonian $V_0$ is block diagonal, Eq. (S.3) is decomposed into each sector as

$$
(H_0|_{A=0} - m\omega)|\phi_\alpha^{m(0)}\rangle = \varepsilon_\alpha^{(0)}|\phi_\alpha^{m(0)}\rangle.
$$

(S.7)

where $H_0|_{A=0}$ is $H_m=0$ at $A = 0$, and is nothing but the Hubbard Hamiltonian $H$. Thus, the zeroth-order eigenstates $|\phi_\alpha^{m(0)}\rangle$ are identified as the eigenstates of $H$, and the Floquet states in Eq. (S.6) are represented in terms of the eigenstates $|i\rangle$ and eigen-energies $E_i$ of $H$.

We assume that the ground state of $H$ is non-degenerated and the resonant transitions do not occur, i.e., $m\omega \neq E_i - E_\alpha$. In Eq. (S.4), one Floquet state $|\alpha\rangle$, which connects to the ground state $|n = 0\rangle|0\rangle$ in the limit of $A \to 0$, is taken into account. This is justified in the small $A/\omega$ region by the calculated results shown in Fig. 3(a) in the main text, in which the weight $|c_\alpha|^2$ for one Floquet state is dominant, and others are much less than one.

By comparing Eq. (S.3) with the following expression:

$$
\bar{K} \approx \sum_{m} J_{m-n}^\alpha(A) \times \left\{ \langle \phi^m_\alpha|H_{\text{kin}}|\phi^m_\alpha\rangle |m-n : \text{even}\rangle, \langle \phi^m_\alpha|(-iJ)|\phi^m_\alpha\rangle \right\} |m-n : \text{odd}\rangle,
$$

(S.8)

we obtain the analytical expression for $c_K$ as follows,

$$
c_K^2 = \frac{1}{K_0} \sum_{(i \neq 0)} \frac{|\langle i|H_{\text{kin}}|0\rangle|^2}{E_0 - E_i} + \sum_{(i \neq 0)} \left[ \frac{|\langle i|J|0\rangle|^2}{(E_0 - (E_i - \omega))^2} + \frac{|\langle i|J|0\rangle|^2}{(E_0 - (E_i + \omega))^2} \right] - \frac{2}{K_0} \sum_{(i \neq 0)} \left[ \frac{|\langle i|J|0\rangle|^2}{E_0 - (E_i - \omega)} + \frac{|\langle i|J|0\rangle|^2}{E_0 - (E_i + \omega)} \right] - \frac{1}{K_0} \sum_{n=\pm 1} \sum_{j(\neq 0)} \frac{(0|J|i\rangle \langle i|H_{\text{kin}}|j\rangle |j|J|0\rangle}{(E_0 - (E_i - n\omega))(E_0 - (E_j - n\omega))}.
$$

(S.9)

The first two terms are Eq. (6) in the main text. In the limits of the low-energy ($\omega \to 0$) and the weak excitation ($A \to 0$), this is
reduced to

$$c_K^2 = 1 + 2 \sum_{i(\neq 0)} \left[ \frac{|\langle i|H_{\text{kin}}|0\rangle|^2}{K_0(E_0 - E_i)} - \frac{2|\langle i|J|0\rangle|^2}{K_0(E_0 - E_i)} + \frac{|\langle i|J|0\rangle|^2}{(E_0 - E_i)^2} \right] - 2 \sum_{i, j(\neq 0)} \frac{\langle 0|J|i\rangle \langle i|H_{\text{kin}}|j\rangle \langle j|J|0\rangle}{K_0(E_0 - E_i)(E_0 - E_j)}. \quad (S.10)$$

On the other hand, in the limit of the high-energy excitation ($\omega \to \infty$), we have

$$c_K^2 = 1 + 2 \sum_{i(\neq 0)} \frac{|\langle i|H_{\text{kin}}|0\rangle|^2}{K_0(E_0 - E_i)}. \quad (S.11)$$