Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model assisted by machine learning

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Photoinduced nonequilibrium states can provide new insight into dynamical properties of strongly correlated electron systems. One of the typical and extensively studied systems is the half-filled one-dimensional extended Hubbard model (1DEHM). Here, we propose that the supervised machine learning (ML) can provide useful information for characterizing photoexcited states in 1DEHM. Using entanglement spectra as a training dataset, we construct neural network. Judging from the trained network, we find that bond-spin-density wave (BSDW) order can be enhanced in photoexcited states if the frequency of a driving pulse nearly resonates with gap. We separately calculate the time evolution of local and non-local order parameters and confirm that the correlation functions of BSDW are actually enhanced by photoexcitation as predicted by ML. The successful prediction of BSDW demonstrates the advantage of ML to assist characterizing photoexcited quantum states.

Introduction. — Nonequilibrium processes in strongly correlated electron systems can provide new insight into dynamical properties of these systems. One such example is nonequilibrium induced phase transitions. As the system is driven away from the equilibrium, under certain conditions, a “crossover” from one state to another (metastable) state may occur, which gives rise to not only a thermally accessible state but also leads to a hidden state of matter.

Not only insulator-to-metal transitions [1–7] but also enhancement of charge and bond orders [4, 8] as well as superconducting correlations [10, 11] have been suggested as an indication of a nonequilibrium induced phase transition in a one-dimensional (1D) Mott insulator. However, characterization of the emergent nonequilibrium state has not yet been well-established. One of the possible strategies for such characterization is the use of machine learning (ML), which can detect hidden features of states without explicitly defining order parameters [12–29].

In this Letter, we investigate photoexcited states of the half-filled 1D extended Hubbard model (1DEHM). We propose that supervised ML can provide new insight into characterization of photoexcited quantum states. Here, entanglement spectrum (ES) of the typical ground states [6, 30–35, 37–44] of the half-filled 1DEHM such as the Mott-insulating (MI) state, charge-density-wave (CDW) state, and bond-charge-density-wave (BCDW) state are used as a training dataset. In addition, we also use ES of bond-spin-density-wave (BSDW) state [45–51], which is stabilized by introducing a correlated-hopping interaction to the 1DEHM. This is because such a correlated-hopping interaction is expected to appear in a Floquet effective model of the periodically-driven Hubbard model. The trained neural network finds that BSDW order can be induced in photoexcited states, although the BSDW state is not a ground state of the 1DEHM. In order to examine the predictions obtained by ML, we separately calculate the time evolution of local order parameters (LOPs) of BCDW, BSDW, and CDW and the parity and string non-local order parameters (NLOPs). We find that order parameters related to BSDW are enhanced by photoexcitation, which is also supported by the Floquet theory. This result is in accordance with the prediction obtained by ML. Thus, ML can successfully characterize photoexcited states of the half-filled 1DEHM.

Model. — The 1DEHM is defined as

$$\mathcal{H} = -t_\hbar \sum_{i,\sigma} B_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_i n_i n_{i+1},$$

where $B_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma}^\dagger c_{i+1,\sigma}$ is the creation operator of an electron with spin $\sigma (=\uparrow, \downarrow)$ at site $i$, and $n_i = \sum_\sigma n_{i,\sigma}$ with $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. We consider the parameter region with $U > 0$ and $V > 0$ at half filling, taking the nearest-neighbor hopping $t_\hbar$ to be the unit of energy ($t_\hbar = 1$). The ground-state phase diagram of the model is well established [6, 30–35, 37–44]. BCDW is an intermediate phase between MI and CDW phases up to a critical value $U = 9.25$. In addition, we can have the ground state with bond order, i.e., BSWB (BCDW) order, if we introduce the correlated-hopping term $\mathcal{H}_X = X \sum_i (n_{i,\uparrow} - n_{i,\downarrow})^2 B_{i,\sigma}$ with $X > 0$ ($X < 0$), where $\uparrow, \downarrow$ is the opposite spin to $\sigma$ [45–51].

Interestingly, such a correlated-hopping interaction appears in the Floquet effective model of the periodically-driven Hubbard model. It has been suggested that periodic driving can induce interaction-/density-dependent photon-assisted tunnelling and exchange in-
system composed of two subsystems A and B, a Schmidt decomposition of a many-body state $|\psi\rangle$ reads $|\psi\rangle = \sum_{i=1}^{N} \rho_i |\psi_i\rangle |\psi_i\rangle^\dagger = \sum_{i=1}^{N} e^{-\xi_i} |\psi_i\rangle |\psi_i\rangle^\dagger$, where $\rho_i$ is the eigenvalue of reduced density matrix $\rho_A = Tr_B |\psi\rangle \langle \psi| = e^{-\xi_A}$ for subsystem A (or $\rho_B = Tr_A |\psi\rangle \langle \psi|$ for subsystem B) and $ES_\xi$ (in ascending order) is the eigenvalue of the entanglement Hamiltonian $H_L$. We take the subsystem A be half of the whole system throughout this paper.

We calculate a gap $\Delta_\xi = \xi_{i+1} - \xi_i$ called the Schmidt gap for the ground state of 1DEHM with the correlated hopping term $H_X$ for system size $L = 20$ under open boundary conditions. The training dataset is extracted randomly from the regions indicated by green rectangles and lines [98].

![FIG. 1. Ground state phase diagram of the half-filled 1DEHM with $H_X$ constructed by ML for (a) $X = -1/4$ and (b) $X = 1/4$. MI, CDW, BCDW, and BSDW are shown by red, yellow, blue, and light blue colors, respectively. Training dataset is extracted randomly from the regions indicated by green rectangles and lines [98].](image)

 interacts [52–73]. For example, when we choose the frequency $\Omega$ such that $U = \Omega (\gg \hbar)$, where $l$ is a natural number, the effective Hamiltonian to the lowest order in $1/\Omega$ is given by $H^{\text{eff}}_{\text{res}} = \sum_i \{ -J_{\text{eff}} g_{i,i+1,1,\sigma} - \Delta_{\text{eff}} [ h_{i,i+1,1,\sigma} + (-1)^l h_{i,i+1,1,\sigma}] + H.c. \} = \sum_i \{ -J_{\text{eff}} [-B_{i,i+1,1,\sigma} \langle \bar{\psi}_i \bar{\psi}_i \rangle + \cdots] + K_{\text{eff}} (n_{i,\sigma} - n_{i+1,\sigma}) \bar{\psi}_i \bar{\psi}_i \}$, where $J_{\text{eff}} = \hbar J_{\text{f}} (A_0 / \Omega)$ and $K_{\text{eff}} = \hbar J_{\text{f}} (A_0 / \Omega)$. Here, $J_{\text{f}}$ is the Bessel function of the first kind of order $l$ and $A_0$ is the amplitude of the vector potential. If $l$ is odd (even), $p = 1$ ($p = 2$). $g_{i,j,\sigma} = (1 - n_{i,\sigma}) c_{i,j,\sigma}^\dagger (1 - n_{j,\sigma}) n_{i,\sigma} c_{i,j,\sigma}^\dagger$ represents the hopping of doublons and holons, and $h_{i,j,\sigma} = n_{i,\sigma} c_{i,j,\sigma}^\dagger (1 - n_{j,\sigma})$ creates a doublon-holon pair. Since $H^{\text{eff}}_{\text{res}}$ contains the correlated hopping term similar to $H_X$, bond-located order can be induced by the driving pulse. In particular, as long as the intensity of the external field is not extremely strong, $J_{\text{eff}}$ remains positive, which corresponds to $X > 0$, and thus the driving pulse may give rise to BSDW.

We demonstrate that BSDW is indeed induced in the 1DEHM driven by a photon pulse. We assume that the pulse has the time dependence determined by the vector potential $A(t) = A_0 \cos(\omega t - \phi)$, where $\phi$ is a constant phase. Spatially homogeneous electric field applied along the chain in the Hamiltonian is incorporated via the Peierls substitution in the hopping terms as $c^\dagger_{i,\sigma} c_{i+1,\sigma} \rightarrow e^{iA(t)} c^\dagger_{i,\sigma} c_{i+1,\sigma}$ [74, 75].

**Machine learning.** — Recent extensive studies have demonstrated that ML can provide new strategies for investigating quantum states [12]. This approach has been successful in characterizing ordered states [13–15], many-body localized states [16, 17], topological states [18–26], Floquet-engineered states [27], and even experimental data [28, 29]. We expect that the supervised ML is also useful for examining photoexcited states.

ES is useful for characterizing phases of not only 1DEHM [76–81], but also various other systems [82–97]. We therefore use ES as a training dataset in the present study. In order to calculate ES, we use the density-matrix renormalization group (DMRG) method. In a

The time evolution of ES is calculated for the (a) for $X = -1/4$ and Fig. 1(b) for $X = 1/4$, which are in good agreement with the phase diagrams obtained previously [49, 101]. One finds that BCDW is stable for $X \leq 0$, while BSDW is stable for $X > 0$ in the intermediate phase.

We apply driving pulse with $A_0 = 0.5, t_d = 0.5$, and $t_0 = 3$ to the 1DEHM for $(U,V) = (10,1.5), (10,4.5)$, and $(10,7)$. Before applying a pulse, the ground state is MI (CDW) state for $(U,V) = (10,1.5)$ and $(10,4.5)$ and ES $(U,V) = (10,7)$. We expect that the photoinduced state is predominantly characterized by some of the phases that are located near the ground state before driving. The time evolution of ES is calculated for the $L = 20$ 1DEHM using the time-dependent DMRG method, which has widely been applied to investigate nonequilibrium phenomena [102–106]. Time evolutions of the likelihood $p_k$ ($k$ indicates each phase) are shown in Fig. 2 for these three sets of $(U,V)$.

If the ground states are driven by a photon pulse with near-resonant frequency such as $\Omega = 6, 4, 10$ and for $(U,V) = (10,1), (U,V) = (10,4.5)$ and $(U,V) = (10,7)$, respectively (see Supplemental Material S1 [100]), the likelihood changes with time. We find that the photoexcited states predicted by ML are different for different values of $V$. The case of $(U,V) = (10,4.5)$ shown in Fig. 2(a) demonstrates that the likelihood obtained by ML correctly predicts photoexcited states, since the photoinduced state driven by a photon pulse with $\Omega = 4$ has been suggested to be CDW [8]. Calculating charge correlation functions, we indeed find the enhancement of CDW order in the photoinduced state for $L = 20$, which demonstrates that ML has the ability to characterize photoexcited states of the 1DEHM. For the case of $(U,V) = (10,1.5)$ shown in Fig. 2(b), $p_{\text{BSDW}}$ first in-
Enhancement of BSDW and CDW orders by photoexcitation just after the photoirradiation but soon decreases, such that the ground states for each U and V are driven with near-resonant frequency. A photon pulse is applied during the yellow-shaded time region. The likelihoods are obtained by ML.

**Photoinduced orders.** — We investigate the time evolution of correlation functions of local order parameters (LOPs) $C_{\text{BCDW}}$, $C_{\text{BSDW}}$, and $C_{\text{CDW}}$ for BCDW, BSDW, and CDW orders, respectively, which can be defined as $C_N = \frac{1}{N} \sum_k C_N(k)$ with $C_N(k) = \sum_{\nu}(1)^{|\nu|-k}\langle \rho_k(j)\rho_N(k) \rangle$, $\nu = \text{BCDW}$, BSDW, and CDW, and $N = L$ ($N = L - 1$) for $\nu = \text{CDW}$ (BCDW and BSDW). LOPs are defined as $P_{\text{BCDW}}(j) = B_{\nu,j+1} + B_{\nu,j+1,\downarrow}$, $P_{\text{BSDW}}(j) = B_{j,j+1} - B_{\nu,j+1,\uparrow}$, and $P_{\text{CDW}}(j) = n_j - 1$. Time-dependent wave function is calculated by the time-dependent DMRG method under open boundary conditions with keeping 1000 to 2000 density-matrix eigenstates. Figures 3(a)–3(c) [3(d)–3(f)] show the time evolution of these correlation functions for $(U,V) = (10,1.5)$ [(U,V) = (10,7)], where the ground state before driving is MI (CDW). We find that $C_{\text{BCDW}}$ in Figs. 3(a) and 3(d) are suppressed (see Supplemental Material S3 [100]), while $C_{\text{BSDW}}$ in Figs. 3(b) and 3(e) are enhanced when the near-resonant conditions are satisfied. Whether $C_{\text{CDW}}$ is enhanced or suppressed depends on $V$: $C_{\text{CDW}}$ for $(U,V) = (10,1.5)$ in Fig. 3(c) is enhanced, while $C_{\text{CDW}}$ for $(U,V) = (10,7)$ in Fig. 3(f) is suppressed. Therefore, BSDW in addition to CDW is enhanced for $(U,V) = (10,1.5)$ and only BSDW is enhanced for $(U,V) = (10,7)$ in the photoexcited state. These results are in good agreement with the prediction by ML. We shall now discuss the mechanism of these photoinduced suppression and enhancement in more detail.

We now consider non-local order parameters (NLOPs) in the photoexcited state, which can detect a photoinduced hidden state. Recently it has been shown that NLOPs give an accurate description of bond-order waves [7, 8]. In addition, NLOPs can detect the presence of non-trivial topological phases [9, 10] and hidden orders not captured by conventional order parameters [11, 112–115]. Furthermore, we can directly compare the calculated NLOPs with experimental observation in optical lattices [116–118]. Thus, we expect that NLOPs are also useful for characterizing photoexcited bond-order waves. Let us introduce the parity (P) and string (S) non-local operators [7, 8, 11]: $P^{(c)}_j = \prod_{k=0}^{j-1} e^{i\pi S^{(c)}_{z,k}}$ and $P^{(s)}_j = \prod_{k=0}^{j-1} e^{i\pi S^{(s)}_{z,k}}$ S^{(c)}_{z,j} = n_j - 1$ and spin operator $S^{(s)}_{z,j} = n_{j,\uparrow} - n_{j,\downarrow}$. If corre-

![FIG. 2. Time evolution of the likelihood $p_k$ with $k = \text{MI}$, CDW, BCDW, and BSDW in the $L = 20$ half-filled 1DEHM for (a) $(U,V,\Omega) = (10,4.5,4)$, (b) $(U,V,\Omega) = (10,1.5,6)$, and (c) $(U,V,\Omega) = (10,7,10)$. Here, $\Omega$ is chosen such that the ground states for each $U$ and $V$ are driven with near-resonant frequency. A photon pulse is applied during the yellow-shaded time region. The likelihoods are obtained by ML.](image)

![FIG. 3. Time evolution of LOPs for (a,d) BCDW, (b,e) BSDW, and (c,f) CDW calculated in the $L = 20$ half-filled 1DEHEM with $(U,V) = (10,1.5)$ for (a)–(c) and $(U,V) = (10,7)$ for (d)–(f). Correlation functions for near-resonant (off-resonant) driving are shown by solid lines (dashed lines). A photon pulse is applied during the yellow-shaded time region. These are calculated by the time-dependent DMRG method.](image)
luation functions $C^\nu_r(r) = \langle P^\nu_p(j) | P^\nu_p(j+r) \rangle$ ($q = P, S$) remain finite in the limit $r \to \infty$, a specific gap in the $\nu$ channel opens [8]. Here we set $r = L/2$. The parity and string NLOPs reveal microscopic information of particle and hole fluctuations on the phases [7, 8, 114, 115]. There are mutual relations between LOPs and NLOPs. For example, MI is related to $C_P^{(c)}$, BCDW to $C_P^{(s)}$ and $C_S^{(s)}$, BSDW to $C_S^{(s)}$, and CDW to $C_P^{(s)}$ and $C_S^{(s)}$ (see Supplemental Material S4 [100]).

We show the $V$ dependence of LOPs (NLOPs) in Fig. 4(a) [Fig. 4(b)], where $\tilde{C}_\kappa (\tilde{C}^{(c)}_\kappa)$ is the time-averaged value of $\kappa$ ($\kappa^{(c)}_m$) over time $0 < t < 20$, and $\tilde{C}_\kappa^{(0)} (\tilde{C}^{(0)}_\kappa)$ is the correlation function in the ground state before driving with $\kappa = \text{BCDW}$, BSDW, and CDW ($q = P$ and $S$, and $\nu = c$ and $s$). Here, we choose frequency $\Omega$ that nearly resonates with the gap: $\Omega = 8, 6, 4, 2$, and $10$ for $(U, V) = (10, 0), (10, 1.5), (10, 4.5), (10, 5)$, and $(10, 7)$, respectively. In these cases, the change of the correlation functions by photoexcitation is the largest. $\tilde{C}_S^{(c)} (\tilde{C}^{(c)}_S)$ is always enhanced (suppressed) by photoexcitation under near-resonant conditions, as $\delta C^{(c)}_S (\tilde{C}^{(c)}_S) = \tilde{C}^{(c)}_S - C^{(0)}_S > 0$ ($\delta C^{(c)}_S = \tilde{C}^{(c)}_S - C^{(0)}_S < 0$) for $0 \leq V \leq 7$, as shown in Fig. 4(b).

Whether $C^{(s)}_P$ is enhanced or suppressed depends on $V$. As shown in Fig. 4(b), $\delta C^{(c)}_P = \tilde{C}^{(c)}_P - C^{(0)}_P > 0$ ($\delta C^{(c)}_P < 0$) for $0 \leq V \leq 5$ ($5 < V \leq 7$), indicating the enhancement (suppression) of CDW. In fact, as shown in Fig. 4(a), we find that $\delta C_{\text{CDW}} = \tilde{C}_{\text{CDW}} - C^{(0)}_{\text{CDW}} > 0$ for $0 \leq V \leq 5$ and $\delta C_{\text{CDW}} < 0$ for $5 < V \leq 7$. The photinduced enhancement of CDW predicted by ML in Fig. 2(a) is thus confirmed by the direct calculation of the order parameters, which is also in good accordance with the previous study [8].

When CDW is enhanced in photoexcited state, both $\tilde{C}^{(c)}_P$ and $\tilde{C}^{(s)}_S$ are simultaneously enhanced. Since the BSDW state is related to $\tilde{C}^{(s)}_S$, BSDW can also be enhanced when CDW is enhanced. Indeed, we find that this is the case, which is also predicted by ML in Fig. 2(b). As shown in Figs. 3(b) and 3(c), after applying the driving pulse, BSDW as well as CDW is enhanced and the time-averaged value of $C_{\text{BSDW}}$ remains finite. We find in Fig. 4(a) that $\delta C_{\text{BSDW}} = \tilde{C}_{\text{BSDW}} - C^{(0)}_{\text{BSDW}} > 0$ for $V = 0$ and $1.5$. However, as shown in Fig. 4(a), $\delta C_{\text{BSDW}} < 0$ for $V = 4.5$ and $5$, where the ground state is located near the phase boundary. Even in such cases close to the phase boundary, we still find that $\delta C_{\text{BSDW}} > 0$ as long as the photon pulse with near-resonant frequency continues to apply (see Supplemental Material S5 [100]). The enhancement of BSDW is also found for $V = 7$, as shown in Figs. 3(e) and 4(a). In this case, CDW is suppressed [see Figs. 3(f) and 4(a)]. This is consistent with $\delta C^{(c)}_P < 0$ and $\delta C^{(c)}_S > 0$ for $V = 7$ [see Fig. 4(b)] and the prediction by ML [see Fig. 2(c)].

**Summary.** — We have proposed and demonstrated that the supervised ML can give useful information for characterizing photoexcited states. Using ES as a training dataset, the neural network is trained to find the quantum state driven by a photon pulse. In the cases of $(U, V) = (10, 1.5)$ and $(10, 7)$, the ML predicts the enhancement of BSDW in photoexcited states. Physically, the enhancement of BSDW can be understood by considering photon-assisted density-dependent hopping. In order to examine the prediction obtained by ML, we have separately calculated the time evolution of various correlation functions. We have found that the correlation functions of BSDW and the corresponding string NLOP are indeed enhanced by photoexcitation, confirming the prediction by ML.

Experimentally, it is interesting to observe photoexcited states by pump-probe experiment in tetracyanoquinodimethane (TCNQ) salts and halogen-bridged transition metal compounds, since optical properties in these materials are well-described by the 1DEHM [119, 120]. Since a CDW to MI transition has already been observed [121], we expect that the enhancement of BSDW in photoexcited states is also detectable in pump-probe spectroscopy.

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We take the following parameter spaces as training dataset: \{4 < U < 8, 0 < V < 1, X = ±1/4\} for MI phase, \{0 < U < 1, 1.5 < V < 5, X = ±1/4\} for CDW phase, \{0 < U < 4, V = U/2, X = −1/4\} for BCDW phase, and \{0 < U < 4, V = U/2, X = 1/4\} for BSDW phase.

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See Supplemental Material for details of the neural network, optical conductivity, BCDW in photoexcited states, NLOPs, and BSDW correlation functions.

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SUPPLEMENTAL MATERIAL

S1. Machine learning

Figure S.1 shows the neural network constructed in this study. The initial vector of the input layer is \( z^{(n=1)} = x \), where a training dataset is substituted in input vector \( x \). Output vector \( z^{(n+1)} \) of the \((n+1)\)-th layer is written as

\[
\begin{align*}
z^{(n+1)} &= f(u^{(n+1)}), \\
u^{(n+1)} &= W^{(n+1)}z^{(n)} + b^{(n+1)},
\end{align*}
\]  

(S1)

where \( f(u_k^{(n)}) \) is the activation function, \( W^{(n+1)} \) is the weight matrix, and \( b^{(n+1)} \) is the bias vector. \( f(u_k^{(n)}) = \max(u_k^{(n)}, 0) \) for the input and hidden layers, while

\[
f(u_k^{(N)}) = \frac{\exp[u_k^{(N)}]}{\sum_{k=1}^{n} \exp[u_k^{(N)}]} \text{ for the output layer.}
\]

Finally, we obtain output vector \( y = z^{(N)} \), where \( N \) is the total number of layers. The output \( y_k \) is regarded as the probability \( p_k \) that the input dataset belongs to class \( k \). Minimizing the loss function that is defined by comparing output label \( y_k \) and input label \( d_k \), \( W^{(n)} \) and \( b^{(n)} \) are optimized. In our case, the number of units in the hidden layers is \( 3/2 \) of that in the input layer, and \( N = 4 \).

In order to increase the accuracy of the prediction by the neural network and also obtain better convergent results, we do not use entanglement spectrum \( \xi_i \) itself, but a Schmidt gap \( \xi_{i+1} - \xi_i \), for the input dataset. This is because the Schmidt gap can capture more appropriate features of the change of quantum states. In addition, by using the Schmidt gap, the dataset is appropriately normalized and standardized as often done in data preprocessing before machine learning. Training and test errors of the network are less than 0.001%.

FIG. S.1. The construction of the neural network is schematically shown. The network consists of input, hidden, and output layers. A input dataset \( x \) is classified as \( y \).

S2. Optical conductivity

Using the method described in Ref [S1–S3], we obtain optical conductivity \( \text{Re}\sigma(\omega) \) of the ground state of the half-filled one-dimensional extended Hubbard model (1DEHM) with system size \( L = 20 \) and open boundary conditions for \((U, V) = (10, 0), (10, 1.5), (10, 4.5), \) and \((10, 5)\). The result is shown in Fig. S.2. We obtain \( \text{Re}\sigma(\omega) \) by calculating time evolution of the charge current. We find exciton peaks at \( \omega = 3.9 \) for \((U, V) = (10, 4.5)\) and \( \omega = 2.3 \) for \((U, V) = (10, 5)\). For \((U, V) = (10, 0)\) and \((10, 1.5)\), \( \text{Re}\sigma(\omega) \) does not show such exciton peaks, but has the largest weight at \( \omega = 8.4 \) and \( \omega = 7.3 \), respectively. This explains that the change of correlation functions are the largest for photoexcitation with near-resonant frequency \( \Omega \) as discussed in the main text.

FIG. S.2. \( \text{Re}\sigma(\omega) \) in the half-filled 1DEHM for \( L = 20 \) with \( U = 10 \) and various values of \( V \).

S3. BCDW in photoexcited states

In the parameter region studied in the main text, BCDW is not enhanced, as shown in Fig. 4(a). However, the enhancement of BCDW has been reported in Ref. [S4] for \((U, V) = (10, 7)\) calculated by the Lanczos method under periodic boundary conditions. We infer that the enhancement of BCDW strongly depends on boundary conditions [S5]. Indeed, our calculations under periodic boundary conditions find that \( C_{\text{BCDW}} \) is enhanced in photoexcited states for \( L = 12 \) and \((U, V) = (10, 7)\). In this case, \( C_{\text{P}} \), \( C_{S} \), and \( C_{\text{BSDW}} \) are also enhanced by photoexcitation. Further investigation is required to understand why a photoexcited state for the CDW phase strongly depends on boundary conditions, which is left for further study.
TABLE S.1. Classification of 1D quantum phases and the corresponding non-local order parameters (NLOPs) from bosonization and renormalization group analysis [S7–S10]. \( \Delta_c \) and \( \Delta_s \) are charge and spin gaps, respectively. Unlocked fields are indicated by \( u \).

| Phase     | \( \phi_c \) | \( \phi_s \) | \( \Delta_c \) | \( \Delta_s \) | NLOP       |
|-----------|-------------|-------------|-------------|-------------|-----------|
| LL        | \( u \)     | \( u \)     | \( 0 \)     | \( 0 \)     | none      |
| MI        | \( 0 \)     | \( u \)     | \( \neq 0 \) | \( 0 \)     | \( C_P^{(c)} \) |
| LE        | \( u \)     | \( 0 \)     | \( \neq 0 \) | \( 0 \)     | \( C_P^{(s)} \) |
| BSDW/HI   | \( \pi/\sqrt{2} \) | \( u \)     | \( \neq 0 \) | \( 0 \)     | \( C_P^{(c)} \), \( C_P^{(s)} \) |
| CDW       | \( \pi/\sqrt{8} \) | \( 0 \)     | \( \neq 0 \) | \( \neq 0 \) | \( C_P^{(c)} \), \( C_P^{(s)} \) |
| BCDW      | \( 0 \)     | \( 0 \)     | \( \neq 0 \) | \( \neq 0 \) | \( C_P^{(c)} \), \( C_P^{(s)} \) |

S4. Non-local order parameters (NLOPs)

The low energy physics of the 1DEHM is described by an effective Hamiltonian obtained by a bosonization treatment [S6]. Upon neglecting terms of higher scaling dimension, the effective Hamiltonian turns out to be the sum of two decoupled sine-Gordon models,

\[
\mathcal{H} = \sum_{\nu=c,s} \frac{v_\nu}{2\pi} \int_0^L dx \left[ K_\nu (\partial_x \theta_\nu)^2 + K_\nu^{-1} (\partial_x \phi_\nu)^2 \right] + \sum_{\nu=c,s} \frac{2m_\nu v_\nu}{(2\pi)^2} \int_0^L dx \cos[\sqrt{8} \phi_\nu(x)], \tag{S2}
\]

where the bosonic fields \( \phi_\nu(x) \) and \( \theta_\nu(x) \) satisfy the commutation relation \( \{\phi_\nu(x), \theta_\nu(x')\} = -i \frac{\pi}{2} \delta_{\nu0} \delta(x-x') \). \( K_\nu \), \( v_\nu \), and \( m_\nu \) are the Luttinger parameters, the velocities, and the masses, respectively, for charge (\( \nu = c \)) and spin (\( \nu = s \)) sectors. An important criterion to classify the various phases is to identify the presence of charge and/or spin gaps. The opening of a gap takes place whenever the vacuum expectation value \( \langle \phi_\nu \rangle \) of the corresponding field pins to a value that minimizes the cosine in Eq. (S2).

As far as the sector is concerned, a gap can open only at half-filling, and there are two possible sets of pinning values for \( \phi_\nu \) depending on the sign of \( m_\nu \). If the spin gap is closed, these pinning values correspond to the two possible insulators, which are denoted as Mott insulator (MI) and bond-spin-density wave (BSDW) also known as charge-gapped Haldane insulator (HI). In contrast, a spin gap always opens when \( m_s < 0 \) due to SU(2) invariance in the spin sector, where only one way of pinning \( \phi_s \) is possible. In this case, when the charge gap is closed, the spin gapped phase is the Luther-Emery (LE) phase. When the charge gap is also open, one has two possible fully gapped phases: for \( m_c > 0 \) the bond-charge-density wave (BCDW) phase and for \( m_c < 0 \) the charge density wave (CDW) phase, whose order parameters can be written as \( \mathcal{O}_{\text{BCDW}}(j) = (-1)^j (B_{j+1}\uparrow + B_{j+1}\downarrow) \propto \cos[\sqrt{2} \phi_c(x)] \cos[\sqrt{2} \phi_s(x)] \) and \( \mathcal{O}_{\text{CDW}}(j) = (-1)^j n_j \propto \sin[\sqrt{2} \phi_c(x)] \cos[\sqrt{2} \phi_s(x)] \), respectively.

We introduce the parity (P) and string (S) non-local operators:

\[
\mathcal{P}_P^{\nu}(j) = \prod_{k=0}^{j-1} e^{i \pi S_{z,k}^{\nu}} \tag{S3}
\]

and

\[
\mathcal{P}_S^{\nu}(j) = \left( \prod_{k=0}^{j-1} e^{i \pi S_{z,k}^{\nu}} \right) S_{z,j}^{\nu} \tag{S4}
\]

with charge operator \( S_{z,j}^{\pm} = n_j - 1 \) and spin operator \( S_{z,j}^{z} = n_j, -n_j \). Their correlation functions \( C_P^{\nu}(r) = \langle \mathcal{P}_P^{\nu}(j) \mathcal{P}_P^{\nu}(j+r) \rangle = \langle e^{i \pi \sum_{i=j}^{j+r} S_{i}^{\nu} } \rangle \) and \( C_S^{\nu}(r) = \langle \mathcal{P}_S^{\nu}(j) \mathcal{P}_S^{\nu}(j+r) \rangle = \langle \mathcal{O}_{\text{BCDW}}^{\nu}(j) \mathcal{O}_{\text{BCDW}}^{\nu}(j+r) \rangle \) remain finite in the limit \( r \rightarrow \infty \), which corresponds to the opening of a specific gap in the \( \nu \) sector. In particular, within the bosonization approximation, \( C_P^{\nu}(x) = \langle \cos[\sqrt{2} \phi_c(0)] \cos[\sqrt{2} \phi_s(x)] \rangle \) remains finite when \( \phi_s(x) \) pins to 0, whereas \( C_S^{\nu}(x) = \langle \sin[\sqrt{2} \phi_c(0)] \sin[\sqrt{2} \phi_s(x)] \rangle \) is finite when \( \phi_c(x) \) pins to \( \frac{\pi}{4} \). Thus, the expectation value of \( C_P^{\nu}(x) \) (\( q = P \) and \( S \)) configures as order parameter for the different gapped phases, and is useful for the classification of 1D quantum phases. As shown in Table S.1, there are Luttinger liquid (LL), three partly-gapped states such as MI, LE, and BSDW/HI states, and
two fully-gapped states, i.e., CDW and BCDW states. These states are characterized by the NLOPs.

In addition, the NLOPs can give crucial informations regarding the microscopic structure encoded in the ground state. Indeed, a finite value of the parity in the charge (spin) sector implies that correlated holon-doublon (up-down spin) virtual excitations are present. On the other hand, a non-zero charge (spin) string or order indicates the presence of dilute holon-doublon (up-down spin) virtual excitations. A finite value of the parity in the charge (spin) sector implies that correlated holon-doublon (up-down spin) virtual excitations are present. Thus, whether $C_p^{(c)}$ is enhanced (suppressed) depends on $V$. The mutual relation between NLOPs and LOPs is summarized schematically in Fig. S.3(c). This relation implies that MI (BSDW) is not enhanced (suppressed) but suppressed (enhanced) in photoexcited states. When $C_p^{(c)}$ is enhanced (suppressed), CDW is expected to be effectively enhanced (suppressed) in photoexcited states. Finally, we should emphasize that the enhancement of BSDW found in our study is interesting not only because BSDW is hidden in the ground state phase diagram of the 1DEHM but also has been discussed in the context of the nontrivial symmetry-protected topological states in the continuum limit [S9–S14].

S5. BSDW correlations in 1DEHM with correlated-hopping interaction

As already described in the main text, the 1DEHM is defined by the following Hamiltonian:

$$
H = -t_0 \sum_{i,\sigma} B_{i,i+1,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_i n_i n_{i+1},
$$

(S5)

where $B_{i,j,\sigma} = c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}$, $c_{i,\sigma}^\dagger$ is the creation operator of an electron with spin $\sigma (=\uparrow, \downarrow)$ at site $i$, and $n_i = \sum_\sigma n_{i,\sigma}$ with $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. The BCDW phase is an intermediate phase between the MI and CDW phases up to a critical value $U = 9.25$. In addition, we can have the ground state with other bond order, e.g., BSDW order, if we introduce the correlated-hopping term

$$
H_X = X \sum_{i,\sigma} (n_{i,\bar{\sigma}} - n_{i+1,\sigma})^2 B_{i,i+1,\sigma}
$$

(S6)

with $X > 0$, where $\bar{\sigma}$ is the opposite spin to $\sigma$. There are two kinds of transitions, a Gaussian transition between the two gapped states and a spin-gap transition belonging to the universality class of the level-1 SU(2) Wess-Zumino-Witten model in the weak coupling region. For $X \leq 0$, the Gaussian transition occurs between the CDW and BCDW phases, and the spin-gap transition occurs between the MI and BCDW phases. For $X > 0$, the order of the Gaussian and spin-gap transitions changes, i.e., the Gaussian transition between the MI and BSDW phases, and the spin-gap transition between the CDW and BSDW phases.

In Fig. S.4(a), we show $X$ dependence of the BSDW correlation function $\langle P_{\text{BSDW}}(j) P_{\text{BSDW}}(L/2) \rangle$ for $(U,V) = (3,1.5)$, where $P_{\text{BSDW}}(j) = B_{j,j+1,\uparrow} - B_{j,j+1,\downarrow}$ is plotted. As expected, the BSDW correlation becomes larger with increasing $X$, revealing the role of correlated-hopping interaction $H_X$ in the 1DEHM. Figure S.4(b) shows the change in the magnitude of BSDW correlation function when $U$ is varied for $V = U/2$ and $X = 0.25$. These results in Fig. S.4 provide a measure of the magnitude of the BSDW correlation function when the ground state is known to be in the BSDW phase.
FIG. S.5. Time evolution of (a) BCDW, (b) BSDW, and (c) CDW correlation functions, i.e., $C_{BCDW}$, $C_{BSDW}$, and $C_{CDW}$, respectively, calculated in the $L = 20$ half-filled 1DEHM for $(U, V) = (6, 1)$. We set $A_0 = 0.3$, $t_d = 2$, and $t_0 = 10$ with $\Omega = 4$ (solid lines) and $\Omega = 0$ (dashed lines). A photon pulse is applied during the yellow-shaded time region. (d) $\langle P_{BSDW}(j)P_{BSDW}(L/2) \rangle$ calculated for time $t = 0$ (before driving), 8, 10, 12, and 14. The model parameters are the same as in (a)–(c) except for $\Omega = 4$.

As discussed in the main text, the correlated-hopping interaction can emerge in the Hubbard model with the help of a photon. We expect that the photon-assisted correlated-hopping interaction plays a role similar to the $X$ term in the 1DEHM. In fact, we find that the BSDW correlation function is enhanced in a wide range of $U > 0$ and $V > 0$ as long as the electric field with near-resonant frequency continues to apply to the 1DEHM. Figures S.5(a)–S.5(c) shows the time evolution of correlation functions $C_{BCDW}$, $C_{BSDW}$, and $C_{CDW}$ (see the main text for the definition) for $(U, V) = (6, 1)$ with $A_0 = 0.3$, $t_d = 2$, and $t_0 = 10$. Notice that here $t_d = 2$ is four time larger than the value set in the main text. The BSDW and CDW correlations are enhanced in the photoexcited state, while the BCDW correlation is suppressed under near-resonant condition. Figures S.5(a)–S.5(c) that the enhancement of BSDW and CDW correlations in the photoexcited state remains even after the pulse is decayed.

Figures S.6(a)–S.6(c) show the time evolution of correlation functions $C_{BCDW}$, $C_{BSDW}$, and $C_{CDW}$ for $(U, V) = (6, 3)$ with $A_0 = 0.3$, $t_d = 2$, and $t_0 = 10$. As in the case for $(U, V) = (6, 1)$, the BSDW and CDW correlations are enhanced in the photoexcited state, while the BCDW correlation is suppressed under near-resonant condition. The enhancement of the BSDW correlation functions in the photoexcited state is focused in Fig. S.6(d) for each time $t = 0$ (before driving), 8, 10, 12, and 14 under the near-resonant condition $\Omega = 0$. Notice that in contrast to the case for $(U, V) = (6, 1)$, the enhancement of BSDW correlations seems limited only during the light irradiation indicated by the yellow-shaded time region in Fig. S.6(b).
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