Photoinduced enhancement of bond-order in the one-dimensional extended Hubbard model

Can Shao,1,* Hantao Lu,2,† Hong-Gang Luo,2,1 and Rubem Mondaini1,‡

1Beijing Computational Science Research Center, Beijing 100084, China
2Center for Interdisciplinary Studies & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, China

We investigate the time evolution of the half-filled one-dimensional extended Hubbard model in the strong-coupling regime, when driven by a transient laser pulse. Starting from a phase displaying charge-density wave (CDW), a robust photoinduced in-gap state appears in the optical conductivity, depending on the parameters of the pulse. Here, by tuning the conditions of the pulse, we maximize the overlap of the time-evolving wavefunction with excited states displaying the elusive bond-ordered wave of this model. Finally, we make a clear connection between the emergence of this order and the formation of the aforementioned in-gap state, suggesting the potential observation of bond-ordered waves in experiments involving molecular crystals.

Introduction. — Driving non-equilibrium behavior in strongly interacting systems has been used as a way to unveil singular information about the different degrees of freedom that give rise to its ordered phases. A clear paradigm of this scenario is given in the context of optical excitations in pump-probe experiments, where one is able to transiently induce ultrafast transitions between different electronic phases, as a result of tuning either its structural, magnetic or electronic properties [1, 2]. Their specific nature depends on the characteristics of the pump pulse and on the material under investigation. For example, one can induce or enhance superconductivity at short time-scales such as to melt some of its competing orders, as the static charge stripes that appear at optimally underdoped cuprates [3–6].

In other situations, magnetic [7, 8] or insulator-to-metal [9–14] transitions are accomplished either by driving with a strong electric field or with a transient laser pulse. All these achievements largely rely on the development in the past few decades of ultrafast X-ray techniques, such as transient transmissivity (reflectivity) spectroscopy measurements, from which time-resolved optical conductivity can be extracted via Kramers-Kronig transformations [15]. A sub-set of these studies concern materials where, due to its peculiar crystal structure, one-dimensional (1D) models are believed to capture the nature of its electronic phases. In particular, molecular solids, as the bis(ethylenedithio)-tetrathiafulvalene-difluoro-tetracyanoquinodimethane (ET-F2TCNQ), are viewed as good examples of 1D Mott insulators whose chains formed by ET molecules possess large on-site and nearest-neighbor (NN) Coulomb repulsions, resulting in electronic immobility [16]. Others, as some halogen-bridged compounds, are good examples of charge-density wave insulators [17].

In both cases, the simplest model potentially describing their equilibrium properties is the extended Hubbard model (EHM), written as

\[ \hat{H} = -t_\h \sum_{i,\sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + V \sum_i \hat{n}_i \hat{n}_{i+1}, \]

(1)

where \( \hat{c}_{i,\sigma}^\dagger \) (\( \hat{c}_{i,\sigma} \)) is the creation (annihilation) operator of an electron with spin \( \sigma \) at site \( i \), and the number operator is \( \hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \); \( t_\h \) denotes the hopping amplitude, while \( U \) and \( V \) the on-site and NN Coulomb repulsions, respectively.

Ultrafast photoirradiation of these materials has revealed unique out-of-equilibrium responses, as the induction of transient metallic behavior [9, 12, 18], generation of insulating behavior with different characteristics, as from a Mott-to-CDW insulators [19], and the change in nature of charge orders, from CDW to charge polarized ones [20]. In other recent pump-probe measurements of the organic Mott insulator ET-F2TCNQ, a new resonance appears after photoexcitation and implies the manifestation of an in-gap state [21], also observed in theoretical analyses [22]. This state is attributed to the electronic delocalization through quantum interference between bound and ionized holon-doublon pairs, transiently induced by the pulse.

The ground-state (GS) phase diagram of the model (1) has been shown to display phases where the onsite and NN Coulomb interactions compete so as to induce insulating behavior with either spin-density wave (SDW) or charge-density wave (CDW) orders at large \( U \) and \( V \), respectively, connected via a first order phase transition at \( U = 2V \) [23]. At smaller values of the interactions, however, an elusive intermediate bond-ordered-wave (BOW) phase has been demonstrated [24–30]. Our main result in this Letter is to argue on the possible observation of in-gap states at the out-of-equilibrium optical conductivity precisely associated to the induction of a BOW phase in a parent equilibrium regime displaying CDW order.
Methods and observables.— We focus our study on the zero temperature strong-coupling region with $U = 10$ — hereafter, we set the energy scale $t_b = 1$ — which is consistent with the estimated on-site interaction of ET-F$_2$TCNQ materials [16]. In theory, a first-order phase transition between the SDW and CDW GSs occurs at $V = 5$ and it avoids any influence of the dimerized BOW phase, which is believed to exist up until a tricritical point at much smaller interaction strengths, $(U_c, V_c) = (5.89, 3.10)$ [30].

The system, when driven out-of-equilibrium by a transient pumping pulse, is affected by a time-dependent electric field expressed in terms of a vector potential $A(t)$, whose introduction into the hopping terms is done via the Peierls substitution:

$$
\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.} \to e^{iA(t)\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.}}. \tag{2}
$$

In terms of the temporal gauge, the vector potential $A(t)$ in (2) is written as $A(t) = A_0 e^{-(t-t_0)^2/2\sigma_0^2} \cos \omega_0 (t - t_0)$, where its temporal distribution is Gaussian centered around $t_0$, with $\sigma_0$ controlling its width, and $\omega_0$ the central frequency. We use extremely short-lived pulses by selecting $t_d = 0.5$ (in terms of the time unit, $t_h^{-1}$) so as to describe the dynamics of ultrafast irradiations.

By employing the time-dependent Lanczos method, the time-dependent wave function $|\psi(t)\rangle$ can be computed starting from the initial GS $|\Psi_0\rangle$ [31], via

$$
|\psi(t + \delta t)\rangle \approx \sum_{\ell=1}^{M} e^{-i\epsilon_\ell \delta t} |\phi_\ell\rangle \langle \phi_\ell |\psi(t)\rangle, \tag{3}
$$

where $\epsilon_\ell$ and $|\phi_\ell\rangle$ are eigenvalues and eigenvectors of the tridiagonal matrix generated in the Lanczos iteration at each instant of time, respectively; $M$ is the dimension of the Lanczos basis, and $\delta t$ is the time stepping. We select $M = 30$ and $\Delta t = 0.02$, where we have checked that increasing the number of states $M$ does not produce substantial quantitative changes in our results for this $\delta t$.

To mitigate the influence of finite size effects in our lattices of length $L$, we further contrast our results with the application of twisted boundary condition (TBC) averaging [32, 33], where the Peierls substitution (2) acquires an extra phase $e^{iA(t)\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.}} \to e^{iA(t)\epsilon_i \hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.}}$, where $\kappa = \phi/L$ and $\phi \in [0, 2\pi)$, enabling the evolution from the $\kappa$-dependent initial state $|\Psi_0^\kappa\rangle$ to $|\psi^\kappa(t)\rangle$.

One of our main concerns is the transport in this strongly interacting system. This can be quantified by the optical conductivity $\sigma(\omega)$, which in equilibrium is given in terms of the Kubo formula [34]. While there is no well-defined out-of-equilibrium optical conductivity, because of the absence of time translation invariance, various methods to calculate the optical conductivity in- and out-of-equilibrium as well as their validity in different limits have been demonstrated in Ref. 35. Here we adopt the method derived rigorously from linear-response theory [36]:

$$
\sigma(\omega, t) = \int_0^t \sigma(t + s, t) e^{i(\omega + i\kappa)s} ds, \tag{4}
$$

and in the diamagnetic term, the stress tensor operator reads $\hat{T} = t_h \sum_{i,\sigma} (\hat{c}_{i+1,\sigma}^\dagger \hat{c}_{i,\sigma} + \text{H.c.})$. The maximum time $t_m$ for the Fourier transformation (Eq. (4)) in our numerical simulation is one hundred times as much as the time unit. The interaction representation of the current operator $\hat{j}(t')$ is defined as $U(t', t) \hat{j}(t')$, where $U(t', t)$ is the time-evolution operator in the absence of probing perturbations [36]. Lastly, the current operator $\hat{j}$ reads $\hat{j} = -it_h \sum_{i,\sigma} [\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} - \text{H.c.}]$.

In what follows, we define the time difference between the central time of pump and the probe time as $\Delta t$, and finally track $\sigma(\omega, \Delta t)$, which is intimately connected to the time-dependent reflectivity in experiments.

FIG. 1. (Color online) Re $\sigma(\omega, \Delta t)$ for a lattice with $L = 14$ and $U = 10$. The standard periodic BC [TBC averaging] is used in (a) [(c)] with $V = 3$ in SDW and (b) [(d)] with $V = 7$ in CDW. The black [red] solid line in (c) and (d) is the averaged result before [after] the pump over ten equidifferent twisted phase $\phi \in [0, 2\pi)$, with the shading marking the corresponding error bar. Parameters of the pump: $A_0 = 0.4$ and $\tau_d = 0.5$, with $\omega_0$ matching the position of the main peak in equilibrium. The broadening factor $\eta$ is taken to be $1/L$.

Results.— We start by comparing the optical conductivity computed from GSs in each side of the transition,
with $V = 3$ and $7$, symmetric in respect to the transition point $V_c = 5$ (for $U = 10$). We report its real part, $\text{Re } \sigma(\omega, \Delta t)$, in a lattice with $L = 14$ and standard periodic BCs, in Figs. 1 (a) and 1 (b), respectively, both before (in equilibrium) and after the pump ($\Delta t = 5, 10, 15$). The size of the optical gap, i.e., the position of the main peak in equilibrium, is $\omega_{\text{gap}} \approx 6.12$ ($\approx 10.12$) for $V = 3$ ($V = 7$). To excite the system, we thus resonantly apply the pump, selecting $\omega_0 = \omega_{\text{gap}}$, also setting $A_0 = 0.4$, so as to enhance the bond-order as will later become clear. In both cases, the original peak at $\omega_{\text{gap}}$ is suppressed after the pump, while another peak arises at smaller energies. We dub these photoinduced states below $\omega_{\text{gap}}$ as the in-gap states. For the situation initially displaying SDW order [Fig. 1(a)], the in-gap peak is extremely close to $\omega = 0$, suggesting it might be indeed zero when approaching $L \to \infty$. In fact, Figs. 1 (c) and 1 (d) display the same as in (a) and (b), but employing the TBC averaging with 10 equidifferent twisted phases $\phi \in [0, 2\pi)$. Although still noisy for this system size, this induced peak at long times approaches $\omega = 0$, indicating a metallic regime. In stark contrast, the in-gap state generated around $\omega \approx 5$ for excitations from the CDW phase does not change regardless of time and TBCs [Figs. 1 (d)], which is indicative it may well exist in the thermodynamic limit.

The question now boils down in understanding the physical nature of the photoinduced in-gap state generated in the CDW regime. For that purpose, we recall the different order parameters associated to the three different insulating phases observed in equilibrium in the case of repulsive interactions: SDW, CDW and BOW. We generically define those in a translationally invariant and staggered fashion as

$$\hat{O}_x = \frac{1}{Lc} \sum_{i=0}^{L-1} \sum_{dx=1}^{L_c} (-1)^{dx} \hat{O}_i \hat{O}_{i+dx},$$

with $\hat{O}_i = \hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}$, for $x=$SDW; $\hat{O}_i = \hat{n}_i - 1$, for $x=$CDW and $\hat{O}_i = \sum_\sigma (\hat{c}_{i+1}^\dagger \hat{c}_i + \text{H.c.})$, for $x=$BOW. $dx$ represents the distance from site $i$ and we introduce an effective cutoff $L_c = \frac{L}{2}$, given the closed BCs $[37]$. 

In Fig. 2, we show the BC averaged time-evolution of these three order parameters, $\langle O_x \rangle_{av} = (1/N_c) \sum_\sigma \langle \psi^\sigma(t)|\hat{O}_x|\psi^\sigma(t)\rangle$, using $N_c$ equidifferent TBCs. For $V = 3$ [Fig. 2(a)], the pump is responsible to induce a metallic behavior as suggested by the optical conductivity peaks. This happens at the expense of substantially reducing the SDW order parameter. Conversely, the CDW and BOW order parameters are slightly changed with extremely long saturation times. A proper finite-size scaling would rule out the manifestation of any order in the thermodynamic limit, but given the metallic behavior suggested by $\sigma(\omega, \Delta t \to \infty)$, one would not expect their concomitant appearance. On the other hand,
when \( V = 7 \) [Fig. 2(b)], there is a considerable increment of the BOW order with little influence of the different TBCs (the shadings are barely visible), at the expense of dramatic reduction of the ruling order parameter in equilibrium, \( \mathcal{O}_{\text{CDW}} \).

Given this enhancement of the BOW order, we are now in position to correlate the appearance of the in-gap state with a photoinduced bond-order. To verify this point, we perform a full exact diagonalization (ED) calculation in a 10-sites lattice, restricted to the \( k = 0 \) momentum subspace. This is the sector where the equilibrium ground-state resides and where the time-evolved wave-function explores, since the pump does not break translation invariance. Figure 3 (a) displays the eigenstate expectation values of the BOW order parameter, for eigenstates \( |\alpha\rangle \)'s of the equilibrium Hamiltonian, as a function of the energy difference \( E_0 - E_0 \), where \( E_0 \) is the GS energy. One finds that the first excited state \( (E_1 - E_0 \simeq 10.13) \) displays the largest bond-order \( \langle |1\rangle \mathcal{O}_{\text{BOW}} |1\rangle \simeq 0.32 \) among all \( |\alpha\rangle \)'s. Besides, Fig. 3 (b) shows the overlap between the evolved wave function at long times after the pump, and all eigenstates, i.e., \( \langle |\alpha\rangle |\psi(\Delta t = 15)\rangle \). The overlap with \( \alpha = 1 \) reaches values up to 0.783 with the optimal pump parameters: \( A_0 = 0.5 \) and \( \omega_0 = 10.12 \). The detailed time evolution of the overlap between \( |\psi(\Delta t)\rangle \) with both the GS and the first excited state is shown in Fig. 3 (c). Their weight switch roles, as the pump reaches its maximum intensity at \( \Delta t = 0 \). Notice as well that \( E_1 - E_0 \simeq 10.13 \) is consistent with the optical gap \( \omega_{\text{gap}} \simeq 10.12 \), indicative that the system displays large resonance so as to absorb energy sufficient to excite this \( |\alpha = 1\rangle \) state [38].

To finally confirm the relation between the pump-enhanced bond-order and the in-gap state observed in the optical conductivity displayed in Fig. 1 (b), we show in Fig. 3 (d) the time-evolved \( \sigma(\omega, \Delta t = 15) \) and the equilibrium \( \sigma(\omega) \) computed from the GS [as in Fig. 1 (b)], accompanied by the equilibrium optical conductivity computed from the first excited state. The similarity between \( \sigma(\omega, \Delta t = 15) \) and \( \sigma(\omega) \) from \( |1\rangle \) makes clear the nature of the in-gap state: it is related to a photoinduced bond order.

The next and final point we address is in systematically finding the optimal parameters of the pump to excite the system so as to enhance the BOW order. In Figs. 4 (a), 4 (b) and 4 (c), we give the contour plots of long time-evolution BOW order parameter, the overlap of \( \langle |\alpha = 1\rangle |\psi(\Delta t = 15)\rangle \) and the injected energy \( \Delta E \equiv \langle \psi(t)|H\psi(t)\rangle - \langle \Psi_0|H|\Psi_0\rangle \), as a function of pump parameters \( A_0 \) and \( \omega_0 \), with \( V = 7 \), respectively. \( \mathcal{O}_{\text{BOW}} \) is obtained after averaging at very long times, \( \Delta t \in [5, 105] \). Here we do not use the twisted BCS because its influence in the order parameter is small, see Fig. 2 (b). The optimal \( \omega_0 \) precisely coincides with \( \omega_{\text{gap}} \) and as Fig. 4 (c) shows, the system absorbs more energy if \( \omega_0 \) is closer to \( \omega_{\text{gap}} \), as one varies \( A_0 \). Lastly, the overlap of the wavefunction at long times and the first excited state in Fig. 4 (b) display remarkable similarity with Fig. 4 (a), confirming the connection between the enhanced BOW order and the overlap increase between the time-evolved wave function and the first excited state.

As a final remark on the generality of our results, Fig. 4 (d) contrasts the equilibrium (before pump) order parameters of the three phases we investigate (solid lines) and \( \mathcal{O}_{\alpha} \), i.e., the long-time average for each of the order parameters (dashed line) as previously defined, always optimizing the pump variables \( A_0 \) and \( \omega_0 \) (with \( A_0 \in [0, 1] \) and \( \omega_0 \in [0, 20] \)) such as to enhance the corresponding order, as a function of \( V \). The enhancement of CDW order in the immediacy of the first order phase transition in SDW side \( (U=10, V=4.5) \) has been discussed in Ref. 39. Remarkably, the enhancement of the BOW order within the equilibrium CDW phase is robust for a wide range of interactions \( V \). Besides, we have further checked that the first excited state in this parameter space always display a considerable bond-order expectation value.

**Summary and discussion.**— By utilizing the time-dependent Lanczos technique, we calculate the nonequilibrium optical conductivity and order parameters for different phases of the 1D EHM. We find that an enhancement of a BOW state can be readily reached from the GS of the equilibrium CDW phase of the model, when
tuning the parameters of the pump so as to (i) be resonant with the main peak of the optical conductivity and (ii) with enough energy to induce a large overlap of the time-evolved wave function with the first excited state. We argue that in the background of alternating doublons and holons, the bond (dimerization) of electrons among the double occupied sites and their nearest empty site is one of the lowest order excitations, which under appropriate photoexcitation, can be dynamically assessed. This provides an unique framework for the observation of the elusive BOW order in experiments involving molecular crystals under ultrafast photoirradiation.

C.S. and R.M. acknowledge support from NSAF-U1530401. R.M. also acknowledges support from the National Natural Science Foundation of China (NSFC) Grant No. 11674021 and No. 11650110441. R.M. acknowledges discussions with C. Cheng; C.S. and H.L. acknowledge T. Tohyama for interactions in related works. The computations were performed in the Tianhe-2JK at the Beijing Computational Science Research Center (CSRC).

*[shaocan2018@csrc.ac.cn]
† luht@lzu.edu.cn
‡ rmmondaini@csrc.ac.cn

1] A. Cavalleri, “Photo-induced superconductivity,” Contemporary Physics 59, 31–46 (2018).

2] M. Buzzi, M. Först, R. Mankowsky, , and A. Cavalleri, “Probing dynamics in quantum materials with femtosecond X-rays,” Nature Reviews Materials 3, 299–311 (2018).

3] D. Fausti, R. I. Tobey, N. Dean, S. Kaiser, A. Dienst, M. C. Hoffmann, S. Pyon, T. Takayama, H. Takagi, and A. Cavalleri, “Light-induced superconductivity in a stripe-ordered cuprate,” Nature 533, 189 (2011).

4] D. Nicoletti, E. Casandrice, Y. Laplace, V. Khanna, C. R. Hunt, S. Kaiser, S. S. Dhesi, G. D. Gu, J. P. Hill, and A. Cavalleri, “Optically induced superconductivity in striped $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ by polarization-selective excitation in the near infrared,” Phys. Rev. B 90, 100503 (2014).

5] W. Hu, S. Kaiser, D. Nicoletti, C. R. Hunt, I. Gierz, M. C. Hoffmann, M. Le Tacon, T. Loew, B. Keimer, and A. Cavalleri, “Optically enhanced coherent transport in $\text{YBa}_2\text{Cu}_3\text{O}_7$ by ultrafast redistribution of interlayer coupling,” Nature Materials 13, 705 (2014).

6] M. Först, R. I. Tobey, H. Bromberger, S. B. Wilkins, V. Khanna, A. D. Caviglia, Y.-D. Chuang, W. S. Lee, W. F. Schlotter, J. J. Turner, M. P. Minitti, O. Krupin, Z. J. Xu, J. S. Wen, G. D. Gu, S. S. Dhesi, A. Cavalleri, and J. P. Hill, “Melting of charge stripes in vibrationally driven $\text{La}_{1.875}\text{Ba}_{0.125}\text{Cu}_4\text{O}_8$: Assessing the respective roles of electronic and lattice order in frustrated superconductors,” Phys. Rev. Lett. 112, 157002 (2014).

7] M. Först, R. I. Tobey, S. Wall, H. Bromberger, V. Khanna, A. L. Cavalleri, Y.-D. Chuang, W. S. Lee, R. Moore, W. F. Schlotter, J. J. Turner, O. Krupin, M. Trigo, H. Zheng, J. F. Mitchell, S. S. Dhesi, J. P. Hill, and A. Cavalleri, “Driving magnetic order in a manganite by ultrafast lattice excitation,” Phys. Rev. B 84, 241104 (2011).

8] C. E. Graves, A. H. Reid, T. Wang, B. Wu, S. de Jong, K. Vahaplar, I. Radu, D. P. Bernstein, M. Messerschmidt, L. Müller, R. Coffee, M. Bionta, S. W. Epp, R. Hartmann, N. Kimmel, G. Hauser, A. Hartmann, P. Holl, H. Gorke, J. H. Mentink, A. Tsukamoto, A. Fognini, J. J. Turner, W. F. Schlotter, D. Rolles, H. Soltau, L. Strüder, Y. Acremann, A. V. Kimel, A. Kirilyuk, Th Rasing, J. Stöhr, A. O. Scherz, and H. A. Dürr, “Nanoscale spin reversal by non-local angular momentum transfer following ultrafast laser excitation in ferrimagnetic GdFeCo,” Nature Materials 12, 293 (2013).

9] S. Iwai, M. Ono, A. Maeda, H. Matsuizaki, H. Kishida, H. Okamoto, and Y. Tokura, “Ultrafast optical switching to a metallic state by photoinduced Mott transition in a halogen-bridged nickel-chain compound,” Phys. Rev. Lett. 91, 057401 (2003).

10] T. Oka, R. Arita, and H. Aoki, “Breakdown of a Mott insulator: A nonadiabatic tunneling mechanism,” Phys. Rev. Lett. 91, 066406 (2003).

11] T. Oka and H. Aoki, “Ground-state decay rate for the Zener breakdown in band and Mott insulators,” Phys. Rev. Lett. 95, 137601 (2005).

12] H. Okamoto, H. Matsuizaki, T. Wakabayashi, Y. Takeda, and T. Hasegawa, “Photoinduced metallic state mediated by spin-charge separation in a one-dimensional organic Mott insulator,” Phys. Rev. Lett. 98, 037401 (2007).

13] Akira Takahashi, Hisashi Itoh, and Masaki Ai-hara, “Photoinduced insulator-metal transition in one-dimensional Mott insulators,” Phys. Rev. B 77, 205105 (2008).

14] M. Eckstein, T. Oka, and P. Werner, “Dielectric breakdown of Mott insulators in dynamical mean-field theory,” Phys. Rev. Lett. 105, 146404 (2010).

15] D. M. Roessler, “Kramers-Kronig analysis of reflection data,” British Journal of Applied Physics 16, 1119 (1965).

16] T. Hasegawa, T. Mochida, R. Kondo, S. Kagoshima, Y. Iwasa, T. Akutagawa, T. Nakamura, and G. Saito, “Mixed-stack organic charge-transfer complexes with intercolumnar networks,” Phys. Rev. B 62, 10050 (2000).

17] T. Sasaki, H. Ozumi, N. Yoneyama, N. Kobayashi, and N. Toyota, “X-ray irradiation-induced carrier doping effects in organic dimer-Mott insulators,” Journal of the Physical Society of Japan 76, 123701 (2007).

18] H.I. Uemura, H. Matsuizaki, Y. Takahashi, T. Hasegawa, and H. Okamoto, “Ultrafast charge dynamics in one-dimensional organic Mott insulators,” Journal of the Physical Society of Japan 77, 113714 (2008).

19] H. Matsuizaki, M. Iwata, T. Miyamoto, T. Terashige, K. Iwano, S. Takaishi, M. Takamura, S. Kumas-gai, M. Yamashita, R. Takahashi, Y. Wakabayashi, and H. Okamoto, “Excitation-photon-energy selectivity of photoconversions in halogen-bridged Pd-chain compounds: Mott insulator to metal or charge-density-wave state,” Phys. Rev. Lett. 113, 096403 (2014).

20] H. Matsuizaki, T. Matsuoka, H. Kishida, K. Takizawa, H. Miyasaka, K. Sugita, M. Yamashita, and H. Okamoto, “Novel optical and magnetic bistability and
photoinduced transition in a one-dimensional halogen-bridged binuclear Pt complex,” Phys. Rev. Lett. 90, 046401 (2003).

[21] S. Wall, D. Brida, S. R. Clark, H. P. Ehrke, D. Jaksch, A. Ardavan, S. Bonora, H. Uemura, Y. Takahashi, T. Hasegawa, H. Okamoto, G. Cerullo, and A. Cavalleri, “Quantum interference between charge excitation paths in a solid-state Mott insulator,” Nature Physics 7, 114 (2010).

[22] H. Lu, C. Shao, J. Bonča, D. Manske, and T. Tohyama, “Photoinduced in-gap excitations in the one-dimensional extended Hubbard model,” Phys. Rev. B 91, 245117 (2015).

[23] P. G. J. van Dongen, “Extended Hubbard model at strong coupling,” Phys. Rev. B 49, 7904–7915 (1994).

[24] E. Jeckelmann, “Ground-state phase diagram of a half-filled one-dimensional extended Hubbard model,” Phys. Rev. Lett. 89, 236401 (2002).

[25] P. Sengupta, A. W. Sandvik, and D. K. Campbell, “Bond-order-wave phase and quantum phase transitions in the one-dimensional extended Hubbard model,” Phys. Rev. B 65, 155113 (2002).

[26] M. Tsuchiizu and A. Furusaki, “Phase diagram of the one-dimensional extended Hubbard model at half filling,” Phys. Rev. Lett. 88, 056402 (2002).

[27] A. W. Sandvik, L. Balents, and D. K. Campbell, “Ground state phases of the half-filled one-dimensional extended Hubbard model,” Phys. Rev. Lett. 92, 236401 (2004).

[28] Y. Z. Zhang, “Dimerization in a half-filled one-dimensional extended Hubbard model,” Phys. Rev. Lett. 92, 246404 (2004).

[29] M. Aichhorn, H. G. Evertz, W. von der Linden, and M. Potthoff, “Charge ordering in extended Hubbard models: Variational cluster approach,” Phys. Rev. B 70, 235107 (2004).

[30] S. Ejima and S. Nishimoto, “Phase diagram of the one-dimensional half-filled extended Hubbard model,” Phys. Rev. Lett. 99, 216403 (2007).

[31] P. Prelovšek and J. Bonča, “in Strongly correlated systems,” in Strongly Correlated Systems-Numerical Methods, edited by A. Avella and F. Mancini, Springer Series in Solid-State Sciences, Vol. 176 (Springer, Berlin, 2013), pp. 1-30.

[32] D. Poilblanc, “Twisted boundary conditions in cluster calculations of the optical conductivity in two-dimensional lattice models,” Phys. Rev. B 44, 9562 (1991).

[33] T. Tohyama, “Asymmetry of the electronic states in hole- and electron-doped cuprates: Exact diagonalization study of the $t-t'-t''-j$ model,” Phys. Rev. B 70, 174517 (2004).

[34] Gerald D. Mahan, Many-Particle Physics, 2nd ed. (Plenum, New York, N.Y., 1993).

[35] C. Shao, T. Tohyama, H.-G. Luo, and H. Lu, “Numerical method to compute optical conductivity based on pump-probe simulations,” Phys. Rev. B 93, 195144 (2016).

[36] Z. Lenarčič, D. Golev, J. Bonča, and P. Prelovšek, “Optical response of highly excited particles in a strongly correlated system,” Phys. Rev. B 89, 125123 (2014).

[37] It is worth stressing that the definition of the order parameters in Refs. [26] and [30] is only suitable for open BCs, while in the case of periodic BCs, with translation invariance, the only possible way to define them is via the summation over correlation functions, as shown in the main text.

[38] One can easily understand this argument directly from the definition of the Kubo formula, provided the optical conductivity is composed of one large single-peak.

[39] H. Lu, S. Sota, H. Matsueda, J. Bonča, and T. Tohyama, “Enhanced charge order in a photoexcited one-dimensional strongly correlated system,” Phys. Rev. Lett. 109, 197401 (2012).