Ultrafast optical excitation of coherent phonons in a one-dimensional metal at the photoinduced insulator-metal transition

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Photoinduced insulator-metal transition from the charge-density wave (CDW) ground state in a one-dimensional electron system is studied within the nonadiabatic theory of electron-phonon coupling. Ultrafast melting and partial recovery of the CDW and its critical slowing down are found to accompany the cooperative lattice response by an electron-phonon energy transfer on the subpicosecond time scale, which is read out by the nonadiabatic depopulation and repopulation of coherent phonons. Further, electron correlation is described in a self-consistent mean-field theory. In the strong electron correlation, the spin-density wave competes with the CDW and the photoinduced responses of the lattice is found to undergo the nonadiabatic-adiabatic transition.

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I. INTRODUCTION

Many intriguing states of the condensed matters cooperatively stem from the electron-phonon coupling, for instance, superconductivity, charge-density wave (CDW), or some exotic orderings of charge, spin, and orbital are driven by mutual interplays of electron and lattice.^{1,2} According to an advancement of the femtosecond (fs) laser technology, an optical pumping with a shorter pulsed laser than a phonon period was found to lead to the coherent oscillation (i.e., coherent phonons) in the optical properties such as reflectivity or transmission.³ Coherent phonons drive abundant physics such as many-body interferences singular at the onset of quasiparticle,^{4,5} or possibilities for controlling coupled degrees of freedom in the ultrafast time span in semiconductors^{6–8} and superconductors.⁹

Generation of coherent phonons is also observed in a broad class of the photoinduced insulator-metal transitions (PIMTs) accompanying the structural changes in terms of the melting of the lattice-induced order.^{10–12} An important profile under debate is that, in a system with strong electron-phonon coupling, the photoinduced ultrafast dynamics show unexpected nonadiabatic behaviors of electrons and phonons depending on the photoexcitation condition,^{12–15} which differs from the case of a standard solid for which the electrons obey the Born-Oppenheimer approximation (BOA).¹⁶ The proper understanding of the interplay of electrons and coherent phonons in the fs time range is still unclear. Further, the underlying nonadiabatic feature makes the problem more challenging.

A CDW system has been focused on as one of the ideal systems for such motivations so that its real-time study has been extensively done.^{17–23} In a recent experiment on a one-dimensional (1D) CDW system $\text{K}_{0.3}\text{MoO}_3$,²² it was argued that the nonthermal melting and partial recovery of CDW occurs on the subpicosecond (sub-ps) time scale without noticeable change of the lattice. Another recent experiment on a two-dimensional (2D) CDW system 1T-TaS_2 has reported the direct observation of highly cooperative electronic and atomic motions during and after the optical excitation. Spin-density wave (SDW) is an ordered ground state that is also frequently met in a low-dimensional system.²⁴

In this paper, we theoretically study the dynamics of the PIMT in a 1D CDW system on a nonadiabatic equal footing of electrons and phonons. We find that the ultrafast melting and partial recovery of the CDW and the critical slowing down proceed together with the lattice response by a rapid electron-phonon energy transfer in $O(100)$ fs time scale. This is read out by the nonadiabatic depopulation and repopulation of coherent phonons in a way of exceptional cooperativity. Electron correlation is described in a self-consistent mean-field theory. As the electron correlation becomes appreciable, SDW gets to compete with CDW and the lattice response is found to undergo the nonadiabatic-adiabatic transition.

We introduce our model in Sec. II. Photoinduced dynamics of the system is described in Sec. III. Beginning with the calculation scheme, we present the photoinduced melting of the CDW and the nonadiabatic-adiabatic transition according to an incorporation of electron correlation. The results are summarized in Sec. IV.

II. MODEL

We start from the Hamiltonian $\mathcal{H}_0$ which describes a 1D half-filled electronic band interacting with the phonon, that is,

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + g \sum_{\mathbf{k}\sigma} \sum_{\mathbf{Q}} c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma} (b_{\mathbf{Q}} + b_{-\mathbf{Q}}^\dagger), \quad (1)$$

where $c_{\mathbf{k}\sigma}^\dagger$ ($c_{\mathbf{k}\sigma}$) is a creation (annihilation) operator of the band electron with the energy $\epsilon_{\mathbf{k}}$ ($= -2t \cos k$; t is the hopping integral) and the spin σ ($= \uparrow$ or $\downarrow$) and $b_{\mathbf{Q}}^\dagger$ ($b_{\mathbf{Q}}$) is a creation (annihilation) operator of the phonon with momentum $\mathbf{Q}$. g is the electron-phonon coupling constant. We may also introduce the Hamiltonian $\mathcal{H}_U$ to describe the electron correlation in a self-consistent decoupling method,²⁵

$$\mathcal{H}_U = U \sum_{\mathbf{k}} \sum_{\mathbf{Q}} (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{Q}\uparrow} \Delta_{\mathbf{Q}\downarrow} + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{Q}\downarrow} \Delta_{\mathbf{Q}\uparrow}). \quad (2)$$

U is the on-site electron correlation and $\Delta_{\mathbf{Q}\sigma} = \sum_{\mathbf{k}} \langle c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle / N$. N is the number of $\mathbf{k}$ points. Photoexcitation by the ultrashort optical pumping $\mathcal{V}$ can be

written as

$$\mathcal{V} = A e^{i\omega\tau} \bar{\Theta}(\tau) \sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{G}\sigma} + \text{H.c.}, \quad (3)$$

where A and ω are the strength and frequency of the optical field and $\bar{\Theta}(\tau) = \Theta(\tau) - \Theta(\tau - \tau_C)$ simulates the pulse length τ_C [$\Theta(\tau)$: Heaviside step function] and $\mathbf{G}$ is the lowest reciprocal lattice vector. The total Hamiltonian $\mathcal{H}$ then becomes $\mathcal{H} = \sum_{\mathbf{k}} [\mathcal{H}_{0\mathbf{k}} + \mathcal{H}_{U\mathbf{k}} + \mathcal{V}_{\mathbf{k}}] + \mathcal{H}_{\Omega}$. Here $\mathcal{H}_{\Omega} = \Omega \sum_{\mathbf{Q}} b_{\mathbf{Q}}^\dagger b_{\mathbf{Q}}$, where Ω is the phonon frequency. The origin of the CDW instability is the nesting property of the 1D Fermi surface by a translation of $|\mathbf{Q}| = 2k_F$, where $k_F (= \pi/2)$ is the Fermi wave vector. This mechanism also operates for the electron correlation, leading eventually to SDW. In addition, we note that the periodicity doubling in the CDW or SDW instability simply gives $|\mathbf{G}| = \pi (= 2k_F)$ in Eq. (3). Hereafter, therefore, instead of a complete $\mathbf{Q}$ summation in $\mathcal{H}_{0\mathbf{k}}$, $\mathcal{H}_{U\mathbf{k}}$, and $\mathcal{H}_{\Omega}$, we keep only $\mathbf{Q} = \pm 2\mathbf{k}_F$.

III. PHOTOINDUCED DYNAMICS

A. Calculation scheme

Dynamics can be described by the time-dependent Schrödinger equation for $|\psi_{\mathbf{k}}(\tau)\rangle$ under $\mathcal{H}_{0\mathbf{k}} + \mathcal{H}_{U\mathbf{k}} + \mathcal{H}_{\Omega} + \mathcal{V}_{\mathbf{k}}$ in the restricted Hilbert space spanned by nonadiabatic electron-phonon coupled bases,

$$\begin{aligned} |\psi_{\mathbf{k}}(\tau)\rangle = & \sum_n \sum_{n'} \alpha_{\mathbf{k}}^{nn'}(\tau) |\mathbf{k}\uparrow\rangle |\mathbf{k}\downarrow\rangle |n\rangle_{\mathbf{Q}} |n'\rangle_{-\mathbf{Q}} \\ & + \sum_n \sum_{n'} \beta_{\mathbf{k}}^{nn'}(\tau) |\mathbf{k}\uparrow\rangle |\mathbf{k} + \mathbf{Q}\downarrow\rangle |n\rangle_{\mathbf{Q}} |n'\rangle_{-\mathbf{Q}} \\ & + \sum_n \sum_{n'} \gamma_{\mathbf{k}}^{nn'}(\tau) |\mathbf{k} + \mathbf{Q}\uparrow\rangle |\mathbf{k}\downarrow\rangle |n\rangle_{\mathbf{Q}} |n'\rangle_{-\mathbf{Q}} \\ & + \sum_n \sum_{n'} \delta_{\mathbf{k}}^{nn'}(\tau) |\mathbf{k} + \mathbf{Q}\uparrow\rangle |\mathbf{k} + \mathbf{Q}\downarrow\rangle |n\rangle_{\mathbf{Q}} |n'\rangle_{-\mathbf{Q}}. \end{aligned} \quad (4)$$

$|\mathbf{k}\sigma\rangle$ and $|\mathbf{k} + \mathbf{Q}\sigma\rangle$ are the electronic states with given momenta and spins. $|n\rangle_{\mathbf{Q}}$ and $|n'\rangle_{-\mathbf{Q}}$ are the phonon states of the mode $\mathbf{Q}$ and $-\mathbf{Q}$ with the phonon numbers n and n' (i.e., $n, n' = 0, 1, 2, \dots, n_{\max}$). $\Delta_{\mathbf{Q}\sigma}$ in $\mathcal{H}_{U\mathbf{k}}$ is obtained by taking $\Delta_{\mathbf{Q}\sigma} = \sum_{\mathbf{k}} \langle \psi_{\mathbf{k}}(\tau) | c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma} | \psi_{\mathbf{k}}(\tau) \rangle / N$ and makes the dynamics of $|\psi_{\mathbf{k}}(\tau)\rangle$ couple to those of $|\psi_{\mathbf{k}'}(\tau)\rangle$. $|\psi_{\mathbf{k}}(0)\rangle$ at $\tau = 0$ should be the ground state obtained by the diagonalization of $\mathcal{H}_{0\mathbf{k}} + \mathcal{H}_{U\mathbf{k}} + \mathcal{H}_{\Omega}$. $\Delta_{\mathbf{Q}\sigma}$ in the ground state can be determined in a self-consistent way. A nonzero value of $\Delta_{\mathbf{Q}\uparrow} - \Delta_{\mathbf{Q}\downarrow}$ implies the existence of SDW. Further, it should be noted that $\Delta_{\mathbf{Q}\uparrow} + \Delta_{\mathbf{Q}\downarrow}$ cannot catch the CDW order because it always vanishes in the nonadiabatic approach. Instead, for a more general purpose, we introduce $C(\mathbf{k}, \mathbf{Q})$ and $S(\mathbf{k}, \mathbf{Q})$ in order to capture the order of CDW and SDW, respectively [i.e., $C(\mathbf{k}, \mathbf{Q}) = \sum_{\sigma} \langle \psi_{\mathbf{k}}(\tau) | c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma} (b_{\mathbf{Q}} + b_{-\mathbf{Q}}^\dagger) | \psi_{\mathbf{k}}(\tau) \rangle$,²⁶ and $S(\mathbf{k}, \mathbf{Q}) = \sum_{\sigma} \sigma \langle \psi_{\mathbf{k}}(\tau) | c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma} | \psi_{\mathbf{k}}(\tau) \rangle$].

In Fig. 1, the competition between CDW and SDW in the ground state is illustrated. In the inset of the left panel, the phase diagram on a plane of g and U is given. The phase boundary is sharply defined for SDW by the mean-field treatment, while the tail of remnant CDW is rapidly suppressed as going into the SDW region.²⁷ In the left and right panels, $\text{Re}[C(\mathbf{k}, \mathbf{Q})]$ and $\text{Re}[S(\mathbf{k}, \mathbf{Q})]$ are given with respect to

FIG. 1. (Color online) Left panel: $\text{Re}[C(\mathbf{k}, \mathbf{Q})]$ in the ground state (i.e., at $\tau = 0$) with respect to $k \in [-k_F, k_F]$ ($k_F = \pi/2$) and U . The inset is the mean-field phase diagram of the SDW in a plane of g and U with a sketch of the order strengths of CDW and SDW with respect to U at $g = 0.1$. Right panel: $\text{Re}[S(k, Q)]$ in the ground state with respect to k and U .

$k \in [-k_F, k_F]$ and U . For the calculation, we considered the number of phonons up to $n_{\max} = 10$ for both modes $\mathbf{Q}$ and $-\mathbf{Q}$ and the number of $\mathbf{k}$ points to be $N = 401$ and took material parameters $g = 0.1$ and $\Omega = 0.025$. A unit of energy is t (i.e., a natural unit of time is $1/t$). If we take $t = 0.25$ eV, most of the material parameters such as bandwidth ($W \sim 0.41$ eV for lower valence band), energy gap [$E_g \sim 175$ meV from Fig. 2(a)], or frequency of relevant phonon ($\Omega = 1.51$ THz) could approximately fall in the real parameter range of 1D CDW system $\text{K}_{0.3}\text{MoO}_3$ (i.e., $W = 0.3 - 0.4$ eV, $E_g = 110 - 120$ meV²⁸ or $\Omega = 1.5 - 2.5$ THz).²⁹ Around the phase boundary (i.e., at $U = 2.32$ or $U = 2.5$), a crossover takes place between CDW and SDW.

B. Photoinduced melting of charge-density wave

The energy band $\varepsilon_{\mathbf{k}}$ before the optical pumping is obtained by the diagonalization of $\mathcal{H}_{0\mathbf{k}} + \mathcal{H}_{U\mathbf{k}} + \mathcal{H}_{\Omega}$ and shows the CDW energy gap in Fig. 2(a). The number of nonthermal

FIG. 2. (Color online) (a) Energy eigenvalues $\varepsilon_{\mathbf{k}}$ before the optical pumping. (b) Number of phonons coupled to $|\psi_{\mathbf{k}}(\tau)\rangle$ [i.e., $n_{\mathbf{Q}}(\mathbf{k})$], with respect to τ . $U = 0$ and $\tau_C = 100$. (c) Partial number of phonons $n_{\mathbf{Q}}^\alpha$, $n_{\mathbf{Q}}^\beta$ ($= n_{\mathbf{Q}}^\gamma$), and $n_{\mathbf{Q}}^\delta$ with respect to τ . (d) Total number of phonons with respect to τ for $\tau_C = 50, 100$, and 150 . $A = 0.5$ and $\omega = 0.4$ are taken for (b)–(d). For $\omega < E_g$ (~ 0.7), dynamics are driven by the two-photon absorption.

FIG. 3. (Color online) (a)–(c) $C(\mathbf{Q})$ and $c \times n_Q^{1/2}$ ($c = 0.65$; up to constant shifts) for a few parameter sets of A and ω . $\tau_c = 100$ and $U = 0$ are adopted. Fast oscillations at $\tau \lesssim 100$ in $C(\mathbf{Q})$ are related to the optical frequency ω . (a')–(c') Frequency-time plot of $C(\mathbf{Q})$ of (a)–(c).

phonons $n_Q(\mathbf{k})$ coupled to $|\psi_k(\tau)\rangle$ is, shown in Fig. 2(b), $n_Q(\mathbf{k}) = \langle \psi_k(\tau) | [b_Q^\dagger b_Q + b_{-Q}^\dagger b_{-Q}] | \psi_k(\tau) \rangle$. Phonons initially accumulated near $|\mathbf{k}| = \pm k_F$ up to $n_Q(\mathbf{k}) \sim 14$ get removed as the optical pumping starts. This can be seen more clearly in the dynamics of the total number of those phonons [see Figs. 2(c) and 2(d)]. The total number of nonthermal phonons n_Q is given by $n_Q = \sum_{\mathbf{k}} n_Q(\mathbf{k})/N = n_Q^\alpha + n_Q^\beta + n_Q^\gamma + n_Q^\delta$, where $n_Q^\alpha = \sum_{\mathbf{k}} \sum_n \sum_{n'} (n + n') |\alpha_{\mathbf{k}}^{nn'}(\tau)|^2 / N$ and the other n_Q^β , n_Q^γ , and n_Q^δ are defined in the same way. In Figs. 2(c) and 2(d), as the optical pumping continues up to τ_c , n_Q decreases. These lattice responses are found to be highly nonadiabatic, as implied from different time dependencies among n_Q^α , n_Q^β , and n_Q^δ in Fig. 2(c).

In Fig. 3, the temporal traces of $C(\mathbf{Q})$, which is an approximate CDW order parameter given by $C(\mathbf{Q}) = |\sum_{\mathbf{k}} C(\mathbf{k}, \mathbf{Q})/N|$, are illustrated. Yusupov *et al.*¹⁹ have recently made an observation of temporal behaviors of the order parameter for TbTe₃, 2H-TaSe₂, K_{0.3}MoO₃, and DyTe₃ and also presented the phenomenological theory. They claimed a common feature in the sequence of events as CDW quenching $\rightarrow$ gap recovery $\rightarrow$ critical slowing down $\rightarrow$ coherent defect annihilation with the oscillatory time response. $C(\mathbf{Q})$ reproduces a sequence of events up to the critical slowing down (i.e., at $\tau_s \sim 100$) (~ 265 fs with $t = 0.25$ eV; τ_s is a time scale for recovery of CDW), which is explicitly demonstrated with respect to the field strength A in Fig. 4. In the figure, the time scale for a recovery of CDW increases toward $A \approx 1$ and decreases as A increases further. Its frequency-time plot in Figs. 3(a')–3(c') also shows the oscillatory (not relaxational) nature with the broadband centered around the phonon frequency (i.e., ~ 6 THz/eV $\times 0.25$ eV = 1.5 THz). Critical slowing down has been also pointed by Hellmann *et al.*²⁰ (~ 900 fs for 1T-TaS₂) and by

FIG. 4. (Color online) $C(\mathbf{Q})$ with respect to the strength A of the optical pump field at $\omega = 0.4$. For a better display of their behaviors, they are arbitrarily shifted along the vertical axis. $\tau_c = 100$ and $U = 0$ are adopted. Dashed line is a guide for the eyes, showing time scales for the CDW recovery.

Tomeljak *et al.*²² (~ 300 fs for K_{0.3}MoO₃). For K_{0.3}MoO₃, our result (~ 265 fs) moderately agrees with the experiment.

Most interestingly, temporal behaviors of $C(\mathbf{Q})$ show remarkable overlaps with those of $c \times n_Q^{1/2}$ up to a constant shift. c is found to be 0.65, independent of A and ω . In a limit of strong electron-phonon coupling, we may note a simple relation of $C(\mathbf{Q}) \propto n_Q^{1/2}$ (i.e., a constant shift gets negligible). Its physical significance could be discussed in two respects of electron-phonon cooperativity. First, $C(\mathbf{Q})$ is the coupled phonon displacement from the definition of $C(\mathbf{k}, \mathbf{Q})$. The coherent boson state $|\xi\rangle$ is mathematically defined by the eigenstate of the boson annihilation operator (i.e., $b|\xi\rangle = \xi|\xi\rangle$),³⁰ where b ($b^\dagger$) is the boson annihilation (creation) operator. $|\xi\rangle$ can be expressed as $|\xi\rangle = e^{-|\xi|^2/2} \sum_{n=0}^{\infty} \frac{\xi^n}{\sqrt{n!}} |n\rangle$. The average boson number in a coherent state is $n_{\text{boson}} = \langle b^\dagger b \rangle = |\xi|^2$ and the average boson displacement $\langle b + b^\dagger \rangle = \xi + \xi^*$. If $\text{Re}[\xi] \gg \text{Im}[\xi]$, one finds that the boson displacement is proportional to $n_{\text{boson}}^{1/2}$. This indicates that it is the coherent phonon that drives the lattice response on the sub-ps time scale from our finding of $C(\mathbf{Q}) \propto n_Q^{1/2}$. Second, $C(\mathbf{Q})$ is the order parameter of CDW. We note that the depopulation and repopulation of coherent phonons match well the melting and partial recovery of CDW. This signifies a sub-ps electron-phonon energy transfer during and after the optical excitation.²³ It is clear that turning off the optical excitation, by the energy conservation, the repopulation of coherent phonons leads to the cool down of electrons to the recovered gap (i.e., through partial recovery of CDW) and their final relaxation in vicinity of the gap. An electron-phonon energy transfer occurs in the time scale of $\tau \sim 100 - 150$ (in Fig. 3) (i.e., $\sim 260 - 400$ fs with $t = 0.25$ eV).

These noteworthy features have been recently observed for 2D CDW system²³ 1T-TaS₂ even if 1T-TaS₂ is a more complicated system with multiple CDW phases compared to a 1D CDW one. In the experiment, a decrease in CDW intensity and an accompanying increase in Bragg intensity of the host

FIG. 5. (Color online) (a) Total number of phonons n_Q with respect to τ for values of U . $A = 0.5$ and $\omega = 1$ are taken except for $U = 3$ (with $\omega = 2$). (b)–(c) Partial numbers of phonons $n_Q^\alpha, n_Q^\beta, n_Q^\gamma$, and n_Q^δ for $U = 2.32$, and $U = 3$, respectively. $A = 0.5$ and $\omega = 1$ are taken for (b), while $\omega = 2$ for (c). (d)–(f) $C(Q)$, $S(Q)$, and $c \times n_Q^{1/2}$ ($c = 0.65$; up to constant shifts) for $U = 1, 2.32$, and 3 . $A = 0.5$ and $\omega = 1$ are taken except for $U = 3$ (with $\omega = 2$). $\tau_c = 100$ is adopted.

lattice, or vice versa, during or after the photoexcitation, have been illustrated. Such highly cooperative, electronically driven atomic motions are concluded to be accompanied by a rapid sub-ps electron-phonon energy transfer (~ 350 fs). Another recent experiment on a 1D CDW system $K_{0.3}MoO_3$ has reported that the melting and partial recovery of the CDW state occurs on the sub-ps time scale and the lattice remains largely unperturbed.²² In our study, the lattice responses at ~ 6 THz/eV do not develop much beyond the sub-ps range as shown in Figs. 3(a')–3(c').

C. Nonadiabatic-adiabatic transition

In Fig. 5(a), in sharp contrast to the depopulation and repopulation of phonons at small U due to the nonadiabatic cooperativity, $U \gtrsim 2.5$ gives monotonous population of phonons (i.e., monotonous heating of lattice from hot electrons), which is the adiabatic signal of electrons and phonons. This is also perfectly in line with the disappearance of critical slowing down as demonstrated in Fig. 5(f). Partial numbers of phonons in Figs. 5(b) and 5(c) reconfirm this finding. In the adiabatic limit (e.g., $U = 3$), $|\psi_k(\tau)\rangle$ in Eq. (4) would be cast to $|\psi_k(\tau)\rangle \approx [\alpha_k(\tau)|k\uparrow\rangle|k\downarrow\rangle + \beta_k(\tau)|k\uparrow\rangle|k+Q\downarrow\rangle + \gamma_k(\tau)|k+Q\uparrow\rangle|k\downarrow\rangle + \delta_k(\tau)|k+Q\uparrow\rangle|k+Q\downarrow\rangle]|\psi_{ph}(\tau)\rangle$, where $|\psi_{ph}(\tau)\rangle$ can be written as $|\psi_{ph}(\tau)\rangle = \sum_n \sum_{n'} d_{nn'}(\tau) |n\rangle_Q |n'-Q\rangle$. In the limit, $n_Q^\alpha(k)$ would be given by $n_Q^\alpha(k) = |\alpha_k(\tau)|^2 \sum_n \sum_{n'} (n+n') |d_{nn'}(\tau)|^2$, and $n_Q^\beta(k)$, $n_Q^\gamma(k)$, and $n_Q^\delta(k)$ would be in the same way. Then, n_Q^α , n_Q^β , n_Q^γ , and n_Q^δ would follow the same time dependence $\propto \sum_n \sum_{n'} (n+n') |d_{nn'}(\tau)|^2 / N$, if the rapid electronic motion is averaged in the phononic time scale. Temporal traces of $C(Q)$, $S(Q)$, and $n_Q^{1/2}$ are displayed in Figs. 5(d)–5(f). $S(Q)$ is defined by $S(Q) = |\sum_k S(k, Q) / N|$ and captures the SDW order. At $U = 1$, SDW does not occur. At $U = 2.32$, both CDW and SDW are quite suppressed during the optical pumping, while CDW tends to more or less revive unlike SDW after the termination of the optical pumping. At $U = 3$, however, we find that the coherent phonon is not a main player of the dynamics of PIMT any more.

IV. CONCLUSION

To summarize, we have examined the dynamics of PIMT in a 1D CDW system within the nonadiabatic theory of electrons and phonons. We have found a rapid electron-phonon energy transfer in $O(100)$ fs time scale to the photoinduced melting and recovery of CDW and its critical slowing down, which can be read out by the nonadiabatic depopulation and repopulation of coherent phonons in a cooperative fashion. As SDW gets comparable to CDW by an increase of electron correlation, the nonadiabatic-adiabatic transition has been found to occur in the photoinduced responses of the lattice.

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- ²⁵ $\mathcal{H}_U$ does not necessarily have to be regarded as an approximation of the 1D Hubbard Hamiltonian. The system is assumed to be a quasi-1D one, which is weakly interacting with the environment. This in fact serves the practical situations and avoids the Mermin-Wagner theorem.
- ²⁶Even if $C(\mathbf{k}, \mathbf{Q})$ may not be generally an order parameter of CDW, it directly scales the CDW energy gap near $\mathbf{k}_F$ given a 1D nesting Fermi surface within the first-order perturbation theory incorporating $|\mathbf{k}\rangle$ and $|\mathbf{k} + \mathbf{Q}\rangle$.
- ²⁷In a recent study of large-scale density-matrix renormalization group for 1D Holstein-Hubbard model, it was argued that there is a possibility of another phase in a narrow region around the border between CDW and SDW (see L. Fehske, H. Hager, and E. Jeckelmann, *Europhys. Lett.* **84**, 57001 (2008)). However, this is beyond our scope of mean field approach.
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