Charge density patterns in spin-selectively photoexcited interacting fermions

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We describe the formation of charge-density patterns induced by spin-selective photoexcitations of interacting fermionic systems with an underlying magnetic microstructure. Using tensor-network methods for one-dimensional model systems, we find stable charge-density patterns for a wide range of parameters. We discuss a generic mechanism explaining this effect for systems that possess a periodic modulation of local observables in any dimension. Realizations in pump-probe experiments on materials and by experiments with ultracold gases on optical lattices are discussed.

Introduction. The emergence of order in nonequilibrium quantum systems has inspired a lot of experimental and theoretical research. Examples are the recent observation of so-called time-crystal phases in Floquet-driven systems [1–10], as well as the experimental finding of metastable, ordered states following a photoexcitation using ultrashort laser pulses in pump-probe setups [11–31]. In these experiments, the possible observation of transient superconducting states at elevated temperatures [22, 23] or the transformation of charge-density-wave (CDW) states has been reported [25–27, 29, 30]. This includes optically driven transitions between ordered states [32], enhancement of existent order [26], or its melting [27, 29, 30] due to the excitation. Identifying theoretical mechanisms predicting the behavior in such nonequilibrium situations is a major challenge and topic of ongoing research [33–44].

In this letter, we report on a theoretical mechanism for the emergence of CDW-like patterns in fermionic systems with periodic structures caused by a spin-polarized light pulse. Although our considerations are applicable in general, for the sake of simplicity, we consider one-dimensional systems for which powerful numerical tools exist, e.g., tensor-network approaches [45], specifically time-dependent density-matrix renormalization group (tDMRG) [46–52]. This allows us to investigate in detail the CDW pattern in real space and to make predictions for ongoing experiments in the context of correlated materials [53], as well as for ultracold gases on optical lattices [54, 55]. In our setup, two ingredients are important for the patterns to emerge: i) the photoexcitation is spin-selective; ii) the particles of the two spin directions are spatially separated before the excitation takes place. Such a situation is, e.g., enforced in the presence of a magnetic microstructure, which has been proposed in Ref. 56 in the context of a toy model for manganites [57, 58]. Alternative realizations can be found in experiments with ultracold gases on optical lattices, in which a superlattice can be created in a controlled way [59–68].

Model. We treat a variant of the one-dimensional Fermi Hubbard model [69, 70], which is subject to a pump pulse, making the hopping amplitude \( t_{\sigma,j}^{\text{hop}}(\tau) \) and the magnetic field \( B(j, \tau) \) dependent on the position \( j \) and time \( \tau \),

\[
\hat{H} = - \sum_{\sigma,j} \left( t_{\sigma,j}^{\text{hop}}(\tau) \hat{c}_{\sigma,j}^\dagger \hat{c}_{\sigma,j+1} + \text{h.c.} \right) + \sum_j \left( U \hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j} + |\Delta_j + B(j, \tau)| \hat{S}_j^z \right).
\]

Here, the annihilation (creation) operators are denoted by \( \hat{c}_{\sigma,j}^{(\dagger)} \) for electrons of spin \( \sigma \) on lattice site \( j \), the particle-density operator for electrons with spin \( \sigma \) is \( \hat{n}_{\sigma,j} = \hat{c}_{\sigma,j}^{\dagger} \hat{c}_{\sigma,j} \), and the spin operator in the direction of the quantization axis \( z \) is \( \hat{S}_j^z = \frac{1}{2} (\hat{n}_{\uparrow,j} - \hat{n}_{\downarrow,j}) \). \( U \) is the strength of the Hubbard interaction, the contribution \( \Delta_j \) to the Zeeman term is in the modeling of Ref. 56 due to Hund’s coupling and forms a time-independent magnetic microstructure caused by the ordering of polarons. Note that there can be further realizations of such microstructures so that the following considerations are not restricted to manganite systems. If not mentioned otherwise, we treat systems at quarter filling. We consider a magnetic microstructure with a unit cell of four sites, in which the sign of \( \Delta_j \) is alternating every two sites, so that in a unit cell we have the pattern \( \Delta, \Delta, -\Delta, -\Delta \). In the following, we call the two adjacent sites with the same sign of \( \Delta_j \) within a unit cell a dimer.

The photoexcitation is modeled by Peierls substitution [71–73]. In this approach, the incident light is considered as a classical field and included in the Hamiltonian via minimal coupling [74]. In the usual modeling, this leads to a position- and time-dependent complex phase in the hopping amplitudes, and to additional local magnetic fields, which are often neglected. In the following, we consider a generalization of the usual ansatz and assume that the effect of the light field can depend on the spin direction of the electrons. This is motivated by the realization of spin-selective photoexcitations, e.g., in spin-polarized ARPES experiments [75–78] and through the tunability of parameters in experiments on optical lattices [55]. Specifically, the photoexcitation leads to a tunneling amplitude

\[
t_{\sigma,j}^{\text{hop}}(\tau) = e^{-i \alpha, \tau} \frac{\sin(A(j, \tau) + A(j+1, \tau))}{2 \pi} t_{\text{hop}},
\]
where $t_{\text{hop}}$ is the hopping amplitude in equilibrium. The coefficient $\alpha_\sigma$ takes either the value one, if the light field couples with the electrons of spin direction $\sigma$, or zero, if the coupling is suppressed. The time and space-dependent vector potential is

$$A(j, \tau) = \frac{E_0 \lambda}{2 \pi c} e^{-\frac{(s_j - c \tau)^2}{\tau^2}} \sin \left[ \frac{2 \pi}{\lambda} (a_j - c \tau) \right], \quad (3)$$

with parameters specified in detail in [79]. With the values chosen, the magnetic field $B(j, \tau) \ll \Delta$ so that it will be disregarded in the following.

We treat this pump excitation via tDMRG. Specifically, we use the two-site time-evolution matrix-product operator (MPO) $W^{\text{II}}$ introduced in Ref. [80] with a time step of $\Delta t = 0.01$. The time-dependent MPO is built from a finite-state machine [81]. Due to the time dependence, a rebuilt of the MPO is necessary at every time step in order to re-evaluate the function $A(j, \tau)$. The maximal bond dimension $\chi = 500$ is sufficient to limit the discarded weight $\epsilon < 2 \cdot 10^{-7}$ in all calculations shown.

**Formation of periodic charge-density patterns through spin-selective photoexcitation.** We first discuss the time evolution of the total energy of the system and of local observables in real space, in particular the particle and spin densities $\langle \hat{N}_j \rangle(\tau)$ and $\langle \hat{S}_j^z \rangle(\tau)$, respectively. In Fig. 1, the first two rows display results at $U = 0$, and $\Delta/t_{\text{hop}} = 0$ and 8, which show the generic behavior when applying a spin-selective photoexcitation. In the top panel of Fig. 1 ($U = \Delta = 0$), the ground state exhibits Friedel-like oscillations in the particle density [82, 83] but its overall time evolution is only weakly affected by the pulse and in particular there is no enhanced charge ordering. Furthermore, we note that there is no visible energy absorption after the pulse has passed. We attribute these observations to our choice of parameters, for which the photoexcitation has approximately no site-dependence throughout the system, so that no significant change in the local observables can be expected. For finite values of $\Delta$, a gap opens, so that the Friedel-like oscillations are strongly suppressed, leading to a constant charge density in the bulk of the system. In contrast, the ground state shows a periodic pattern in the local spin densities $\langle \hat{S}_j \rangle$, which follows the magnetic microstructure. A finite amount of energy is absorbed by the system from the pulse, leading to a highly excited state. The values of the local observables are significantly modified and remain time-dependent also after the pulse has left the system. One of the main results of our work is that a periodic pattern in the charge density is induced, which follows the periodicity of the Zeeman term, and is very stable on the time scales treated here, also at finite values of $U$, as shown in the third panel of Fig. 1.

The formation of this CDW-like pattern occurs together with the weakening of the spin pattern. In the bottom panel of Fig. 1, we present the time evolution with the photoexcitation coupling to both spin directions ($\Delta/t_{\text{hop}} = 8$). Even though a significant energy absorption takes place, no stable pattern is obtained. In this case, we also observe a weakening of the spin pattern. However, this does not suffice to create the CDW-like pattern; the spin-polarized excitation is essential. Similar behavior is also obtained when changing the magnetic microstructure, e.g., by using a larger unit cell, as discussed in [79].

**Mechanism for the formation of the CDW.** Due to the spin-selective excitation, particles of only one spin-direction are moved to the neighboring dimer with opposite local magnetic field. In this way, a new state is
obtained, which is at higher energy, has a weaker spin pattern, and a density modulation. This is also seen in the analytical solution of the non-interacting case, which we derive in detail in the supplemental material for the scenario of an infinitesimally small Peierls pulse (a “kick”) and whose main features we discuss in the following: In the limit $2t_{\text{hop}}/\Delta \to 0$ the ground state of each fermion species exhibits a CDW pattern with strong localization in the occupied dimers, mimicking the Zeeman interaction in the specific spin direction. Because a unit cell consists of four sites, the dispersion has four bands, which are all separated by a gap. The instantaneous action of the spin-selective Peierls pulse on the ground state can be modeled by the time-independent perturbation $T_\phi = t_{\text{hop}} \sum_i \left( e^{i\phi} \hat{c}_{i+1} \hat{c}_{i+1}^\dagger + e^{-i\phi} \hat{c}_{i+1}^\dagger \hat{c}_{i+1} \right)$ at time $\tau = \tau_0$.

We focus on the situation at quarter filling ($\bar{N} = \ell/2$), at which the lowest of the four bands is completely filled. In this case, any phase $\phi \neq 0$ leads to a scattering of particles from the lowest band to excited states, which can occur in any of the remaining three bands, where the maximal mixing is obtained at $\phi = k\pi/2$ with integer $k$.

In the non-interacting case, the time evolution in the quenched fermionic species is dominated by oscillations with frequencies given by the energy differences of the four bands. However, due to the absence of any interaction between both spin directions, the state of the particles of the other species remains unaltered. In this way, the CDW pattern in the ground state of the unaffected species becomes visible. Without interactions, the band populations are conserved quantities. Thus, excitations cannot relax back to the lowest band, and the CDW pattern remains stable up to arbitrary times.

In Fig. 2 we further elucidate this scenario by considering the frequencies of the density oscillations on a dimer, which we obtain by first subtracting the double occupancies and then Fourier transforming the result. The non-interacting band structure at $\Delta/t_{\text{hop}} = 8$ is shown in the inset, and the results are compared to those at finite $U$. The oscillation frequencies of the particle density within a dimer and the associated averaged band gaps are marked and show excellent agreement. This analysis for the non-interacting case can now be used as a starting point to investigate the behavior in the interacting case.

**Effect of interactions.** The main effect of a finite Hubbard interaction is to induce scattering between the two fermion species and thereby to transfer energy between them, opening a decay channel for the CDW pattern of the fermion species that is not excited by the pulse. However, the Hubbard term also enforces the formation of local moments with finite $\langle \hat{S}^z \rangle$, which lower the energy in the staggered field and in this way stabilize the periodic pattern for each fermion species. Thus, localization of single fermions within the dimers is enforced by the repulsion. Therefore, we expect the description in terms of the non-interacting system to give at least a qualitative understanding of the dynamics. Indeed, at large $U$ a mean-field decoupling in the spins $\langle \hat{S}^z \rangle \propto \Delta$ shows that the Zeeman interaction is shifted according to $\Delta \to \Delta^* = \frac{1}{2} (\Delta + 4U)$ while a strong on-site potential $\propto U$ localizes the fermions and correlates the motion between the two species. Thus, in the strong coupling limit, the single-particle dynamics for the excited dimers is also dominated by the frequencies of the non-interacting system, indicating a strong localization of single particles on the dimers and hence a stabilization of the CDW pattern. From Fig. 2 we see that in the regime of intermediate interaction $U \approx \Delta$ there are more decay channels for single-particle excitations. However, there is still the dominant contribution at $\omega \approx 2$, i.e., the low energy excitation of the non-interacting single-particle description.

In order to better understand the connection between the two limits we consider the mean field decoupling for $t_{\text{hop}} \ll U$ in more detail. Within this limit, a Peierls pulse redistributes the amplitude of the local moments $\langle \hat{S}^z \rangle$ over the dimers. The mean-field Hamiltonian (see ) essentially resembles a Heisenberg $XX$ chain with a strong, staggered magnetic field $\Delta$. Thus, relaxation of the local moments after the quench is suppressed with $\Delta$. The corresponding observable can be written in terms of the local particle densities via $\langle \hat{S}^z \rangle^2 = \frac{1}{2} (\hat{n}_{\uparrow, j} - \hat{n}_{\downarrow, j})^2 \propto \hat{n}_j - 2\hat{n}_{\uparrow, j}\hat{n}_{\downarrow, j}$. Since the states obtained after the excita-
tion are to a good approximation invariant under translation by one unit cell at all instances of time, the total number of particles in one unit cell can be considered to be conserved, so that we can identify the doublon density $n_{\uparrow,j} n_{\downarrow,j}$ and its dynamics as the dominating decay channel. Subtracting the doublon density from the local density, we expect to obtain the single-particle dynamics. Indeed, in Fig. 2 we see that on the time scales reached by our simulations, the doublon-purified density follows the single-particle dynamics for any value of the interaction strength. The question arises how interaction effects during the pulse may correlate the fermion species, thereby reducing the amplitude of the CDW pattern.

In Fig. 3, we show tDMRG results for the averaged amplitude of the CDW, $\bar{P} = \int_{\tau_1}^{\tau_2} \frac{d\tau}{\tau_2 - \tau_1} \sum_j \langle \hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j} \rangle(\tau)$ (green squares) averaged from time $\tau_1 = 17.5$ to $\tau_2 = 20$ ($\tau_1 = \tau_2 - \tau_1$), and amplitude of the CDW in the center of the system $\bar{P}$ (blue triangles, see text), also averaged over time as function of the interaction strength $U/\hbar\omega$. The strength of the magnetic microstructure is $\Delta/\hbar\omega = 8$ and the Peierls pulse is spin selective.

The average doublon density $\bar{D} = \int_{\tau_1}^{\tau_2} \frac{d\tau}{\tau_2 - \tau_1} \sum_j \langle \hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j} \rangle(\tau)$ (green squares) averaged from time $\tau_1 = 17.5$ to $\tau_2 = 20$ ($\tau_1 = \tau_2 - \tau_1$), and amplitude of the CDW in the center of the system $\bar{P}$ (blue triangles, see text), also averaged over time as function of the interaction strength $U/\hbar\omega$. The strength of the magnetic microstructure is $\Delta/\hbar\omega = 8$ and the Peierls pulse is spin selective.

The absorbed energy $\Delta E = |E_0 - E_\tau/\hbar\omega = 20|$ (purple circles) at time $\tau/\hbar\omega = 20$ as function of the interaction strength $U/\hbar\omega$. Total number of doublons $\bar{D} = \int_{\tau_1}^{\tau_2} \frac{d\tau}{\tau_2 - \tau_1} \sum_j \langle \hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j} \rangle(\tau)$ (green squares) averaged from time $\tau_1 = 17.5$ to $\tau_2 = 20$ ($\tau_1 = \tau_2 - \tau_1$), and amplitude of the CDW in the center of the system $\bar{P}$ (blue triangles, see text), also averaged over time as function of the interaction strength $U/\hbar\omega$. The strength of the magnetic microstructure is $\Delta/\hbar\omega = 8$ and the Peierls pulse is spin selective.

Spin-selective excitations can be realized by polarized light in ARPES experiments [78] and the presented considerations are expected to hold even if the excitation is not completely spin polarized. In cold-gas experiments, the underlying magnetic (or ionic) pattern can be realized by a superlattice [59–68]. For the spin-selective photoexcitation one can treat a more simplified situation, in which the lattice of only one species is shaken [96–99]. This leads to similar behavior, see the Supplemental Material [79], which can be investigated using quantum-gas microscopes [100–105]. However, in materials, additional effects like the dynamics of the spin structure and phonons will eventually enter into play and destroy the pattern. As this happens on the Frank-Condon time scale, we expect a lifetime of ~ps for the pattern to persist in this context. It would be interesting to explore this prediction in materials, e.g., by time-resolved x-ray diffractions, time-dependent ARPES, or reflectivity measurements.
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SUPPLEMENTAL MATERIAL

Parameters

In this section we present the Hamilton operator of our model system,
\[
\hat{H} = - \sum_{\sigma,j} (t_{\sigma,j}^{\text{hop}}(\tau) \hat{c}_{\sigma,j} \hat{c}_{\sigma,j+1} + \text{h.c.}) + \sum_j \left( U \hat{n}_{\downarrow,j} \hat{n}_{\uparrow,j} + [\Delta_j + B(j,\tau)] \hat{S}_j^z \right),
\]
(S1)
in more detail. The annihilation (creation) operators are denoted by \( \hat{c}_{\sigma,j} \) for electrons of spin \( \sigma \) on lattice site \( j \), the particle-density operator for electrons with spin \( \sigma \) is \( \hat{n}_{\sigma,j} = \hat{c}_{\sigma,j} \hat{c}_{\sigma,j}^\dagger \), and the spin operator in the direction of the quantization axis \( z \) is \( \hat{S}_j^z = \frac{1}{2} (\hat{\sigma}_{\downarrow,j} - \hat{\sigma}_{\uparrow,j}) \). \( U \) is the strength of the Hubbard interaction and the magnetic microstructure is defined by the parameter \( \Delta_j \). In the case of a four site unit cell \( \Delta_j = (\Delta, \Delta, -\Delta, -\Delta) \). The Peierls substitution introduces a position- and time-dependent hopping amplitude \( t_{\sigma,j}^{\text{hop}}(\tau) \) and magnetic field \( B(j,\tau) \). The hopping amplitude,
\[
t_{\sigma,j}^{\text{hop}}(\tau) = e^{-i\alpha \frac{\sin}{\lambda}(A(j,\tau)+A(j+1,\tau)) t_{\text{hop}}},
\]
(S2)
includes a position- and time-dependent vector potential \( A(j,\tau) \). The time-dependent vector potential \( A(j,\tau) \) and magnetic field \( B(j,\tau) \) are specified by
\[
A(j,\tau) = \frac{E_0}{2\pi c} e^{-\frac{[aj-c\tau-\tau_0]^2}{\lambda^2}} \sin \left[ \frac{2\pi}{\lambda} (aj - c\tau) \right],
\]
(S3)
\[
B(j,\tau) = \frac{E_0 g_2 \mu_B}{c} e^{-\frac{[aj-c\tau-\tau_0]^2}{\lambda^2}} \cos \left[ \frac{2\pi}{\lambda} (aj - c\tau) \right].
\]
(S4)
The parameters are defined as follows: \( c \) denotes the speed of light; \( \lambda \) the wavelength of the incoming light, which we assume for the sake of simplicity to be monochromatic; \( e_{el} \) is the charge of the electron; \( a \) is the lattice constant. We assume the light-pulse to have a Gaussian envelope with amplitude \( E_0 \), peak at time \( \tau = \tau_0 \) and width \( s \). \( \hbar \) is Planck’s constant. We work in units, in which \( \hbar = e_{el} = c = 1 \), leading to the values displayed in table I. These values are used in the main text and in this supplementary material if not stated otherwise.

Note that with these values the magnetic field induced by the pulse typically is \( B(j,\tau) \ll \Delta \) and can therefore be safely disregarded.

CDW-pattern when varying the unit cell and the filling

As an example that a charge-density wave (CDW) also occurs for other unit cells of the magnetic microstruc-

| Parameter | Value |
|-----------|-------|
| \( \lambda \) | 500 [nm] |
| \( E_0 \) | 20 [V/m] |
| \( \tau_0 \) | 10 [\hbar] |

| Parameters | Value |
|-----------|-------|
| \( e_{el} \) | 3374.85 |
| \( \mu_B \) | 13.04 |
| \( a \) | 1 \times 10^{-6} [m] |

In table I we show in Fig. S1 the particle density for a system in which \( \Delta \) has a periodicity of 8 instead of 4, i.e., \( \Delta_j = (\Delta, \Delta, \Delta, \Delta, -\Delta, -\Delta, -\Delta, -\Delta) \). All other parameters are similar to the main results, i.e., \( \Delta/\text{hop} = 8 \), \( L = 40 \), and \( U/\text{hop} = 0 \) and 8.

FIG. S1. Time evolution of system Eq \((\text{S1})\) with \( L = 40 \) sites from tDMRG with a unit cell of 8 sites, i.e., \( \Delta = \{8, 8, 8, 8, -8, -8, -8, -8\} \) at (top) \( U = 0 \) and (bottom) \( U/\text{hop} = 8 \) induced by a spin-selective pump-pulse as discussed in the main text. First column: total energy of the system (black) and the modulation of the vector potential (blue). Second column: particle density \( \langle \hat{N}_j \rangle(\tau) \) in the bulk (sites 8-32). In the case of \( U = 8 \) the discarded weight \( \epsilon \) grows faster than in the noninteracting case and reaches \( \epsilon \approx 7 \times 10^{-6} \) at the end of the simulation.

Again, a stable pattern occurs in the particle density. In this case, the pattern is more pronounced at the edges of the magnetic domains.

A further magnetic pattern is a Néel-type single-site staggered magnetic structure. Here, we also obtain a CDW pattern as shown in Fig. S2, for non-interacting fermions as well as at finite \( U/\text{hop} \).

At half filling, all excited particles will lead to a dou-

blon, and as discussed in the main text below, this leads to a fast decay of the CDW pattern. We complement this discussion by comparing our results at \( U/\text{hop} = 4 \) and \( \Delta/\text{hop} = 8 \) obtained at quarter filling with the ones at half filling, shown in Fig. S3. As can be seen, on the time scale displayed, at both values of the filling a CDW-pattern is obtained. However, due to the exclusive formation of doublons at half filling, the CDW is less stable in this case and will decay soon.
Effect of the wavelength of the incident light

In Fig. S4 the amount of absorbed energy $\Delta E$ as a function of the wavelength $\lambda$ is shown for two interaction strengths $U/t_{\text{hop}} = 0$ and $4$. One obtains a non-trivial dependence of the absorption from the parameters of the system. However, at the wavelength of our choice (see Table I) $\lambda = 500$ nm, a significant energy absorption in both cases takes place, so that we expect the effects studied in the main text to be representative for the wavelengths, at which absorption takes place. Furthermore, Fig. 3 in the main text shows the complete $U$ dependence at $\lambda = 500$ nm. A full scan of the $\lambda$, $U$-dependence of the absorbed energy would be helpful for further studies as the $U$-dependence differs considerably for other wavelengths.

Doublon-cleaned particle densities

As discussed in the main text, the observed CDW pattern decays through doublon delocalization. Here, we consider the doublon densities, their behavior in time, and the resultant charge densities after removing the doublon part in some detail. In Fig. S5 we show the long-time behavior of the particle density, the double occupancy and the particle density after removing the double occupancy for different values of the interaction $U/t_{\text{hop}} = 0, 2, 4, 20$, and 100. The first observation is that at $U = 0$ all affected spin down particles create double occupancies as the particle density on the particle rich dimers stays constant and the CDW is only visible due to the particle poor dimers in the doublon-purified particle density. At finite interaction this is no longer the case and the amplitude of the CDW is increased. On the other hand, the creation of double occupancies is suppressed with further increasing the value of the interaction $U/t_{\text{hop}}$, a superposition of particles each located on one of the sites of a dimer is preferred instead.

FIG. S2. Time evolution of system Eq ((S1)) with $L = 40$ sites from tDMRG with a unit cell of 2 sites, i.e., $\Delta = \{8, -8\}$ at (top) $U = 0$ and (bottom) $U/t_{\text{hop}} = 8$ induced by a spin-selective pump-pulse as discussed in the main text. First column: total energy of the system (black) and the modulation of the vector potential (blue). Second column: particle density $\langle \hat{N}_j \rangle(\tau)$ in the bulk (sites 8-32).

FIG. S3. Time evolution of system (S1) with $L = 40$ sites from tDMRG with $U/t_{\text{hop}} = 4$ and $\Delta/t_{\text{hop}} = 8$ at (top) quarter filling and (bottom) half filling induced by a spin-selective pump-pulse as discussed in the text. First column: total energy of the system (black) and the modulation of the vector potential (blue). Second column: particle density $\langle \hat{N}_j \rangle(\tau)$ in the bulk (sites 8-32). Third column: local magnetizations $\langle \hat{S}_j^z \rangle(\tau)$, also only in the bulk. The color bars on the right indicate the values for $\langle \hat{N}_j \rangle(\tau)$ and $\langle \hat{S}_j^z \rangle(\tau)$, respectively. Note that the maximum of the color bar for the particle density is doubled compared to Fig. 1 to capture the results at half filling.

FIG. S4. Absorbed energy $\Delta E = |E_0 - E_{150}|$ as function of the wavelength $\lambda$. Here we used the parameters $\Delta/t_{\text{hop}} = 8$, $U/t_{\text{hop}} = 4$ with quarter filling. The Peierls phase is only acting on the spins down direction. Most of the calculations in this manuscript are performed at $\lambda \sim 500$ nm, so that a substantial amount of energy is absorbed. Note that for clarity not all computed data points are shown, furthermore a spline interpolation (over all computed data points) is used as guide for the eye.

FIG. S5. Time evolution of system (S1) with $L = 40$ sites from tDMRG with a unit cell of 2 sites, i.e., $\Delta = \{8, -8\}$ at (top) quarter filling and (bottom) half filling induced by a spin-selective pump-pulse as discussed in the main text. First column: total energy of the system (black) and the modulation of the vector potential (blue). Second column: particle density $\langle \hat{N}_j \rangle(\tau)$ in the bulk (sites 8-32). Third column: local magnetizations $\langle \hat{S}_j^z \rangle(\tau)$, also only in the bulk. The color bars on the right indicate the values for $\langle \hat{N}_j \rangle(\tau)$ and $\langle \hat{S}_j^z \rangle(\tau)$, respectively. Note that the maximum of the color bar for the particle density is doubled compared to Fig. 1 to capture the results at half filling.
Hence, subtracting the doublon contribution from the charge density is insightful in the presence of interactions, as the double occupancy will eventually spread equally over the whole system, because, as discussed in the main text, the magnetic microstructure does not constitute a barrier for its motion and it also does not decay. Therefore, only the density without the double occupancy is indicative for the long time behavior of the CDW.

Oscillations on a dimer

In order to compare the non-interacting case to the interacting case, we find it useful to consider the spectral properties of the temporal oscillations on the dimers induced by the photoexcitation, see Fig. 2 in the main text and its discussion. In particular, we consider the Fourier-transform of the difference of the particle densities of the two sites on a dimer at the center of the chain. The result is presented in Fig. S6 and shows a peak at $\omega = 2$ for all values of $U$ and several (smaller) peaks at various frequencies $\omega$ when changing $U/t_{\text{hop}}$.

As we have seen above, the doublon delocalization will reduce the amplitude of the CDW but will not destroy it completely. Therefore, we also consider the same quantity after subtraction of the doublon density in Fig. S6. Two important observations are: i) the wide peaks around $\omega = 3$ ($\omega = 5$) for $U/t_{\text{hop}} = 2$ ($U/t_{\text{hop}} = 4$) are gone. These are due to the doublon motion and correspond to the period seen in Fig. S5 (center row). ii) The peaks given by the band structure (see main text) are still present.

We can also attempt to estimate a lifetime of these oscillations, by estimating the full width at half maximum (FWHM). However, we find that the so-obtained lifetime would correspond to the order of the maximal time reached in our simulations. While this indicates that no significant decay is taking place on this time scale, the present data therefore only allows us to estimate the lifetime of the CDW pattern to be at least the duration of our simulation time, and probably much longer as we do not find any hint for a decay on this time scale.

Time averaging the doublon density and the CDW amplitude

In order to get values for the doublon density and the CDW amplitude after the pulse, which can be related to each other, we perform a time average in the window from $\tau_1 = 17.5$ to $\tau_2 = 20$, which is sufficiently late after the pulse. An example for the full dynamics of the doublon population and the time window for the average are displayed in Fig. S7 for $U/t_{\text{hop}} = 4$ and $\Delta/t_{\text{hop}} = 8$.  

FIG. S5. Local particle density (top), local double occupancy (middle), and the local, doublon-cleaned particle density (bottom) for systems with $\Delta/t_{\text{hop}} = 8$, $L = 40$, and $U/t_{\text{hop}} = 0$, 2, 4, 20, and 100. In the case of small but finite $U$ the CDW seems to decay in the local particle density plots. Considering the double occupancy plots it becomes clear that this decay is only due to the creation of the space invariant background. Hence, in the doublon-cleaned particle density the decay is absent. Note that for $U = 0$ the double occupancy is trapped on the dimer to which the spin down particles were moved and that at large $U$ nearly no double occupancies were created in the first place. In order to obtain longer times the bond dimension $\chi$ is increased by a factor of 10, i.e., $\chi = 5000$, to reach a discarded weight $\epsilon < 10^{-7}$. 

$\langle \hat{N}_j \rangle = \frac{\langle \hat{n}_i, \uparrow \hat{n}_j, \uparrow \rangle - 2 \langle \hat{n}_i, \uparrow \rangle \langle \hat{n}_j, \uparrow \rangle}{\langle \hat{n}_i, \uparrow \hat{n}_j, \uparrow \rangle}$
Alternative to a photoexcitation: periodic modulation of the lattice in cold-gases experiments

![Figures S6, S7, and S8](image)

FIG. S6. Fourier transformed of the local density (top) and the doublon-purified local density (bottom) for different values of $U/t_{\text{hop}} = 0, 2, 4, 20,$ and 100 with $\Delta/t_{\text{hop}} = 8$.

FIG. S7. Dynamic of the doublon density for $U/t_{\text{hop}} = 4$ and $\Delta/t_{\text{hop}} = 8$. The window for the time average is shown by the blue dotted line ($\tau_1 = 17.5$) and the red dashed line ($\tau_2 = 20$).

FIG. S8. Periodic modulation of the lattice of only one species of particles also leads to a CDW pattern. (left) Energy of systems with $\Delta/t_{\text{hop}} = 8$ and (top) $U/t_{\text{hop}} = 0$ and (bottom) $U/t_{\text{hop}} = 8$. (center) Particle density for these systems. (right) Spin density for the systems above. In the interacting case ($U/t_{\text{hop}} = 8$), the discarded weight $\epsilon$ grows rapidly and reaches a value of $\epsilon \sim 10^{-5}$ at the end of the simulation.

In Fig. S8 we present our results, in which the spin-selective photoexcitation is emulated by a periodic modulation of the lattice of only one fermionic species, which can be realized in experiments with ultracold quantum gases on optical lattices. As can be seen, the CDW-pattern emerges also in this setup, indicating that the details of the excitation are not crucial, as long as it is acting on only one fermion species. As in the case of a Peierls-pulse treated in the main text, at finite $U$ the absorbed energy is larger than at $U = 0$.

Spatial dependence of the Peierls pulse

In Fig. S9 the vector potential Eq. (S3) of the Peierls pulse including the spatial dependence is shown. The potential is shown at site 0 and 40, which are the two edges of the system and therefore represent the largest difference for the spatial dependence of $A(j, \tau)$. In the inset the actual difference can be spotted but it is, with the parameters from table I, very small.

“Kick”-excitation in the non-interacting case and Mean-field treatment at low fillings

We consider the analytically solvable case $U = 0$ and write the system in terms of two independent chains of
The vector potential has nearly the same value at all sites $j$ because the wavelength is much larger than the spatial extent of the chain. In the inset the small – but finite – difference between the vector potential on the two ends of the system is visible. This small difference is due to fact that the wave packet traverses through the chain only with the speed of light $c$.

spinless fermions,

$$\hat{H} = \hat{H}_\uparrow + \hat{H}_\downarrow$$

$$\hat{H}_\sigma = -\sum_j t_\text{hop} \left( c_{\sigma,j}^\dagger c_{\sigma,j+1} + \text{h.c.} \right) + \Delta_{\sigma,j} \hat{n}_{\sigma,j} \ , \quad (S5)$$

with $\Delta_{\uparrow,j} = \Delta_\uparrow/2$ and $\Delta_{\downarrow,j} = -\Delta_\downarrow/2$. We discuss the system at quarter filling, i.e. from $\langle \hat{N}_\sigma \rangle = 0$ follows $\langle \hat{N}_\sigma \rangle = \ell/4$. In order to rewrite the Hamiltonians $\hat{H}_{\uparrow,\downarrow}$ in terms of the enlarged four-site unit cell we introduce vector-valued operators

$$\hat{u}_j = \sum_{a=0}^3 \hat{u}_{j,a} \xi_a = \sum_a \hat{c}_{\uparrow,j+a} \xi_a \quad \text{(S7)}$$

$$\hat{d}_j = \sum_{a=0}^3 \hat{d}_{j,a} \xi_a = \sum_a \hat{c}_{\downarrow,j+a} \xi_a \ . \quad (S8)$$

Exemplary, we will continue the discussion treating only spin-up fermions. The kinetic term can then be rewritten as

$$\hat{H}_{\uparrow,\text{hop}} = -t_\text{hop} \sum_j \left( \hat{u}_j^\dagger \hat{u}_{j+1} + \hat{u}_j \hat{W} \hat{u}_j + \text{h.c.} \right) \ , \quad (S9)$$

with the matrices

$$J = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \ , \quad W = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \ . \quad (S10)$$

The magnetic contribution is diagonal, i.e.,

$$\hat{H}_\text{magn} = \sum_j \hat{u}_j^\dagger \Delta_j \hat{u}_j$$

with $\Delta_j \equiv \delta_{ab} \Delta_{\sigma,a}$. Since the system is at quarter filling we obtain, due to translational invariance of the coarse-grained system,

$$\langle \hat{u}_j^\dagger \hat{u}_j \rangle = \sum_a \langle \hat{n}_{\uparrow,j,a} \rangle = 1 \ . \quad (S12)$$

Now we define the Fourier modes of the components of the vector-valued operators via

$$\hat{u}_{j,a} = \frac{2}{\sqrt{L}} \sum_q \hat{u}_{q,a} e^{i q r_j}$$

with the sum over the reduced Brillouin zone $q \in \{-\pi/4, \ldots, \pi/4\}$ and $r_{j,a} = r_j + r_a = 4 \cdot j + a$. Note that the reduced Brillouin zone follows from the fact that the Fourier modes in the sublattices are connected by symmetry, i.e., $\hat{u}_{q,a+1} = \hat{u}_{q,a} e^{i \pi/2}$. Thus, we can rewrite the kinetic terms according to

$$\sum_j \hat{u}_j^\dagger \hat{u}_{j+1} + \hat{u}_j^{\dagger} \hat{W} \hat{u}_j$$

$$\sum_j \hat{u}_j^{\dagger} W \hat{u}_j$$

$$\sum_{q,a,b} \hat{u}_{q,a}^{\dagger} (W_{a,b} e^{i q r_j} + W_{b,a} e^{-i q r_j}) \hat{u}_{q,b}$$

$$\Rightarrow \hat{H}_{\uparrow,\text{hop}} = -t_\text{hop} \sum_q \hat{u}_{q,a}^{\dagger} (J(q) \hat{u}_{q,a})$$

$$\quad = \sum_q \sum_{a,b} \hat{u}_{q,a}^{\dagger} (W_{a,b} e^{i q r_j} + W_{b,a} e^{-i q r_j}) \hat{u}_{q,b}$$

$$\Rightarrow \hat{H}_{\uparrow,\text{hop}} = -t_\text{hop} \sum_q \hat{u}_{q,a}^{\dagger} J(q) \hat{u}_{q,a}$$

$$\quad = \sum_q \sum_{a,b} \hat{u}_{q,a}^{\dagger} (W_{a,b} e^{i q r_j} + W_{b,a} e^{-i q r_j}) \hat{u}_{q,b}$$

In summary we obtain

$$\hat{H}_\uparrow = \hat{H}_{\uparrow,\text{hop}} + \hat{H}_\text{magn} = -t_\text{hop} \sum_q \hat{u}_{q,a}^{\dagger} \Gamma_{\uparrow}(q) \hat{u}_{q,a}$$

with

$$\Gamma_{\uparrow}(q) = \frac{J(q)}{4} + \Delta_{\uparrow} / t_\text{hop}$$

$$= \begin{pmatrix} \Delta_{\uparrow,1} / t_\text{hop} & \cos(q) & 0 & \cos(q) \\ \cos(q) & \Delta_{\uparrow,1} / t_\text{hop} & \cos(q) & 0 \\ 0 & \cos(q) & \Delta_{\uparrow,2} / t_\text{hop} & \cos(q) \\ \cos(q) & 0 & \cos(q) & \Delta_{\uparrow,2} / t_\text{hop} \end{pmatrix} \ . \quad (S19)$$

Finding the eigenmodes $\hat{\psi}_{\alpha,\uparrow,q}$ of this single particle Hamiltonian permits to construct the ground state by populating eigenmodes until $\langle \hat{N}_\sigma \rangle = \ell/4$. 
Let us discuss the limits $\Delta/2t_{\text{hop}} \to 0$ (vanishing magnetic microstructure) and $2t_{\text{hop}}/\Delta \to 0$ (atomic limit) both from now on in both spin directions. The first case yields the formation of four dispersive bands which, by sublattice symmetry, resemble the usual cosine dispersion of spinless fermions. Since we are at quarter filling the ground state is a sea of non-interacting fermions created by filling up the lowest band (until $q = \pm \pi/4$). The corresponding eigenmodes of $\Sigma(q)$ are completely delocalized over the sublattice sites. Since the dispersion is gapless, impurities, e.g., boundaries, induce (weak) Friedel oscillations in the ground state particle density [83].

On the other hand, in the atomic limit $2t_{\text{hop}}/\Delta \to 0$ the eigenmodes $\tilde{g}_{a,\sigma,q}$ are strongly localized at the sublattice sites. To be more precise we consider degenerate perturbation theory by decomposing the sublattice hopping matrix for each fourier mode $q$ according to

$$
\Sigma_{\sigma}(q) = \begin{pmatrix} A_{\sigma}(q,\varepsilon) & 0 \\ 0 & B_{\sigma}(q,\varepsilon) \end{pmatrix} + \varepsilon \cos(q) \begin{pmatrix} 0 \\ \sigma \end{pmatrix}
$$

$$
\equiv \Delta \left( \Sigma_{\sigma}^{(0)}(q,\varepsilon) + \varepsilon \Sigma(q) \right), \quad \varepsilon = \frac{2t_{\text{hop}}}{\Delta}
$$

where we treat $\Sigma(q)$ as the perturbation and $\sigma$ is the first Pauli matrix. Diagonalization of the unperturbed problem $\Sigma_{\sigma}^{(0)}(q,\varepsilon)$ (yet still depending on $\varepsilon$) yields eigenvalues $\gamma_{\sigma}^{(0)}(q,\varepsilon)$ and eigenvectors $(\tilde{u}_0, \ldots, \tilde{u}_3)$ of the form

$$
\gamma_{\sigma}^{(0)}(q,\varepsilon) = \text{diag}(\pm 1, \mp 1, 1, -1)
$$

$$
\tilde{U} = (\tilde{u}_0 \ldots \tilde{u}_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}
$$

with $\text{sgn}(\sigma) = \pm 1$ for $\sigma = \uparrow, \downarrow$. The spin dependent, unperturbed ground states are obtained by filling the lowest band and are localized within adjacent halves of the unit cell,

$$
\tilde{g}_{0,\uparrow}^{(0)} = \tilde{u}_0, \quad \tilde{g}_{0,\downarrow}^{(0)} = \tilde{u}_2.
$$

First order corrections to the unperturbed ground state are now obtained by standard perturbation theory evaluating the matrix elements $\langle \tilde{g}_{a,\sigma}^{(0)} | V(q) | \tilde{g}_{a,\sigma}^{(0)} \rangle$ and are given via

$$
\tilde{g}_{a,\sigma,q}^{(1)} = \tilde{g}_{a,\sigma,q}^{(0)} - \varepsilon \sigma \gamma_{\sigma}^{(0)}(q,\varepsilon) \tilde{g}_{a,\sigma,q}^{(0)}
$$

with the states $\tilde{g}_{a,\uparrow}^{(0)} = \tilde{u}_2$ and $\tilde{g}_{a,\downarrow}^{(0)} = \tilde{u}_0$. Note that $V(q)$ does not break parity in the sublattice while $\Sigma_{\sigma}^{(0)}(q,\varepsilon)$ is invariant under parity transformation only within the dimers. As a consequence both the perturbed and exact eigenstates decompose into 2-dimensional representations of the parity in the sublattice.

To first order in $2t_{\text{hop}}/\Delta$ the ground state exhibits a charge ordering in the dimers

$$
\langle \tilde{n}_{a,\downarrow} \rangle = \frac{4}{L} \sum_{q,a} e^{i pr \cdot a} \langle \tilde{d}_{a,\downarrow} \rangle = \left( \begin{array}{cc} 1 & \varepsilon \cos(\varphi_{1,a}) \\ \varepsilon \cos(\varphi_{1,a}) & 1 \end{array} \right)
$$

$$
\langle \tilde{n}_{a,\uparrow} \rangle = \frac{4}{L} \sum_{q,a} e^{i pr \cdot a} \langle \tilde{d}_{a,\uparrow} \rangle = \left( \begin{array}{cc} \varepsilon \cos(\varphi_{1,a}) & 1 \\ 1 & \varepsilon \cos(\varphi_{1,a}) \end{array} \right)
$$

with some phase $\varphi_{1,a}$.

Now we compute the time evolution after applying a light pulse, which we assume to last infinitesimally short (a “kick”). In this scenario, we apply a perturbation $\hat{T}_\phi$ to the ground state in the limit $2t_{\text{hop}}/\Delta \ll 1$

$$
\hat{T}_\phi = t_{\text{hop}} \sum_i e^{i \phi_i} \hat{d}_{i+1}^\dagger \hat{d}_i + e^{-i \phi_i} \hat{d}_i \hat{d}_{i+1}
$$

$$
= 2t_{\text{hop}} \sum_q \hat{d}_q \hat{d}_q^\dagger \hat{d}_{q+\phi} + \hat{d}_{q+\phi} \hat{d}_q^\dagger
$$

yielding

$$
|\psi_\phi \rangle = \hat{T}_\phi \prod_q \hat{\psi}_{q+\phi}^\dagger |0\rangle = 2t_{\text{hop}} \prod_q \hat{d}_q \hat{d}_{q+\phi} |0\rangle
$$

$$
= 2t_{\text{hop}} \prod_q \cos(\phi) \hat{d}_q \hat{d}_q^\dagger (\hat{g}_0^{(1)} + \hat{g}_0^{(1)} + \mathcal{O}(\epsilon^2)) |0\rangle.
$$

Using the connection $\hat{d}_{q,a+1} = \hat{d}_{q,a} e^{i \phi/2}$ we find that depending on $q+\phi$ all eigenmodes $\hat{\psi}_{q+\phi}^\dagger$ can be populated. For instance, when shifting the ground state by $\pi/2$ one finds

$$
e^{i \pi/2} \hat{d}_q^\dagger \hat{g}_0^{(1)} = (1 - x) \hat{d}_q^\dagger \left( \hat{g}_0^{(1)} + \hat{g}_0^{(1)} \right) + (1 + x) \hat{d}_q^\dagger \left( \hat{g}_0^{(1)} - \hat{g}_0^{(1)} \right), \quad \text{with} \quad x = \varepsilon \frac{\cos(q)}{2}.
$$

Note that $|q| < \pi/4$ and therefore a complex phase is required to mix the different sectors of parity within the
dimers. If, for instance, $\phi = 0$ then only states within the same parity sector can be populated, i.e., from the ground state these are $\hat{a}^{(1)\uparrow,q}_0 \hat{a}^{(1)\downarrow,q}$. The corresponding time evolution is that of a two level system with frequency $\omega = \Delta$. However, in the case of the Peierls pulse Eq. (S3) transitions between all bands can be observed (see Figs. S6 and S6).

Mean-field decoupling at low fillings

Finally we briefly discuss the limit $t_{\text{hop}}/U \ll 1$ in which we can rewrite the Hubbard interaction in terms of local spin operators

$$\hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j} = -\frac{1}{2} \left( \hat{n}_{\uparrow,j} - \hat{n}_{\downarrow,j} \right)^2 - (\hat{n}_{\uparrow,j} + \hat{n}_{\downarrow,j})$$

$$= \frac{1}{2} \hat{n}_j - 2 \left( \hat{s}_j^z \right)^2 \quad (S30)$$

$$\Rightarrow \hat{H} = -t_{\text{hop}} \sum_{\sigma,j} \left( \hat{c}_{\sigma,j}^\dagger \hat{c}_{\sigma,j+1} + \text{h.c.} \right) + \cdots$$

$$+ \sum_i \Delta_j \hat{s}_j^z - 2 \left( \hat{s}_j^z \right)^2 + \frac{1}{2} \hat{n}_j. \quad (S32)$$

We note that for large $U$ the formation of local moments $\left( \hat{s}_j^z \right)^2$ with strong polarization in the expectation values of $\hat{s}_j^z$ minimizing the Zeeman coupling is beneficial. Therefore we can perform a mean-field decoupling around the saturated local expectation values $\hat{s}_j^z = \langle \hat{s}_j^z \rangle + \delta \hat{s}_j^z$ and neglect contributions $\propto \delta^2$, leading to

$$\hat{H}_{\text{int}} \approx \sum_{j} \delta \hat{s}_j^z \left( \frac{\Delta_j}{2} - 4U \langle \hat{s}_j^z \rangle \right) + \cdots$$

$$+ \langle \hat{s}_j^z \rangle \left( \frac{\Delta_j}{2} - 2U \langle \hat{s}_j^z \rangle \right) + U \hat{n}_j. \quad (S33)$$

Inserting for the local expectation values the SDW pattern in the unit cell $\langle \hat{s}_j^z \rangle = m (-1/2, -1/2, 1/2, 1/2)$, where $m$ is to be determined self consistently, we see that the second summand is only a constant. Defining the renormalized Zeeman coupling $\tilde{\Delta} = \frac{1}{2}(\Delta + 4U)$ and $\tilde{\Delta}_{\sigma,j} = \Delta_{\sigma,j} \text{sgn}(\sigma)$ we obtain

$$\hat{H}_{\text{int}} = \sum_{\sigma,j} \hat{n}_{\sigma,j} \left( U + \delta \tilde{\Delta}_{\sigma,j} \right) + \text{const} \quad (S34)$$

and thereby (up to an on-site potential $\propto U$) we rewrote the interaction in terms of an effective Zeeman coupling for which we can use the noninteracting solution above.