Magnetism of one-dimensional Wigner lattices and its impact on charge order

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The magnetic phase diagram of the quarter-filled generalized Wigner lattice with nearest- and next-nearest-neighbor hopping $t_1$ and $t_2$ is explored. We find a region at negative $t_2$ with fully saturated ferromagnetic ground states that we attribute to kinetic exchange. Such interaction disfavors antiferromagnetism at $t_2 < 0$ and stems from virtual excitations across the charge gap of the Wigner lattice, which is much smaller than the Mott-Hubbard gap $\propto U$. Remarkably, we find a strong dependence of the charge structure factor on magnetism even in the limit $U \rightarrow \infty$, in contrast to the expectation that charge ordering in the Wigner lattice regime should be well described by spinless fermions. Our results, obtained using the density-matrix renormalization group and exact diagonalization, can be transparently explained by means of an effective low-energy Hamiltonian.

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I. INTRODUCTION

In a Wigner lattice (WL), long-range Coulomb repulsion dominates over the kinetic energy of electrons and leads to strong and well-defined charge order.\textsuperscript{12} Originally introduced for the electron gas with a homogeneous neutralizing background, this concept was generalized to electrons on a lattice by Hubbard.\textsuperscript{2} Evidence for quasi-one-dimensional (1D) Wigner lattices has been found in organic\textsuperscript{3,4,5,6} and anorganic\textsuperscript{7,8,9,10} chain compounds, nanowires\textsuperscript{11} and in carbon nanotubes.\textsuperscript{12} Low-dimensional WLs are favored by reduced screening.\textsuperscript{2} Moreover, strong correlations induced by large local Hubbard interaction $U$ suppress screening further and protect the long-range nature of the Coulomb repulsion.\textsuperscript{6} It is, however, not straightforward to distinguish a true WL from a quantum-mechanical charge-density wave (CDW) simply on the basis of the periodicity of the charge modulation. In fact, it turns out that the modulation period of the WL coincides with that of the 4$F$ CDW.\textsuperscript{2,4,14,15,16} This may be surprising, as the microscopic origin of the charge order in the two cases is fundamentally different.\textsuperscript{2}

(i) The mechanism for the WL is based solely on the classical Coulomb repulsion and is dependent only on the charge of electrons and not on their fermionic nature. The periodicity follows simply from the configuration of charges with minimal energy.\textsuperscript{2} (ii) Instead, the quantum mechanical CDW depends on the Fermi surface topology and the instability and modulation reflects the Fermi momentum $k_F$.

If we allow for nearest-neighbor (NN) and next-nearest-neighbor (NNN) hoppings $t_1$ and $t_2$, we arrive at an even more interesting model which, depending on the relative size and sign of $t_1$ and $t_2$, may have an electron dispersion with two minima instead of one.\textsuperscript{17,18} Actually, it has been proposed that the edge-sharing CuO chain compounds are described by such models with $|t_2| > |t_1|$. It is then immediately obvious that in the case of a four-Fermi-point topology the periodicities of WL and CDW no longer coincide. We note that the experimentally observed charge modulations in the edge-sharing compounds Na$_{1+x}$CuO$_2$\textsuperscript{19,20,21} are strong and their periodicity consistent only with that of the WL. Another possible type of instability in the presence of strong correlations, namely, the 2$F$ Peierls and spin-Peierls modulations\textsuperscript{16,22} which requires a distortion of the lattice, appears to be ruled out in these systems. Doped edge-sharing chains are also building blocks of the Ca$_{2+x}$Y$_{2-x}$Cu$_5$O$_{10}$\textsuperscript{9,23} and the Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$\textsuperscript{7,8,24} systems, and pronounced charge order has been observed in these compounds as well.

Here we shall investigate the intrinsic mechanisms for the magnetism of generalized Wigner lattices. It is well known that NNN hopping $t_2$ has nontrivial consequences for magnetism in the 1D Hubbard model at general filling and may lead to ferromagnetic (FM) states in certain cases.\textsuperscript{25,26,27,28,29} It should be kept in mind that, according to the Lieb-Mattis theorem,\textsuperscript{30} ferromagnetism is excluded at any filling in the 1D Hubbard model with NN hopping (i.e., $t_2 = 0$). For the 1D Hubbard model with NN and NNN hopping, Pieri \textit{et al.}\textsuperscript{27} and Daul and Noack\textsuperscript{28} found that ferromagnetic ground states appeared above a critical $U$ in those regions of the $t_1$-$t_2$ plane where four Fermi points exist. These results were obtained in the metallic regime where the relevance of Fermi surface topology is suggestive; however, the implications for the localized electrons of a Wigner crystal are unclear.

The magnetism of generalized WLs is typically discussed in terms of effective Heisenberg models where the position of the spins is dictated by the charge order pattern of the WL.\textsuperscript{10,11,31} The prevailing superexchange interactions are antiferromagnetic. However, there are also ferromagnetic couplings in edge-sharing...
chains due to the Hund interaction at the oxygen ligands that may be larger than the AF interactions and render, e.g., the nearest-neighbor interaction $J_1$ ferromagnetic\textsuperscript{10,33,34}. These features lead to frustration, and the resulting helical spin states have been observed in the spin-1/2 edge-sharing chain compounds LiCu$_2$O$_2$\textsuperscript{35} and NaCu$_2$O$_2$\textsuperscript{36-38}.

In this paper, we show that, for a Wigner crystal at quarter-filling, there is another intrinsic mechanism that may lead to ferromagnetism. By means of a density-matrix renormalization group (DMRG) study of the $t_1-t_2$ Hubbard-Wigner model, which includes local Hubbard $U$ and long-range Coulomb interactions $V_I = V/l$, we show that there is a regime of fully polarized FM states at negative $t_2$. Subsequently, we derive an effective magnetic Hamiltonian for the Wigner-lattice regime, i.e., $|t_1|, |t_2| \ll V < U$, and show that the emergence of ferromagnetism can be explained by an effective kinetic exchange mechanism mediated by NNN hopping $t_2$. The associated magnetic exchange constant $\propto t_2^2l_2^2/e_0^2$ depends on the sign of $t_2$ and therefore kinetic exchange is found to favor ferromagnetism for negative $t_2$ and antiferromagnetism for positive $t_2$. Kinetic exchange involves excitations across the charge gap $e_0$ of the WL but not across the usually much larger Mott-Hubbard gap $\sim U$, as is the case for AF superexchange or for many realizations of FM three-particle ring exchange.\textsuperscript{39} The charge gap $e_0$ of the generalized WL depends sensitively on the commensurability with the underlying crystalline lattice. At quarter-filling this gap is particularly large $e_0 \sim V/2$.

If the charge gap $e_0 \sim V/2$ of the WL is much larger than the hopping amplitudes $t_1$ and $t_2$ and any expected magnetic couplings, a separation of charge and magnetic energy scales appears straightforward. Hence, charge ordering in a WL is usually discussed in terms of spinless fermions. Magnetism, e.g., antiferromagnetic (AF) superexchange or ferromagnetic (FM) Hund’s rule and three-site ring exchange is then treated as a perturbation given a particular charge-ordering pattern. One would, however, not expect the magnetic order to have a strong impact on the underlying charge order, because the magnetic energy scale is so much smaller than the dominant Coulomb repulsion for all these processes.\textsuperscript{41} The motivation for this work was the initial observation that the charge structure of the WL, measured by the charge structure factor $N(q)$ at $q = \pi$, is strongly affected by electron spin, in disagreement with the calculation for spinless fermions. Yet there is a region in the $t_1-t_2$ phase diagram at negative $t_2$ where $N(\pi)$ is the same for spinless fermions and for fermions with spin, and, moreover, $N(\pi)$ does not depend on $t_2$ in that parameter range. The obvious conjecture is that the ground state should be fully spin-polarized in this regime.

We show here that, due to the kinetic exchange mechanism, these FM ground states emerge and that the kinetic exchange processes have a surprisingly strong impact on the charge ordering in spite of the classical origin of the WL. Indeed, the AF state at $t_2 > 0$ has dramatically weaker charge order than the ferromagnetic or spinless states. While the charge order is reduced $\propto t_2$ for positive $t_2$, it does not depend on $t_2$ in the FM regime $t_2^2 > t_2 > |t_2|$ with negative $t_2$. Remarkably, for negative $t_2$ values below $t_2^2$, AF reappears, yet the charge order then increases with increasing modulus $|t_2|$. The boundaries of the FM phase follow from the effective spin Hamiltonian as $t_2^2 \sim -3t_2^2/U$ and $t_2^2 \sim -(U/e_0^2)t_2^2$, and match the magnetic phase boundaries found using the DMRG. This peculiar behavior is due to a purely quantum effect involving destructive interference of kinetic exchange processes in the FM state due to the Pauli principle and constructive interference for the AF case.

The paper is organized as follows: After introducing the Hubbard-Wigner Hamiltonian in Sec. \textsuperscript{II} we present results for the charge structure factor for spinless fermions interacting via long-range Coulomb interaction in Sec. \textsuperscript{III}. We shall see that the results for spinless fermions coincide with results for electrons with spin in some region of the $t_1$-$t_2$ phase diagram, while they are substantially different in other parts of the phase diagram. We derive an effective Heisenberg Hamiltonian in Sec. \textsuperscript{IV} and show that the magnetic phase diagram, i.e., the appearance of the fully saturated FM phase and its phase boundaries, can be naturally explained. Next we show that the peculiarities found numerically for the the charge structure factor find a straightforward analytical description in the framework of the effective Hamiltonian. Finally, we discuss and summarize our results in Sec. \textsuperscript{V}.

[FIG. 1: (Color online) Schematic depiction of relevant $t_1^2t_2^2/e_0^2$ kinetic exchange processes. We start from perfect charge order (a and e), where circles denote empty sites ($\text{Cu}^{3+}$ atoms in Na$_{1+x}$Cu$_2$O$_2$), and arrows denote occupied sites (Cu$^{2+}$). NN hopping $t_1$ induces excitations (a→b and e→f) with two domain walls (dashed lines) and cost $e_0$. Two different $t_2$ processes, one with (f→g) and one without (b→c) electron exchange, become possible. For FM spins (triplet channel) or spinless fermions, however, these two processes (a→d) and (e→h) cancel exactly because of the relative Fermi sign in the next-nearest-neighbor hopping process.]
II. HUBBARD-WIGNER MODEL

The Hubbard-Wigner Hamiltonian investigated in this paper is motivated by the one-dimensional edge-sharing CuO-chains. Edge-sharing chains are formed by CuO₃ squares just as in the CuO planes of the high-
Tc compounds, but these units are differently linked. The edge-sharing arrangement leads to small nearest-neighbor hopping matrix element t₁ due to the almost 90° Cu-O-Cu coordination, and some contribution to t₂ stems from direct Cu d-d overlap. Moreover, the structure leads to a comparatively large matrix element t₂ between second neighbor Cu ions stemming from a Cu-O-O-Cu path. Thus edge-sharing chains, in contrast to the 180° bonded high-Tc cuprates, fulfill the fundamental criterion for a WL, namely that the kinetic energy is small compared to the nearest-neighbor Coulomb interaction, in an optimal way. While the Coulomb repulsion is screened by a static dielectric constant in these insulators, the one over distance decay of the interaction is preserved and must be taken into account. Truncation of the interaction may have serious consequences for the charge-order pattern of generalized WLs as well as for their charge excitations.

The relevant states of Cu that need to be included in a low-energy model are: Cu²⁺ or, more precisely, the Cu d⁰-ligand hole singlet state, Cu²⁺ with spin-1/2, and Cu¹⁺, corresponding to the filled d shell. These states can be expressed in the frame of a single-orbital Hubbard model with 0,1 or 2 electrons per site. Thus we consider the Hubbard-Wigner Hamiltonian, where the extension Wigner indicates that the long-range Coulomb interaction is included. This model has the form:

\[ H = -t_1 \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) - t_2 \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+2,\sigma} + \text{h.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{l=1}^{L/2} V_l \sum_i (n_i - \bar{n})(n_{i+l} - \bar{n}) , \]

where the operators \( c_{i,\sigma}^\dagger \) (\( c_{i,\sigma} \)) create (destroy) electrons with spin \( \sigma \) at lattice site \( i \) with \( i = 1 \ldots L \). The local density is given by \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \), \( n_i = n_{i,\uparrow} + n_{i,\downarrow} \), and the average density is \( \bar{n} = N_e/L \) for \( N_e \) electrons. The kinetic energy term includes NN hopping \( t_1 \) and NNN hopping \( t_2 \), which are both typically much smaller than either the on-site Coulomb repulsion \( U \) or the NN-Coulomb interaction \( V \) that parametrizes the long-range Coulomb interaction \( V_l = V/l \). In the case of finite rings of length \( L \), we truncate the 1/1 behavior at \( L/2 \), which is equivalent to replacing \( V/l \) by \( \max(V/l, V/(L-l)) \) for \( 0 < l < L \). We have verified that small modifications to the 1/1 behavior do not affect our results. In fact, truly long-range Coulomb repulsion is not crucial for the results presented here: At quarter filling, both the FM kinetic exchange and the weakened charge order can also be seen for on-site \( U \) and NN Coulomb repulsion \( V_1 \) only.

In the following, we consider the model with long-range Coulomb interaction and use the NN Coulomb repulsion \( V_1 = V \) as unit of energy. Without loss of generality, \( t_1 \) is chosen to be positive.

The Hamiltonian in Eq.(1) contains two ingredients that have been shown to favor FM correlations in Hubbard-like models: Strong on-site and longer-range Coulomb repulsion\(^{25} \) and, perhaps more importantly, NNN hopping\(^{26,27,28,29} \). In this paper we address the most transparent instance of the WL, namely quarter filling \( \bar{n} = 0.5 \) for Hamiltonian (1). We explore the magnetic properties within the WL regime, i.e., \( t_1, t_2 \ll V \ll U \), which have not been explored before, and find FM ground states in a region of the \( t_1-t_2 \) phase diagram with negative \( t_2 \). Quite unexpectedly, we also find a strong influence of magnetism on WL charge order. For comparison, we will first discuss the charge ordering for spinless fermions at half filling, corresponding to the fully spin-polarized case with \( \bar{n} = 0.5 \). At small \( t_1 \) and \( t_2 \), the alternating charge order is very rigid and its lowest charge excitations are domain walls (DWs) with fractional charge\(^{30,31} \). DWs can be induced in a perfectly ordered state via NN hopping \( t_1 \), as schematically illustrated in Fig.1. Their creation costs energy \( c_0 \approx V/2 \) in the case of long-range Coulomb interaction, and once created they can move easily through the lattice via \( t_1 \) hopping processes. Their fractional charge \( \pm 1/2 \) is responsible for the distinctive WL features in the optical conductivity and in photoemission\(^{32,44,48} \).

We investigate this model with exact diagonalization (ED) for spinless Fermions and chains of up to \( L = 28 \) sites. We use the Lanczos algorithm with a numerical accuracy of \( \approx 10^{-6} \) and check its validity by use of full diagonalization for up to 18 sites. These ED calculations were done for both the ground state \( (T = 0) \) and for small but finite temperatures \( (T = 10^{-4} - 10^{-3}) \), leading to practically identical results at small \( t_1 \) and \( t_2 \) because there is a finite charge gap \( c_0 \approx V/2 \), which blocks changes at temperatures with an energy scale smaller than this. For electrons with spin, we use the DMRG with chains of \( L = 24, 32, 40 \), and find results consistent with the ED for spinless fermions. In the DMRG, we keep 200 to 1200 states at each step, perform up to 10 finite-size sweeps and the neglected weight is \( \lesssim 10^{-5} \). For parameters with a FM ground state, the energy obtained with the DMRG agrees with the ED result.

III. CHARGE ORDER

Increasing the NN hopping \( t_1 \) gradually reduces the charge ordering\(^{42} \) until, at \( t_1 \approx 0.2V \), the charge gap vanishes\(^{42} \). This is reflected in the charge structure factor

\[ N(q) = \langle \rho_{-q} \rho_{q} \rangle, \text{ with } \rho_{q} = 1/N_e \sum_r \exp(-qr)n_r , \]

which, for perfect charge alternation, is peaked at \( q = \pi \) with \( N(\pi) = 1 \). As can be seen in Fig.2 the results...
with $\Delta = \epsilon_0$ (FM) and $\Delta = \epsilon_0 - 2t_2$ (AF), respectively.

for spinless fermions, obtained using Lanczos diagonalization, show that $N(\pi)$ is strongly reduced even before the gap vanishes, giving a weaker charge density wave. We find that, for spinless fermions, the melting of WL charge order with $t_1$ does not depend on $t_2$. The behavior of $N(\pi)$ can be described analytically because only few DWs are present at small $t_1$. To leading order, virtual DW excitations contribute

$$E_c \sim -N_c 2t_1^2/\epsilon_0$$

(3)
to the ground state energy. With $N_c = L/2$, we obtain

$$N(\pi) \simeq \frac{1}{1 + (4t_1/\Delta)^2},$$

(4)given the charge gap $\Delta = \epsilon_0 \sim V/2$. This expression is indicated by the dashed line in Fig. 2 and agrees with the numerical data.

In marked contrast to the gradual change that occurs with $t_1$, NNN hopping $t_2$ is frustrated for spinless fermions until $N(\pi)$ drops sharply at a level-crossing transition at $t_2^* \sim 0.15V$, see also Fig. 3. At the level crossing, the ground state changes fundamentally: $N(\pi)$ develops a broad continuum with a maximum between $\pi$ and $\pi/2$ (moving to $\pi/2$ at large $t_2$) rather than at $\pi$. Just as $t_2$ does not influence the charge order, weakening with $t_1$, the level-crossing transition driven by $t_2$ is hardly affected by $t_1$. This can be seen by comparing the $t_1 = 0.02V$ and $t_1 = 0.07V$ curves for spinless fermions in Fig. 3. Consequently, the WL phase is bounded by vertical and horizontal lines in the $t_1$–$t_2$ plane, see Fig. 3.

While the transition between the two CDW phases with $q = \pi$ and $q \neq \pi$ depends on both $t_1$ and $t_2$, it is remarkable that the WL is never affected by the combination of hopping processes. We would actually expect some cooperative effects between $t_1$ and $t_2$ because NNN hopping is no longer frustrated in the presence of $t_1$, see Fig. 3. Due to the DW delocalization, (b↔c), two-DW states should gain energy with $t_2$, and nonzero $t_2$ should thus help destabilize the charge ordering. The solution is found in the process shown in (f→g): For spinless fermions (all arrows in Fig. 1 pointing up), process (a↔e) and process (f→g) are equivalent. Since two electrons swap places in the second case, the resulting Fermi sign leads to destructive interference and the lowest-order processes associated both with $t_1$ and with $t_2$ cancel out.

After this discussion of the spinless model, we now turn to electrons with spin. Due to the dominance of the Coulomb repulsion and the classical nature of WL ordering, we might not expect charge ordering to be affected significantly by the spin degree of freedom as long as $U \gg V$. However, the behavior of $N(\pi)$ obtained using the DMRG for electrons with spin indicates that there

FIG. 3: (Color online) The charge structure factor $N(\pi)$ versus $t_2$. Note that it does depend on the sign of $t_2$ for fermions with spin and does not for spinless fermions. The results for spinless fermions were calculated using exact diagonalization ($L = 18$), and the results for electrons with spin using the DMRG ($t_1 = 0.02V$, $U = 4V$, $L = 24$ and $t_1 = 0.07V$, $U = 100V$, $L = 32$).

FIG. 4: Phase diagram for spinless fermions determined from the charge structure factor $N(\pi)$, see Eq. (2). WL (dark gray): strongly charge-ordered WL with $N(\pi) > 0.7$, $\pi$-CDW (light gray): CDW with periodicity $\pi$, but $N(\pi) < 0.7$. (This choice corresponds approximately to the inflection point of $N(\pi)$ as a function of $t_1$.) In the white area, $N(\pi)$ has its maximum at $\pi/2 \leq q < \pi$, at $\pi/2$ for large $t_2$. In the exact diagonalization, we take $N_e = 8$ fermions on $L = 16$ sites.
is a surprisingly strong influence even for $U = 100V$. In contrast to spinless fermions, where $t_2$ does not affect the behavior of $N(\pi)$ as a function of $t_1$, we find the charge order to be considerably weakened at $t_2 > 0$ for electrons with spin, see Fig. 2. We can understand this by considering the processes of Fig. 1. The states depicted in (c) and (g) differ by their sequence of up and down spins. Process (b→c) is then no longer canceled by (f→g), as it is for spinless fermions. Consequently, a kinetic energy contribution $\propto t_1^4 t_2^2/\epsilon_0^2$ is no longer forbidden by the Pauli principle.

Our interpretation is corroborated by analytic considerations: The additional DW motion due to $t_2$ favors two-DW states and changes the gap relevant to Eq. (4) from $\Delta = \epsilon_0 \sim V/2$ to $\Delta = \epsilon_0 - 2t_2$. This leads to the dash-dotted line in Fig. 2 which indeed describes the weakened charge order seen in the DMRG at $t_2 > 0$. For $t_2 < 0$, however, the DMRG results are described by the spinless gap $\Delta = \epsilon_0$. Since spinless fermions are equivalent to the fully polarized FM state, this indicates ferromagnetism, see below. For $U = 4V$ and small $t_1 \lesssim 0.07V$, where AF superexchange $\sim 4t_1^2/U$ destroys the polarized state, processes $\propto t_1^4 t_2^2$ retain their impact and strengthen charge order, see the full line in Fig. 2.

For fermions with spin, the sharp transition as a function of $t_2$ shown in Fig. 3 becomes asymmetric with respect to the sign of $t_2$. Even for very small $t_1 = 0.02V$, the cooperation between $t_1$ and $t_2$ is enough to render the breakdown of the WL charge order more gradual for $t_2 > 0$ than for $t_2 < 0$. For $t_1 = 0.07V$, charge order is strongly reduced for $t_2 > 0$, and the sharp drop in $N(\pi)$ as a function of $t_2$ has disappeared, in stark contrast to the spinless model.

IV. MAGNETISM

One expects AF interactions for the WL due to superexchange in the generalized Hubbard model. Yet our observation that the charge structure factor at negative $t_2$ agrees closely with results for spinless fermions, see Figs. 2 and 3, is already an indication that the ground state in this regime is FM. This is indeed the case, and our DMRG studies in fact yield fully polarized ground states for some parameter sets at negative $t_2$. As can be seen in Fig. 5, the FM interval increases with $t_2$.

In the following, we analyze the magnetic exchange by using perturbation theory valid when $t_1, t_2 \ll V \ll U$. The robust WL charge order leads to a modulated Heisenberg chain with spins at every second lattice site. Magnetism is therefore described by an effective Heisenberg-like Hamiltonian

$$H_J = J \sum_i (S_i \cdot S_{i+2} - \frac{1}{4} n_i n_{i+2}) \ ,$$

where $i$ runs only over the even sites, where the $L/2$ spins forming the WL are located. The total ground-state energy then is $E = \langle H_J \rangle + E_{FM}$, where $E_{FM}$ is the energy of the fully spin-polarized state, which is equivalent to the ground-state energy of spinless fermions. There are two distinct mechanisms that contribute to the exchange constant $J = J_{SE} + J_{KE}$. The first term is the usual superexchange, which involves a doubly occupied intermediate state and therefore has the energy scale $U$ in the denominator:

$$J_{SE} \simeq \frac{4t_1^2}{U} + \frac{12t_1^4}{\epsilon_0 U} + \frac{8t_1^2 t_2}{\epsilon_0} + \ldots$$

The second term $J_{KE}$—denoted as the kinetic exchange—arises from a spin exchange without any doubly occupied sites, i.e., exactly from the same effect that weakens the charge order for $t_2 > 0$: Quantum interference between processes (a→c) and (f→g) in Fig. 1 is destructive in the polarized FM state and constructive in the AF singlet, which leads to an exchange energy

$$J_{KE} \simeq \frac{2t_1^2}{\epsilon_0} \left( \frac{1}{1 - 2t_2/\epsilon_0} - 1 \right) \simeq \frac{4t_1^2 t_2}{\epsilon_0} + \ldots$$

that depends on the sign of $t_2$. The NN correlation function of the 1D quantum antiferromagnet is given by $\kappa = -\ln 2 + 1/4 \approx -0.443$, corresponding to $(S_i \cdot S_{i+2})$ for our modulated chain. Inserting $\kappa$ as well as Eqs. (9) and (7) into Eq. (5), we obtain an analytic estimate, valid at small hopping, for the energy of the AF state

$$E_{AF} \simeq \frac{L}{2} (J_{SE} + J_{KE})(\kappa - 1/4) + E_{FM} \ .$$

We compare this analytic result to numerical DMRG data for $t_1 = 0.05V$ and $t_2 = 0.07V$, in Fig. 5. This figure shows that the analytic curves given by $E_0 = \min(E_{AF}, E_{FM})$ closely model the numerical ground-state energies for not-too-large $t_2$ with no fitting parameters. Moreover, the analytical boundaries of the FM
phase, namely $t_2^2 \sim -3t_1^2/U$ and $t_2^4 \sim -(U/c_0^2)t_1^2$, match the magnetic phase boundaries found using the DMRG.

This may be compared with the boundaries in the $t_1$-$t_2$ plane describing the appearance of four Fermi points, namely $t_2 \leq -(t_1/4)\sec(\pi n/4)^2$ and $t_2 \geq (t_1/4)\csc(\pi n/4)^2$, where $n$ is the filling. For the quarter-filled case, i.e., $n = 1/2$, only the first relation is of interest and yields the condition $-\infty \leq t_2 \leq -0.293t_1$ for the appearance of FM in the Hubbard model, as observed in Refs. 27 and 28. It is perhaps not surprising that the boundary relevant for the Hubbard model, which is linear in $t_1$, is completely different from the boundaries obtained for the Wigner lattice, which are both quadratic in $t_1$. Nevertheless, ferromagnetism at quarter-filling is found at negative $t_2$ in both cases!

The phase diagram in Fig. 6 shows the total spin in the ground state of a chain with $L = 24$ for the range of $t_1$, $t_2$ corresponding to the WL regime. The dashed lines represent the analytical boundaries $t_2^2$ and $t_2^4$ of the FM region. Kinetic exchange $t_2^4$—the only magnetic interaction surviving for $U \to \infty$—is AF for $t_2 > 0$. For $t_2 < 0$, $J_{KE}$ raises the energy of the AF state over that of the FM state, see Fig 5. In the FM state itself, this effective FM exchange is, ironically, absent, because the Pauli principle forbids the ring exchange in the polarized state. At large negative $t_2$ and not-too-large $U$, AF superexchange 4 once again dominates.

The phase diagram Fig. 6 also contains contour lines $N(q = \pi, t_1, t_2) = C$ with the constant $C = 0.9, 0.8, ..., 0.4$, which indicate the strength of the alternating ($q = \pi$) charge order of the Wigner lattice. In accordance with Figs. 2 and 3, we find that the charge order dies off most quickly in the singlet states in the $t_2 > 0$ region. The analytic contour lines $t_1^4$ versus $t_2$

following from Eq. (4) for $t_2 > 0$ have the form

$$t_1^4 \simeq \frac{1}{4}(\epsilon_0 - 2t_2)\sqrt{1/N(\pi) - 1}.\quad (9)$$

They agree with the DMRG data, just as Eq. (4) agrees with $N(\pi)$ in Fig. 2. Since our analytic result describes the unbiased DMRG simulations so well, we conclude that the kinetic exchange indeed drives the suppression of charge order in the AF regime for $t_2 > 0$.

V. DISCUSSION AND CONCLUSIONS

We have investigated charge order and magnetism of the 1D quarter-filled Wigner lattice with nearest and next-nearest neighbor hopping. Starting from the regime $t_1, |t_2| \ll V$ with extremely strong alternating charge order stabilized by the long-range Coulomb repulsion, we find that increasing NN hopping $t_1$ drives a crossover to a $4k_F$ charge density state with weaker charge order but unchanged modulation period, whereas increasing NNN hopping $t_2$ leads to a sudden level-crossing transition, destroying the alternating charge order. For $t_1, |t_2| \ll V$ and spinless fermions, we find that there are no mixed processes involving both $t_1$ and $t_2$ because destructive interference removes the lowest order processes $\propto t_1^2t_2$. Consequently, the WL is bounded by a vertical crossover line and horizontal phase transition lines in the $t_1$-$t_2$ phase diagram for spinless fermions, see Fig. 4.

However, in the case of real electrons with spin, we find that processes $\propto t_1^2t_2^2$ are absent in the FM state (as for spinless fermions) but not in the AF state (as illustrated in Fig. 4). This results in an effective magnetic exchange $\propto 4t_1^2t_2^2/c_0^2$ which favors the AF relative to the FM state for positive $t_2$ and disfavors the AF state for negative $t_2$. This peculiar effect is corroborated by DMRG data, where we indeed find AF as well as FM ground states which depend on $t_1$ and $t_2$. The phase boundaries of the FM phase obtained here for the quarter-filled WL are distinct from those obtained for the $t_1$-$t_2$ Hubbard models driven by large $U$ and Fermi surface topology, where ferromagnetism is found whenever the fully polarized Fermi sea is split in two. This is perhaps not that surprising, as the charge order in the WL is not caused by a quantum mechanical Fermi-surface instability but by the strong Coulomb repulsion, which does not depend on the Fermi surface. Thus, the situation in the WL is very different from charge and magnetic order driven by Fermi surface instabilities in the Hubbard model with purely on-site Coulomb repulsion, which was studied extensively in Ref. 16.

Magnetism in the WL is not driven by Fermi-surface instabilities, but actually has more in common with the FM reported for a model of coupled chains with a symmetry-breaking on-site potential. In these coupled chains, charge order is stabilized by a strong on-site potential, which corresponds to the spontaneous symmetry breaking by long-range Coulomb repulsion in the case of
the WL, and is likewise independent of the Fermi surface. Starting from strong charge order, we have been able to derive the effective magnetic exchange terms using perturbation theory, and find the resulting magnetic energy to be in good agreement with DMRG data, see Fig. 5. The most important terms in the effective exchange Hamiltonian are the AF superexchange $\propto t_2^2/U$ involving a doubly occupied site and the kinetic exchange term $\propto t_1^2t_2/V^2$. A related FM exchange mechanism based on strong charge ordering and NN hopping has been invoked for two-dimensional kagome lattices.

Since neither charge order nor magnetism are driven by a Fermi surface instability but are determined by the Coulomb interactions, one might not expect that the charge order depends significantly on the magnetic correlations. Indeed, Wigner lattices are often discussed in terms of spinless fermions, and the magnetic exchange is added only in terms of a modulated Heisenberg model for the given charge order. Our calculations show that this picture is too simple: Figures 2 and 3 reveal that magnetic correlations have a very strong impact indeed on charge order. In fact, the weakening of charge order depends significantly on the magnetic correlations. In fact, the spin degrees of freedom have such a strong impact in the AF regime that charge ordering cannot be described reliably in terms of spinless fermions, even in the extreme WL regime $t_1, |t_2| \ll V \ll U$. As this effect is intimately related to the kinetic exchange mechanism, it may also be relevant in higher dimensions, e.g., the above-mentioned kagome systems.

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