Interaction driven phases in the honeycomb lattice from exact diagonalization

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We investigate the fate of interaction driven phases in the half-filled honeycomb lattice for finite systems via exact diagonalization with nearest and next nearest neighbour interactions. We find evidence for a charge density wave phase, a Kekulé bond order and a sublattice charge modulated phase in agreement with previously reported mean-field phase diagrams. No clear sign of an interaction driven Chern insulator phase (Haldane phase) is found despite being predicted by the same mean-field analysis. We characterize these phases by their ground state degeneracy and by calculating charge order and bond order correlation functions.

I. INTRODUCTION

The role of electron-electron interactions in graphene has been a fruitful subject of research even before this material was discovered. Although important progress has been made towards a full understanding of their effect, there are still fundamental questions that need to be clarified. One of such open questions regards the fate of band electrons in graphene’s honeycomb lattice when subject to repulsive interactions at half-filling. The plethora of techniques available to study the effect of interactions in this system has produced a range of interesting predictions. In particular, in a series of works, several groups have produced compatible mean-field phase diagrams that suggest that electrons in a honeycomb lattice with extended Hubbard interactions at half filling stabilize a Chern insulator (CI) phase with topological character and quantized Hall conductance at half filling stabilize a Chern insulator (CI) phase in a honeycomb lattice with extended Hubbard interactions (Haldane phase) is found despite being predicted by the same mean-field analysis. We characterize these phases by their ground state degeneracy and by calculating charge order and bond order correlation functions.

state of the system might not be adiabatically connected to mean-field state with a local order parameter and (iii) the mean field phase can be over/under estimated in the parameter region of the phase diagram.

To test the mean-field picture it is necessary to employ different tools as independent checks for the presence of the mean-field phases. One of such tools is exact diagonalization (ED) which we explore in this work. It is based on the ED of the Hamiltonian for finite lattice sizes and it provides, in principle, an unbiased analysis of interactions. The main limitations for ED in two-dimensional quantum systems are the smallness of system sizes that can be studied. Finite size effects might well out-range the energy scale of a potential many-body gap of incompressible ground states, so that the incompressibility cannot be recognized. Therefore, the limitations of ED and the mean-field approach are to a large extend complementary. If both methods yield the same phase for a region in parameter space, this provides strong evidence that the true ground state in the thermodynamic limit will be of this nature. Phases that cannot be easily detected with neither ED nor the mean-field approach include those with incommensurate long-range order. For example, depending on the system size and the particular geometry, ED might favor commensurate phases against frustrated phases and one has to be careful to explore (whenever possible) different sizes, and/or aspect ratios to pin down the relevant competing phases. Indeed, ED has proven useful in studies of the Haldane-Hubbard model and the π-flux model complementing other techniques such as quantum Monte-Carlo and variational cluster approximation used in studies of the Hubbard and Kane-Mele-Hubbard model in the Honeycomb lattice.

Motivated by these results, and in particular by the interaction driven phases found in existing mean-field calculations, in this work we study the spinless extended Hubbard model with both NN and NNN interactions in the honeycomb lattice at half filling via ED of small finite size systems. We will investigate and characterize the phase diagram for electronic phases that are driven by Coulomb interactions in the honeycomb lattice as an

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[54x416]of interesting predictions. In particular, in a series of effects in this system has produced a range of phase diagram mean-field phase diagrams that suggest that electrons

[54x336]phase

[54x348]tivity. This phase is nothing but the celebrated Haldane

[54x359]tions at half filling stabilize a Chern insulator (CI) phase

[54x382]with topological character and quantized Hall conduc-

[54x393]mean-field phase diagrams that suggest that electrons

[54x69]energy physics have been considered,

[10]tainty that all local order parameters relevant to the low

[54x103]perspective. However, the results are subject to the

[54x126]fate of band electrons in graphene’s honeycomb lat-

[54x161]limit.

[54x206]that compensates for the large

[54x218]V

[54x229]charge modulated phase (CMs)

[54x241]of NN interaction energy to be paid. A sublattice

[54x252]the two different sublattices that reduces the amount

[54x259]of system sizes that can be studied. Finite size effects

[54x262]V

[54x264]at

[54x267]V

[54x267]≫

[54x312]>V

[54x313].

[54x315]V

[54x315]2

[54x318]V

[54x318]1

[54x319]V

[54x323]and next to nearest neighbor (NNN) V

[54x326]2

interactions but always with V

[54x326]2

> V

[54x328]1.

Interestingly, the CI phase is embedded in a rich

structure of other competing orders in the phase dia-

gram. The first of these is a charge density wave order

(CDW) at V

1

≫ V

2

with charge imbalance between the two different sublattices that reduces the amount of NN interaction energy to be paid. A sublattice charge modulated phase (CMs) was also found for V

2

≫ V

1

with charge imbalance over the same sublattice that compensates for the large V

2

cost. At sufficiently large V

2

~ V

1

, a Kekulé bond order emerged characterized by a Z

3

order parameter which can lead to fractionalized excitations of ± e/2 at the long wavelength limit. These phases have the additional interest of being also examples of an interaction driven gap for low energy quasiparticles in the honeycomb lattice. Together, these works provide a clear consistent picture of the possible phases available within the mean-field perspective. However, the results are subject to the limitations of mean field theory, for (i) there is no certainty that all local order parameters relevant to the low energy physics have been considered (ii) the ground

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independent check for the mean-field picture. We will provide evidence for the appearance of some of the phases that were previously obtained in mean-field calculations. These include the CDW, the Kekulé bond order and the CMs phases which surround a trivial semi-metal (SM) phase. Surprisingly, for the studied lattice sizes, we find no clear sign of the previously reported interaction driven CI phase. As for the phases that do appear, we will characterize them by their ground-state degeneracy and by computing the charge density and bond order correlation functions.

In section III we introduce the model and establish notation conventions. In section IV we present the complete phase diagram of the honeycomb lattice at half filling with NN and NNN interactions. We will discuss the main properties and characterize each of the appearing phases. In section V we relate our findings with previous works and discuss the absence the interaction driven CI phase. Finally, in section VI we summarize our main findings.

II. THE MODEL

We start with the spinless extended Hubbard model for electrons in a honeycomb lattice with nearest neighbor (NN) interaction $V_1$ and next to nearest neighbor (NNN) interaction $V_2$. The Hamiltonian in real space reads:

$$ H := -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + h.c.) + V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle \langle i,j \rangle \rangle} n_i n_j $$

where $t$ is the nearest neighbor hopping and $c_i$ annihilates an electron at the $i$-th site of the honeycomb lattice. Each of the two triangular sublattices A and B is spanned by the basis vectors $a_1 = \delta_2 - \delta_3$ and $a_2 = \delta_3 - \delta_1$ defined through the three nearest neighbors $\delta_i = a(0,-1)$.

III. PHASE DIAGRAM

In order to implement the ED of Hamiltonian (2) we discretize the Brillouin zone (BZ) with a lattice $\Omega = L_1 \times L_2$ of points that span the BZ area. The band structure of graphene and two different set of lattice sizes are shown in Fig. 2. For the $\Omega = 3 \times 3$ lattice there are 9 points per band in the BZ each to be filled with one electron. There is one at the $\Gamma$ point, two at the $K$ and $K'$ points, and a set of six energetically degenerate points. For a given particle $i$, we label its momentum by its coordinates in momentum space $q_1^{(i)}$, $q_2^{(i)}$ or, alternatively, with the discrete one-dimensional integer label $Q^{(i)} = k_1^{(i)} + L_1 k_2^{(i)}$. In this notation and for this
lattice the \( \Gamma \) point corresponds to momentum (0, 0), or \( Q^{(i)} = 0 \), and the \( K \) and \( K' \) points are at (1, 1), or \( Q^{(i)} = 4 \), and (2, 2), or \( Q^{(i)} = 8 \), respectively [see Fig. 2(a)]. In general \( k^{(i)}_1 \in [0, L_1 - 1] \), \( k^{(i)}_2 \in [0, L_2 - 1] \) and \( Q^{(i)} \in [0, L_1 L_2 - 1] \).

Since the interaction in Hamiltonian \( \hat{H} \) conserves the total momentum, in ED we can diagonalize independently each total momentum sector subspace \( Q = \sum_i Q^{(i)} \) with \( Q \in [0, L_1 L_2 - 1] \), where the momentum is defined modulo \( \Omega \). Therefore all eigenvalues and eigenvectors that we obtain are labelled by \( Q \). The phase diagram for \( \Omega = 3 \times 3 \) with \( N = 9 \) particles (i.e., \( \nu = N/(2\Omega) = 1/2 \) filling) and representative eigenvalue spectra as a function of \( Q \) are shown in Fig. 3(i). By focusing on the ground state degeneracy we identify a phase by the number of ground states over which there is the highest gap. In what follows we will distinguish and characterize the four distinct phases. We will argue that they correspond to the SM, Kekulé, CDW, and CMs phases and discuss their main signatures. We note that the phase boundaries might be altered by going to larger systems or applying alternative definitions to identify the phases.

In the following section we will use these findings to relate to previous works to finally compare with the mean-field diagram in Fig. 3(ii) of Ref. [10] which includes all possible (non-superconducting) mean-field decouplings with a tripled unit cell. In particular, this phase diagram is consistent with past mean-field studies for which the absence of the Kekulé or CMs phases in the mean-field phase diagrams was due to the fact that these works did not allow for these mean-field solutions.

### A. Semi-metal phase

This phase, labelled SM and shown in red in Fig. 3(a) is straightforward to characterize since it stems from the noninteracting \( (V_1 = V_2 = 0) \) limit of Hamiltonian \( \hat{H} \). For \( \Omega = 3 \times 3 \) at half filling \( (N = 9) \) there are \( 2\Omega = 18 \) lattice sites to fit 9 particles. Seven of them sit at the lower states, one at the \( \Gamma \) point at \( (0, 0) \) and six particles go to the six degenerate momenta at \( (1, 0), (2, 0), (0, 1), (2, 1), (0, 2), (1, 2) \). We have two particles left for four degenerate single-particle states, two at the \( K \) point and two at the \( K' \) point, since at these points there are two degenerate states, one from each band. This gives a freedom to choose the ground state. We have 2 particles to fill 4 states, the degeneracy of which is given by the binomial coefficient \( C(4, 2) = 6 \) which is the ground-state degeneracy for the non-interacting case. Out of these six possibilities, four of them have a particle at \( K \) and a particle at \( K' \) and thus a total momentum of \( Q = 0 \). The remaining two configurations have two particles at the same valley. Having both at \( K = (1, 1) \) results in a total momentum \( (2, 2) \) or \( Q = 8 \). Similarly placing the two last particles at \( K' = (2, 2) \) we expect to have a single state at momentum \((1, 1)\), or \( Q = 4 \).

To summarize, the non-interacting Hamiltonian in ED has a sixfold quasi degenerate ground-state at half-filling with four states at \( Q = 0 \), one state at \( Q = 4 \) and one state at \( Q = 8 \).

We observe this structure for a finite region of parameters colored red in Fig. 3(a) connected to the non-interacting Hamiltonian and thus we interpret this phase as a SM phase. The spectrum for such phase is shown in Fig. 3(d) where the six-fold quasi degenerate ground-state are observed at the momenta discussed above.

### B. Charge Density Wave phase

The second phase that we identify is labelled CDW and shown in light blue in Fig. 3(a). Its spectrum shows a two-fold degenerate ground state at \( Q = 0 \) [Fig. 3(e)] and would break spontaneously the sublattice symmetry in the thermodynamic limit. The most transparent way to understand that this phase is indeed a CDW is to investigate the strong coupling limit at \( V_1/t \to \infty \) with \( V_2 = 0 \) to which this phase is adiabatically connected. Calculating the degeneracy of such a strong coupling state is a classical problem, the ground state of which is represented in Fig. 4.

As only one sublattice is occupied in either of these classical ground states, both of them are zero-energy eigenstates of the NN interaction \( V_1 \). We expect this state to appear at total momentum \( Q = 0 \) since it is a charge density wave (CDW) order state within the unit cell. Indeed, the ED of the Hamiltonian with \( V_1 \neq 0 \) and \( V_2 = t = 0 \) yields exactly this two fold degenerate ground-state at zero energy. The excited states that can be computed classically also coincide both in energy and degeneracy in this limit.

It is possible to connect this strong coupling phase to the two-fold degenerate phase shown in Fig. 3 simply by increasing the hopping continuously to see that both phases are indeed connected without ever closing the many-body gap. From this fact alone we can already conclude that this state is a CDW state. A further check of this picture comes from calculating the charge density wave modulation in the same spirit as described in Ref. [27]. Suppose that we have a phase with a set of (quasi-)degenerate ground states \( |m\rangle \), \( m = 1, \cdots, N_{gs} \). For these, we define the sublattice-staggered electron density matrix

\[
\rho_{\ell}^{m'm} := \frac{1}{\Omega} \sum_k e^{i(Q_m - Q_{m'}) \cdot r} \\
\times |m\rangle \langle a_k^\dagger (Q_m - Q_{m'}) a_k - b_k^\dagger (Q_m - Q_{m'}) b_k |m'\rangle .
\]

For the CDW case we have in particular that \( m = 1, 2 \) with both \( Q_1 = Q_2 = 0 \). Note that since \( Q_1 = Q_2 \) it is not possible to build a linear combination of ground
The defining feature of the CDW phase. For example, imbalances. Therefore if finite, the eigenvalues are the size of the many-body gap ∆/t. With a staggered chemical potential ±m.

Finally, a transparent way to understand this state is represented in Fig. 4 confirming the CDW interpretation state with particles localized in sublattice B (A) as a single state of total momentum Q = Q1 + L1Q2 for the (b) CMs phase, (c) Kekulé (d) SM phase and (e) CDW phase. The small numbers indicate the degeneracy of each state. The zero of energies is chosen to be the ground state energy. The phases are identified by the number of ground states over which there is the highest gap.

![Fig. 4](image)

The next phase that we identify is labelled Kekulé phase shown in green color in Fig. 3(a). It has a four-fold degenerate ground state [Fig. 3(c)] at Q = 0(×2), 4, 8 corresponding to two states at the Σ point and one state at both K and K'. As mentioned above, ED of finite systems can only yield precursors of spontaneous symmetry breaking in the thermodynamic limit. This means that if the Kekulé order is present, it should appear in all of its linearly independent forms. Therefore, if finite, the eigenvalues are the defining feature of the CDW phase. For example, for V1 = 5t and V2 = 0 we find that λ1 = −0.99 and λ2 = 0.97. The former (latter) corresponds to a state with particles localized in sublattice B (A) as represented in Fig. 4 confirming the CDW interpretation of the state.

![Fig. 3](image)

C. Kekulé phase

We now diagonalize the 2 × 2 matrix ρr for representative points inside the CDW phase. This generates two r-independent eigenvectors and eigenvalues, v1 and λi (i = 1, 2). The former represent the two independent super-positions of the two-fold degenerate ground states while the latter represent the two possible sublattice imbalances. Therefore if finite, the eigenvalues are the defining feature of the CDW phase. For example, for V1 = 5t and V2 = 0 we find that λ1 = −0.99 and λ2 = 0.97. The former (latter) corresponds to a state with particles localized in sublattice B (A) as represented in Fig. 4 confirming the CDW interpretation of the state.

Finally, a transparent way to understand this state is to relate it with the non-interacting honeycomb lattice with a staggered chemical potential ±m in the A(B) sublattice, i.e. the non-interacting version of the CDW state. Upon filling the band structure for this simple case at half-filling and for Ω = 3 × 3 the two particles highest in energy have momenta K and K', thus corresponding to a single state of total momentum Q = 0. Within the interacting model and since symmetry breaking is absent for finite systems, by ED of the interacting Hamiltonian we find both ±m and ±m configurations which then give a degeneracy of two.
wave matrix (3) this time for the hopping amplitudes

\[ t^{m,m'}_r = \frac{1}{\Omega} \sum_k \langle m | a_k^{\dagger} (Q_m - Q_{m'}) b_k | m' \rangle e^{i(Q_m - Q_{m'}) \cdot r} \]

(4)

with the same notation as above but now for \( m = 1, 2, 3, 4 \) quasi-degenerate ground states. In this case the momentum differences \( Q_m - Q_{m'} \in \{0, K, K'\} \) allow for a Kekulé bond order. As before, we diagonalize the matrix (4) and label the system of four eigenvalues and eigenvectors \( \lambda_r \) and \( \mathbf{v}_r^{(m)} \). This time, the eigenvectors depend on position. If present, the Kekulé bond order will appear as a superposition of the allowed phase factors \( e^{i(Q_m - Q_{m'}) \cdot r} \). We can construct four independent superpositions corresponding to the four eigenvectors such that:

\[ t^m_r = 2 \cos(v^{(m)}_{r,1} + v^{(m)}_{r,2} + v^{(m)}_{r,3} + v^{(m)}_{r,4}). \]

(5)

with \( m = 1, 2, 3, 4 \). When evaluated at the three different links \( t^m_r, t^m_{r+a_1}, t^m_{r+a_2} \) the underlying hopping lattice of this phase is revealed. There are four of such patterns, one for each value of \( m \).

However, if in the Kekulé phase, this procedure will in general produce an arbitrary superposition of all the possible Kekulé structures of Fig. 5(i). The four independent superpositions are shown in Fig. 5(ii) where the three different colors represent different bond strengths. Note that each of these patterns has a tripled unit cell periodicity with the right Kekulé orders, inherited from the \( r \)-dependent vectors \( \mathbf{v}_r^{(m)} \). Indeed, by forming linear combinations of these, one can obtain all the “pure” (coherent) Kekulé patterns in Fig. 5(i). We find the analysis of this section to be consistent with the presence of the Kekulé phase in this part of the phase diagram.

D. Sub-lattice charge modulation (CMs)

We finally address the last phase that remains to be characterized which we shall name as sublattice charge modulation or CMs appearing at the upper left corner of the phase diagram in Fig. 3(a). This phase, unlike the CDW, does not correspond to the naive classical strong coupling phase in the corresponding strong coupling limit. Rather, the limit \( V_2/t, V_2/V_1 \to \infty \) has an extensive classical ground state degeneracy so that quantum corrections will determine the form of the actual ground state for arbitrarily small non-zero values of \( t/V_2 \) and \( V_1/V_2 \). The classical counting yields a 666 fold degenerate ground state with energy \( 18V_2 \) for a \( \Omega = 3 \times 3 \) lattice. This information serves in fact as a consistency check just as in the CDW case. Indeed, we recover numerically the correct degeneracy and ground state energy in the limit \( V_1/t \to 0 \) and \( V_2 \neq 0 \).

The question then becomes, what phase will be selected by the quantum fluctuations out of the classical ground state manifold. From a large system with periodic boundary conditions a natural phase to be expected at half-filling for large \( V_2/V_1 \) is that with a charge modulation within the same sublattice, the CMs phase. This phase, discussed in detail in Ref. 10 reduces \( V_2 \) by paying an additional \( V_1 \) cost. Pictorially the state is shown in Fig. 6 where it is evident that it has a degeneracy of 18 because of the rotational symmetry of the Hamiltonian. We find a phase consistent with this picture at large \( V_2/V_1 \) in ED with a quasi-degeneracy of 18. Such a degeneracy slowly becomes more exact as one increases \( V_2/V_1 \), although the gap to the excited states also decreases such that in the limit \( V_1/t \to 0 \) and \( V_2 \neq 0 \) the strong coupling phase is recovered. Note also that, just as the Kekulé, the CMs state has also a tripled unit cell periodicity \( \Omega \) which is consistent with having the ground states at momenta \( Q \in \{0, K, K'\} \).
not only it contains the $K$ phases, all but the CI phase.

in Fig. 3 (ii). We have found, out of the five mean-field phases, all but the CI phase.

The $\Omega = 3 \times 3$ lattice studied above is special in that not only it contains the $K$ and $K'$ which enables clear physical interpretation of the emerging phases, but also it fits phases with a tripled unit cell without frustration, such as the Kekulé or the CMs phases. Therefore, such a lattice size has a natural bias towards these phases as compared to the CI phase, which does not break translational symmetries. This might be the reason why the Kekulé phase is so prevalent as compared to the mean-field phase diagram in Fig. 3 (ii). It is also interesting to note that the Kekule phase shifts to higher values of $V_2$ reducing the region for the charge modulated phase when comparing with the mean field result. Since both phases are favored by the $\Omega = 3 \times 3$ lattice size this result seems robust.

To investigate further the presence of the CI phase we have studied the $\Omega = 3 \times 4$ and $4 \times 3$ lattices for $V_1 = 0$, where the CI phase is expected to appear from the mean-field analysis at intermediate $V_2$. These lattice size frustrates the Kekulé and can leave phase space for other phases (such as the CI phase) to appear.

The CI phase for a finite system would appear as a two-fold quasi degenerate ground-state one for each sign of the flux, in a similar way as the CDW shows a two-fold degenerate ground-state corresponding to $\pm m$ or $\mp m$ charge in the A and B sublattices. However, we find no evidence of such signature and thus we conclude that this phase is absent also from the ED of $\Omega = 3 \times 4$ and $4 \times 3$ lattices. Taking the $3 \times 4$ as an example, the spectra along the $V_2$ line shows first a single ground-state at $Q = 6$ for low $V_2$, as expected for the trivial SM phase just by adding all the non-interacting momenta in Fig. 2(b). At $V_2 \sim 7t$ the gap closes and reopens with a six fold quasi-degenerate ground-state. The lowest pair of these states lie at $Q = 6$, as would be expected for the CI phase. Therefore, it remains an open question whether this six-fold degeneracy becomes two-fold by increasing the lattice size, which could in principle lead in the thermodynamic limit to the appearance of the Hal-dane phase.

Finally we comment on a different route towards achieving interaction driven topological phases in the extended Hubbard model on the honeycomb lattice which involves moving away from half-filling. An example of these topological phases were shown to appear at higher fillings from a mean-field calculation in Ref 10. These are generalizations of the Haldane phase at fillings $\nu \gtrsim 2/3$ and with a tripled unit cell, which could also be present via ED. However, identifying these phases by characterizing the ground state properties from ED is challenging due to band folding.

FIG. 6: (Color online) CMs patterns with their corresponding degeneracies due to a sixfold rotational symmetry.

IV. DISCUSSION:

Despite the small system size, it is remarkable that the phase diagram Fig. 2(i) resembles very closely the mean-field phase diagram of Ref. 10 at half-filling shown in Fig. 3(ii). We have found, out of the five mean-field phases, all but the CI phase.

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V. CONCLUSIONS

We have investigated the effect of extended Hubbard interactions on spinless electrons on the honeycomb lattice at half filling via exact diagonalization (ED). We have found that four out of the five predicted mean-field phases are present. These are the semi-metal (SM), CDW, the Kekulé bond order and the sublattice charge modulation (CMs) phases. First, we have shown that the six-fold degeneracy of the SM ground-state can be understood entirely from the non-interacting band structure. For the CDW phase we have proven that it is connected to the strong coupling phase at $V_1/t \to \infty, V_2 = 0$ and we have characterized it finding a finite sublattice charge imbalance through the charge order correlation function, the hallmark for the CDW phase. The two-fold degeneracy is a sign of the two possible orders that the system can choose in the thermodynamic limit by spontaneously breaking the sublattice symmetry. Similarly, we have disentangled the Kekulé bond order phase by calculating the bond order correlation function which reveals the underlying superposition of four independent Kekulé patterns which conform the fourfold quasi-degenerate ground-state. Finally, we have argued that for $V_2 > V_1$ the CMs phase is expected to have a 18-fold degeneracy favoured by the costly NNN interaction, which is consistent with what we observed in ED.

Importantly, the fact that the discussed phases appear both in ED and in mean-field suggests that they are stable up to the thermodynamic limit. The appearance of the Kekulé phase dominating a wide region of the phase diagram opens up the possibility of realizing this exotic phase in cold atoms with a scheme along the lines of Ref. 7. Despite the fact that we have not found evidence for the Chern Insulator (CI) phase, it is still possible that it is realizable in the thermodynamic limit. Different approaches such as cluster mean-field, 28 can also prove useful to ascertain the presence of the CI phase. We hope that the conclusions of the present work will motivate further explorations of the extended Hubbard model on the honeycomb lattice.

Note added: During the completion of this work we learned from a complementary analysis in that focuses on
the line $V_2 \neq 0, V_1 = 0$ in the phase diagram. The results are consistent with those presented here, in particular, with the absence of the CI phase and the appearance of the CMs state.

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\end{enumerate}