Diversity of charge orderings in correlated systems

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The phenomenon associated with inhomogeneous distribution of electron density is known as a charge ordering. In this work, we study the zero-bandwidth limit of the extended Hubbard model, which can be considered as a simple effective model of charge ordered insulators. It consists of the on-site interaction $U$ and the intersite density-density interactions $W_1$ and $W_2$ between nearest-neighbors and next-nearest neighbors, respectively. We derived the exact ground state diagrams for different lattice dimensionalities and discuss effects of small finite temperatures in the limit of high dimensions. In particular, we estimated the critical interactions for which new ordered phases emerge (laminar or stripe and four-sublattice-type). Our analysis show that the ground state of the model is highly degenerated. One of the most intriguing finding is that the nonzero temperature removes these degenerations.

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I. FORMULATION OF THE PROBLEM

The solutions of the extended Hubbard model predicts an existence of the states with the inhomogeneous spatial distribution of electrons [1–9]. This phenomenon is known as the charge ordering and can be observed in variety of compounds, e.g., cuprates [10–13], multiferroics [14, 15] and other intensively studied materials [16–18]. The simplest example of such an order is an alternate modulation of electron concentration on the biparticle lattice. In such a setup one can distinguish two equivalent sublattices, where every site in each sublattice is occupied by the same number of particles. This is so-called two sublattice assumption. In more general systems in which longer-range interactions play an important role the two-sublattice solutions does not capture the full basis of charge ordered phases [19–23]. In order to properly describe these orderings one needs to take into account more than two inequivalent sites. The most conspicuous classes of such materials are those where laminar or stripe orderings appear, e.g., manganites [24, 25], cobaltites [26], and other transition-metal compounds [27].

The exact solution of the extended Hubbard model is still unknown, even in one dimension. A good testing field for approximate solutions would be results obtained for simplified, but exactly solvable model (in arbitrary dimensions). The Hubbard model (without intersite interactions) has been exactly solved in one dimension [28, 29] and in the limit of infinite dimension [30–32]. Another approach is to neglect the hopping term instead of longer-range interactions. Similar conditions can be met in narrow band materials [3]. One of the main goals of the present work is to provide the exact solutions that can be compared with approximate results for more complex systems (such as models taking into account quantum fluctuations introduced by the hopping term).

In this work we investigate the extended Hubbard model in the atomic limit taking into account the next-nearest-neighbour density-density interactions. We assume that the mean-field solutions (with an exact treatment of the on-site terms) are contained within the four-sublattice system. This assumption is justified as long as we do not take into account interactions with longer range than the next-nearest neighbour. Phase diagrams in this approach are obtained for full range of model parameters. We note that the presented ground state solutions are exact for arbitrary dimensionality of the lattice. In a case of the high-dimension limit ($d \to +\infty$) we also present the effects associated with finite temperature. In addition, we discuss the qualitative differences of ordering range depending on dimensionality of the considered system.

The extended Hubbard model in the zero-bandwidth limit with interactions restricted to the second neighbors

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can be expressed as:

$$\hat{H} = U \sum_{i} n_{i} n_{i} + \frac{W_{1}}{2z_{1}} \sum_{\langle i,j \rangle_{1}} n_{i} n_{j}$$

$$+ \frac{W_{2}}{2z_{2}} \sum_{\langle i,j \rangle_{2}} n_{i} n_{j} - \mu \sum_{i} n_{i},$$

(1)

where $c_{i}^{\dagger}$ denotes the creation operator of an electron with spin $\sigma$ at the site $i$, $n_{i} = \sum_{\sigma} n_{i\sigma}$, $n_{i\sigma} = c_{i}^{\dagger} c_{i\sigma}$, $U$ is the on-site density interaction, and $W_{1}$ and $W_{2}$ are the intersite density-density interactions between nearest neighbours (NNs) and next-nearest neighbours (NNNs), respectively. $z_{1}$ and $z_{2}$ are numbers of NNs and NNNs, respectively. $\mu$ is the chemical potential determining the total concentration $n$ of electrons in the system by the relation $n = \frac{1}{L} \sum_{i} \langle n_{i} \rangle$, where $0 \leq n \leq 2$ and $L$ is the total number of lattice sites. We inspect phase diagrams emerging from this model. The analyses are performed in the grand canonical ensemble.

Model (1) with neglected next-nearest interactions ($W_{2} = 0$) was intensively studied using various methods. In particular, the exact solutions for a one-dimensional ($d = 1$) chain were obtained using the transfer-matrix method [33–35] or equations of motion and Green’s function formalism [36–39]. The rigorous ground state phase diagrams as a function of $\mu$ were performed using various methods [43, 44]. The model on the Bethe lattice was also analysed [45, 46]. The only known work beyond mean-field approaches for $W_{2} \neq 0$ treated the model within the transfer-matrix method for $d = 1$ chain [47, 48] and the checker-board estimate with respect to lattice planes [40].

Using the mean-field method for alternate lattices it was shown that the system can exhibit several homogeneous charge-ordered phases as well as various phase separated states [49–52]. A case of $W_{2} \neq 0$ within a mean-field approach was investigated in Refs. [51, 52]. However, these analyses were restricted to the two-sublattice assumption. This restriction is sufficient only for attractive $W_{2}$, where there are no physical mechanisms supporting the four-sublattice type order. In the present work we perform the studies of the model for the full range of parameters including repulsive $W_{2} > 0$. Our preliminary results only for $U < 0$ have been presented in Ref. [53]. One of the conclusions of the mentioned work was that the magnitude of on-site attractive $U$ does not change the diagrams of the model qualitatively. Therefore, in the present work we mainly focus on repulsive $U$. We show that at particular values of $U > 0$ new phases emerge.

The mean-field expressions

The grand thermodynamic potential per site $\Omega_{0}$ for model (1) in the grand canonical ensemble and in the mean-field four-sublattice approximation at $T = 0$ can be expressed as

$$\Omega_{0} = \langle \hat{H} \rangle / L = E_{U} + E_{W} + E_{\mu},$$

(2)

where

$$E_{U} = \frac{1}{2} U \left[ n_{A} (n_{A} - 1) + n_{B} (n_{B} - 1) \right] + n_{C} (n_{C} - 1) + n_{D} (n_{D} - 1),$$

(3)

$$E_{W} = \frac{1}{8} W_{1} (n_{A} n_{B} + n_{A} n_{D} + n_{B} n_{C} + n_{C} n_{D}),$$

(4)

$$E_{\mu} = -\frac{1}{2} \mu (n_{A} + n_{B} + n_{C} + n_{D}),$$

(5)

and $n_{\alpha}$ denotes the average number of particles in each sublattice $n_{\alpha} = \frac{1}{4} \sum_{i} \langle n_{i} \rangle$, $\alpha \in \{A, B, C, D\}$. In this work we adopted the convention that the NNNs for any site from $A (B)$ sublattice are those and only those sites, which are located in $C (D)$, respectively sublattice.

For finite temperatures, the expressions given in Ref. [51] in the four-sublattice assumption takes the following forms. For $n_{\alpha}$ one gets

$$n_{\alpha} = \frac{1}{Z_{\alpha}} \left[ \exp (\beta \mu_{\alpha}) + \exp (2 \mu_{\alpha} - U) \right].$$

(6)

For a grand canonical potential (per lattice site) one obtains:

$$\Omega = -\frac{1}{8} \sum_{\alpha} \Phi_{\alpha} n_{\alpha} - \frac{1}{4 \beta} \sum_{\alpha} (\ln Z_{\alpha}),$$

(7)

where $\beta = 1/(k_{B} T)$ is inverted temperature, $\mu_{\alpha} = \mu - \Phi_{\alpha}$, and

$$Z_{\alpha} = 1 + 2 \exp \beta \mu_{\alpha} + \exp \beta (2 \mu_{\alpha} - U),$$

(8)

$$\Phi_{A} = \frac{1}{2} W_{1} (n_{A} + n_{D}) + W_{2} n_{C},$$

(9)

$$\Phi_{B} = \frac{1}{2} W_{1} (n_{A} + n_{C}) + W_{2} n_{D},$$

(10)

$$\Phi_{C} = \frac{1}{2} W_{1} (n_{B} + n_{D}) + W_{2} n_{A},$$

(11)

$$\Phi_{D} = \frac{1}{2} W_{1} (n_{A} + n_{C}) + W_{2} n_{B}.$$  

(12)

II. PHASE DIAGRAMS AT HIGH DIMENSIONS

In this paragraph we present the ground state solutions of model (1) in the limit of high dimensions i.e. $d \to +\infty$.
(or equivalently the limit of large coordination number: 
\( z_1 \rightarrow +\infty \) and \( z_2 \rightarrow +\infty \)) and compare them to the 
results obtained for finite temperatures. We present the 
phase diagrams for fixed chemical potential as well as 
for fixed total electron concentration. In the following 
analyses \( |W_1| \) is used as the energy unit. The solutions 
for repulsive \( W_1 > 0 \) and attractive \( W_1 < 0 \) are analysed 
separately.

In our system only six (inequivalent) homogeneous 
phases can occur at \( T = 0 \). They are determined by the 
relations between \( n_\alpha \)'s (but several equivalent solutions 
exist due to cyclic change of sublattices indexes \( \alpha \)). 
For intuitive understanding of rather complicated 
phase diagrams each pattern is marked with adequate 
abbreviation. Nonordered (NO), checker-board-ordered 
(CBO), and stripe-ordered (STO) phases can be realized 
using two sublattices, while the letter “F” (in the names 
of the FNO, FCBO, and FSTO phases) indicates that 
these types of ordering requires the four-sublattice 
assumption. All these phases are schematically depicted 
in Fig. 1. Each pattern can be realised in a few distinct 
forms depending on specific electron concentrations on 
each sublattice (cf. Tables I and II). Table I also contains 
the degeneracy of the ground state solutions (including 
charge- and spin-degrees of freedom).

A. Analysis for fixed chemical potential for 
repulsive \( W_1 \)

First, we focus on the case of repulsive \( W_1 > 0 \). We 
discuss the qualitative changes of a phase diagrams with 
respect to on-site Coulomb interaction \( U \) as a function of 
chemical potential and next-nearest neighbour inter-
site interactions \( W_2 \). Below we present phase diagrams 
for a few representative on-site interactions, where qual-
itative differences occur. The diagrams are plotted for 
a full range of NNN interaction \( W_2 \) and shifted chemical 
potential \( \bar{\mu} (\mu = \mu - \frac{1}{2}U - W_1 - W_2) \). Notice that 
the model exhibits the particle-hole symmetry and thus 
all phase diagrams are symmetric towards \( \bar{\mu} = 0 \) (or 
\( n = 1 \)) with \( n_n \leftrightarrow 2-n_n \) transformation if one changes 
\( \bar{\mu} \leftrightarrow -\bar{\mu} \) (or \( n \leftrightarrow 2-n \)).

The qualitative changeover occurs for on-site energy 
\( U = 0.5|W_1| \). For this value of interaction two electrons 
occupying one site in the FNO2 phase can be separated 
to form the stripe-ordered STO1 (1100) phase and thus 
for larger \( U \) the STO1 phase is stable. We note that ad-
ditional two phases (the FNO2 (1110) and NO1 (1111) 
phases) without double occupied sites emerge on bound-
daries around \( W_2 = 0.5|W_1| \) and \( -0.25|W_1| < \bar{\mu} < 0 \). For 
\( U > 0.5|W_1| \) the FNO3 and NO1 phases occurs in finite 
range of model parameters. With further increasing of \( U \)
the region of the FCBO (2010) phase shrinks. The region 
of this phase occurrence at \( U = 1.00|W_1| \) is reduced to 
a single point. For \( U > 1.00|W_1| \) the NO1–CBO1 transi-
tions appears and for larger values of \( U \) the diagram does 
not change, qualitatively. Remarkably, the FCBO phase 
exists only for define range of on-site interaction, while 
the FSTO phase is present for arbitrarily large \( U \).

Notice that all boundaries between ground state phases 
in Fig. 2 are discontinuous (first order transitions associ-
ated with discontinuous change of at least one of the 
\( n_\alpha \)'s). At the boundaries two phases possess the same 
energy. If two phases coexist in the system the inter-

| Phase | \( n_A \) | \( n_B \) | \( n_C \) | \( n_D \) | \( d_x \times d_y \) | \( D_x \times D_y \) |
|-------|--------|--------|--------|--------|----------------|----------------|
| NO0   | 0 0 0 0 | 1 x 1  | 1 x 1  | 1 x 1  |
| NO2   | 1 1 1 1 | 1 x 16 | 1 x 2L |
| CBO1  | 1 0 1 0 | 2 x 4  | 2 x 2L |
| CBO2  | 2 0 2 0 | 2 x 1  | 2 x 1  |
| STO1  | 1 1 0 0 | 4 x 4  | 4 x 2L |
| STO2  | 2 2 0 0 | 4 x 1  | 4 x 1  |
| FNO1* | 0 0 0 0 | 4 x 2  | 2N/2L  |
| FNO2* | 2 0 0 0 | 4 x 1  | 2N/2L  |
| FNO3* | 1 1 1 0 | 4 x 8  | 2N/2L  |
| FCBO  | 2 0 1 0 | 4 x 4  | 4 x 2L |
| FCBO* | 2 1 0 0 | 4 x 4  | 4 x 2L |
| FSTO* | 2 0 0 0 | 8 x 2  | 2N/2L  |
| FSTO* | 2 1 1 0 | 4 x 4  | 2N/2L  |

\* The long-range charge-order is “reduced” in the phase 
constructed from this elementary blocks in \( d = 1, 2 \).

b This phase constructed from this elementary block does not 
or in the ground state.

TABLE I. The definitions of phases \((d \leq 3)\) or elementary 
blocks \((d = 1, 2)\) occurring in the ground state for total \( n \leq 1 \). 
Notation: \( 2 \) – doubly occupied site, \( 0 \) – empty site, \( 1 \) – singly 
occupied site. The degeneration \( d_x \times d_y \) of the elementary 
blocks (equal to the degeneration of the ground state for \( d \rightarrow \infty \) limit) 
degeneration \( D_x \times D_y \) of the ground state 
phases constructed from the corresponding blocks for \( d = 2 \) 
\((L = N^2)\) is given (with respect to charge- and spin-degrees 
of freedom).
faces between them are formed. To determine the state of the system in such conditions one needs to estimate the additional energy required for formation of the phase interface. If creation of the interface between two phases does not require additional energy, then these two phases can coexist on a microscopic level. In other words the four-site building blocks of each phases can be aligned arbitrary next to each other. More detailed discussion of this issue is included in Section III.

The situation is more complex for nonzero interface energies. In this case the phases cannot be mixed on a microscopic level. Nevertheless, if the size of the interface energies. In this case the phases cannot be mixed on a microscopic level. Nevertheless, if the size of the interface
increases as $L^\gamma$ with $\gamma < 1$ (where $L$ is the number of lattice sites) the contribution of the interface energy to the total energy of the system vanishes in the thermodynamic limit. In such a case, the macroscopic phase domains will be formed. A formation of these regions with different orderings is known in physics as the (macroscopic) phase separation (PS) (the only one possible type of a coexistence of two phases in $d \to +\infty$ limit). Otherwise, for $\gamma > 1$ the formation of the interfaces is disfavoured and the coexistence of the phases is not allowed in the system. In such situation, even though both phases have the same energy, only one type of the ordering is realized in all volume of the system. We note, however, that we did not find such behaviour in the considered model.

Effects of finite temperatures (fixed $\mu$)

So far we considered the ground state ($T = 0$), where all phase transitions are associated with a discontinuous change of at least one sublattice concentration $n_\alpha$. In this subsection we discuss the influence of a finite temperatures on phase transitions slightly above the ground state. The phases are found by numerically solving the set of four self-consistent equations in a form of (6) and finding the solution corresponding to the lowest $\Omega$ determined by (7).

For attractive $W_2$ the behaviour of the system does not change qualitatively at small temperatures, and all phase transitions remain first-order. At critical $W_2 = 0$ the order of all transitions changes into the second one. A more complex situation occurs for repulsive $W_2$. Our analysis shows that all ground state FNO–STO boundaries (namely, (2000)–(2200), (1000)–(1100), and (1110)–(1100)) and boundary lines which are not dependent on the chemical potential (horizontal lines in Fig. 2) remain first-order. All other transitions for $W > 0$ are second-order at small $T > 0$. At finite temperature, the FNO phases are no longer stable, and they are converted into FCBO phases, i.e. $(n_A000)_{T=0} \to (n_An_Bn_Cn_B)_{T>0}$. As a result the ground state FNO$_1$–FNO$_2$ ((1000)–(2000)) and FNO$_2$–FCBO ((2000)–(2100)) boundaries no longer exist at $T > 0$ (Fig. 2(b)). The similar situation takes place for the CBO$_1$–CBO$_2$ boundary for $W_2 = 0$ [52].

Additionally, we noticed that finite temperature, for small $W_2 > 0$, gives rise to checker-board orderings between NO and FNO phases. Namely, NO–FNO boundaries change into the NO–CBO–FNO sequence of second-order transitions with changing chemical potential. In particular, the following sequences emerge: NO$_0$–CBO$_2$–FNO$_2$, NO$_0$–CBO$_1$–FNO$_1$, FNO$_3$–CBO$_1$–NO$_1$ (cf. Ref. [53] for the $U < 0$ case). For larger values of $W_2$, the CBO phases are absent and only second-order transitions between corresponding NO and FNO phases occur.

B. Analysis for fixed electron concentration for repulsive $W_1$

Here we consider the mutual relations between homogeneous phases and phase separated states for fixed total concentrations $n$. To do this one needs to first establish which homogeneous phases have the lowest energies and then compare them to the energies of phase separated states. The first step is illustrated in Fig. 3, which presents the phase diagrams as a function of electron concentration. Each rectangular region of the diagrams is labeled by the abbreviation of homogeneous phase with the lowest free energy. The meaning of each label is given in Table II. The free energy per site of homogeneous phases at $T = 0$ within the mean-field approximation can by obtained as $f_0 = U D_{\text{occ}} + E_W$, where $E_W$ is expressed by Eq. (4). The double occupancy $D_{\text{occ}}$ and $n_\alpha$ are also collected in Table II. On the vertical boundaries (for commensurate particle fillings $n = i/4$, $i = 1, 2, 3, 4$) the homogeneous phases occur. These phases can be read from Table I and Fig. 2. For $n = 1/2$ on the boundary between FSTO$_0$ and FSTO$_r$ regions the STO$_1$ phase occurs (Fig. 3(f)). On the horizontal boundaries the phases from both neighboring regions have equal energies, and they coexist.

So far we labelled only homogenous phases with the lowest energies. The comparison of them with the phase separated states shows that for $W_2 < 0$ the homogeneous phases are unstable (i.e. $\partial u/\partial n < 0$) and thus only the PS states are present. These regions in Fig. 3 are marked by a slantwise pattern. The obvious exclusion from this pattern occurs for vertical boundaries between two types of PS states where homogenous phases are stable below $W_2 = 0$. We determined that at $T = 0$ and $W_2 \geq 0$ homogenous phases and PS states have the same energy. The corresponding PS states in each region of Fig. 3 are given in the last column of Table II. We would like to emphasize that the system cannot be simultaneously in a homogenous phase and a PS state. Thus even though energies of PS states and homogeneous phases at $T = 0$ are equal, the system must “choose” one of the solutions. This type of degeneracy is removed by the finite temperature. The free energies of the (macroscopic) PS states are calculated from the expression $f_{PS} = m f_+(n_+) + (1-m) f_-(n_-)$, where $f_\pm(n_{\pm})$ are free energies of separating homogeneous phases and $m = (n-n_-)/(n_+-n_-)$ is a fraction of the system which is occupied by the phase with concentration $n_+$.

Additionally, we note that for fixed $W_2$ transitions between homogeneous phases (horizontal lines in Fig. 3) are associated with continuous change of sublattice concentrations, whereas for fixed $n$ (vertical boundaries) the sublattice concentrations change discontinuously (at commensurate fillings only at points indicated by square symbols in Fig. 3). All transitions between the phases exhibit discontinuous change of chemical potential.

Notice also that mean-field results presented in Fig. 3 ($W_1 > 0$) are coincided with some exact results obtained...
for a one-dimensional chain at $T = 0$ and arbitrary $n$. In particular, the mean-field approximation used in the present work predicts properly the values for (free) energy, double occupancy correlation function, and nearest- and next-nearest two-point correlation functions [38, 48]. Ref. [38] predicts also that at $T = 0$ and for $W_2 = 0$ ($W_1 > 0$) the long-range checker-board order exist in the following range of model parameters: (i) $0 < U < W_1$ and $1/2 < n < 1$, (ii) $U > 0$ and $n = 1/2$, (iii) $U < W_1$ and $n = 1$. We found the similar behaviour for $W_2 > 0$ in the FCB0B and FCB0G regions (Fig. 3(b)–(d)), where the long-range checker-board order is expected for $d = 1$ and $d = 2$ at zero temperature. For (a) $W_1 > 0$ and $W_2 < 0$ as well as (b) $W_1 < 0$ and any $W_2$ at $T = 0$ and $d = 1, 2$ the macroscopic phase separation involving the checkerboard order would occur (for incommensurate fillings).

**Influence of finite temperatures (fixed $n$)**

For $W_2 < 0$ the finite temperature does not change qualitative behavior of the system and the PS are still stable. For $W_2 \geq 0$, infinitely small $T > 0$ breaks the energy equality between homogeneous phases and PS states and only one of them is stable. Namely, the PS states between FNO and STO phases emerge at the regions filled by grating pattern for $W_2 > 1/2$, whereas in empty regions in Fig. 3 the homogeneous phases are favoured. For $W_2 = 0$ only the homogeneous CBO phases are present. Remarkably, the regions of the PS states occurrence (slantwise and grating patterns) are separated by homogeneous phases (empty regions) at $T > 0$. The stability of the PS states at $T > 0$ in these regions is a result of discontinuous transitions with changing $\tilde{\mu}$, e.g., Refs. [51, 52]. Note that at $T > 0$ the separating homogeneous phases are the phases with particle concentrations different than those at the ground state, and they can be determined by the so-called Maxwell’s construction (cf., e.g., Ref. [51]).

Due to the fact that at finite temperatures sublattice concentrations change continuously for fixed $W_2/|W_1|$ (vertical lines between nonfilled regions in Fig. 3) only boundaries between different types of phases still exist. Boundaries between the same type of phases (e.g., FCB0B–FCBOG) are smeared out. We also note that $T > 0$ transforms all FNO phases into FCBO phase. Therefore, ground state FNO–FCBO boundaries are also smeared (vanish) at nonzero temperatures. One should be aware of the type of phase occurring at commensurate filling (at vertical boundaries of diagrams in Fig. 3). For example, at the ground state FCB0B–FCBOG boundary.

### TABLE II. The definitions of homogeneous phases which can occur in the mean-field ground state of the model as a function of $n$ and ranges $[n_s, n_f]$ of electron concentration where the phases are defined properly. For each phase the double occupancy $D_{occ}$ defined as $D_{occ} = \frac{1}{2} \sum_i (n_i + n_i)^2$ is also calculated (exact result for $d \to +\infty$). At the last column the corresponding phase separated states are mentioned (cf. Table I).

| Phase   | $n_A$ | $n_B$ | $n_C$ | $n_D$ | $D_{occ}$ | $n_s$ | $n_f$ | PS state       |
|---------|-------|-------|-------|-------|-----------|-------|-------|---------------|
| NOA     | $n$   | $n$   | $n$   | $n$   | $n/2$     | $0$   | $2$   | NO$_0$/NO$_2$ |
| NOB     | $n$   | $n$   | $n$   | $n$   | $0$       | $0$   | $1$   | NO$_0$/NO$_1$ |
| CBOA    | $2n$  | $0$   | $2n$  | $0$   | $n/2$     | $0$   | $1$   | NO$_0$/CBO$_2$|
| CBOB    | $2n$  | $0$   | $2n$  | $0$   | $0$       | $0$   | $1/2$ | NO$_0$/CBO$_1$|
| CBOC    | $2n$  | $0$   | $2n$  | $0$   | $n - 1/2$ | $1/2$ | $1$   | CBO$_1$/CBO$_2$|
| CBO$_D$ | $1$   | $2n - 1$ | $1$   | $2n - 1$ | $0$       | $1/2$ | $1$   | CBO$_1$/NO$_1$ |
| STOA    | $2n$  | $2n$  | $0$   | $0$   | $n/2$     | $0$   | $1$   | NO$_0$/STO$_2$|
| STOB    | $2n$  | $2n$  | $0$   | $0$   | $0$       | $0$   | $1/2$ | NO$_0$/STO$_1$|
| STOC    | $2n$  | $2n$  | $0$   | $0$   | $n - 1/2$ | $1/2$ | $1$   | STO$_1$/STO$_2$|
| STOD    | $1$   | $2n - 1$ | $2n - 1$ | $1$   | $0$       | $1/2$ | $1$   | STO$_1$/NO$_1$ |
| FNOA    | $4n$  | $0$   | $0$   | $0$   | $n/2$     | $0$   | $1/2$ | NO$_0$/FNO$_2$|
| FNOB    | $4n$  | $0$   | $0$   | $0$   | $0$       | $0$   | $1/4$ | NO$_0$/FNO$_1$|
| FNO$_C$ | $4n$  | $0$   | $0$   | $0$   | $n - 1/4$ | $1/4$ | $1/2$ | FNO$_0$/FNO$_2$|
| FCBOA   | $2$   | $0$   | $4n - 2$ | $0$   | $n/2$     | $1/2$ | $1$   | FNO$_0$/CBO$_2$|
| FCBO$_B$| $2$   | $0$   | $4n - 2$ | $0$   | $n - 1/2$ | $3/4$ | $1$   | FCBO$_1$/CBO$_2$|
| FCBOC   | $2$   | $0$   | $4n - 2$ | $0$   | $1/4$     | $1/2$ | $3/4$ | FNO$_0$/FCBO  |
| FCBO$_D$| $1$   | $0$   | $4n - 1$ | $0$   | $0$       | $1/4$ | $1/2$ | FNO$_0$/CBO$_1$|
| FCBO$_E$| $1$   | $0$   | $4n - 1$ | $0$   | $n - 1/2$ | $1/2$ | $3/4$ | CBO$_1$/FCBO  |
| FCBOF   | $1$   | $4n - 2$ | $1$   | $0$   | $0$       | $1/2$ | $3/4$ | CBO$_1$/FNO$_0$|
| FCBO$_G$| $1$   | $4n - 3$ | $1$   | $1$   | $0$       | $3/4$ | $1$   | FNO$_0$/NO$_1$ |
| FSTOA   | $2$   | $4n - 2$ | $0$   | $0$   | $n/2$     | $1/2$ | $1$   | FNO$_0$/STO$_2$|
| FSTOB   | $2$   | $4n - 2$ | $0$   | $0$   | $1/4$     | $1/2$ | $3/4$ | FNO$_0$/FSTO  |
| FSTOC   | $2$   | $4n - 2$ | $0$   | $0$   | $n - 1/2$ | $3/4$ | $1$   | FSTO$_1$/STO$_2$|
| FSTOD   | $1$   | $4n - 1$ | $0$   | $0$   | $0$       | $1/4$ | $1/2$ | FSTO$_1$/STO$_1$|
| FSTOE   | $1$   | $4n - 1$ | $0$   | $0$   | $n - 1/2$ | $1/2$ | $3/4$ | STO$_1$/FSTO  |
| FSTOF   | $1$   | $1$   | $4n - 2$ | $0$   | $0$       | $1/2$ | $3/4$ | STO$_1$/FNO$_0$|
Fig. 3(c)) the FCBO phase occurs and thus this boundary vanishes at $T > 0$. The situation changes for FCBO$_D$–FCBO$_E$ and FCBO$_D$–FCBO$_F$ boundaries (e.g. Fig. 3(d)), where for $n = 1/2$ the CBO$_1$ phase occurs at $T = 0$. As a result at small $T > 0$ the FCBO–CBO–FCBO sequence of transitions with changing $n$ is present. For the ground state FNO$_C$–FSTO$_B$ boundary (Fig. 3(b)), the FNO$_2$ phase is stable at $n = 1/2$ and
Finally, let us comment on transitions with changing $W_2/|W_1|$ for fixed $n$. All horizontal ground state boundaries, for $W_2 \neq 0$ remain discontinuous at $T > 0$. At the specific case of $W_2 = 0$ the CBO–FCBO and CBO–FNO boundaries are second order at nonzero temperatures (cf. also Ref. [53]). Moreover, the ground state CBO$_A$–CBO$_B$ and CBO$_A$–CBO$_C$ boundaries vanish at any finite $T$ for $W_2 = 0$ (cf. Refs. [49, 51, 52]).

C. The case of attractive $W_1$

To provide the full picture of the system ground state we present results obtained for the attractive nearest-neighbour interaction ($W_1 < 0$).

This case is less complex than a case of $W_1$ as the qualitative behaviour of the system is not dependent on a magnitude of the on-site interaction (only the sign of $U$ is relevant). For attractive $W_1$ only possible phases are either nonordered or stripe-ordered (STO) phases. In the case of $U < 0$ only phases with empty or double-occupied sites are realized (Fig. 4(a)), whereas for $U > 0$ the phases with single-occupied sites emerge (Fig. 4(b)). All phase boundaries are discontinuous. The above behaviour of the system is preserved also at small, but finite temperatures.

Similarly to the previous analyses, in Fig. 5 we present the phase diagrams as a function of concentration $n$. In this case the corresponding PS states (cf. Table II) possess lower energies than homogeneous phases in the full range of the model parameters (excluding vertical boundaries in Fig. 5). The attractive $W_2$ favours the PS states between nonordered phases, whereas repulsive $W_2$ gives rise to PS states involving various STO phases. Homogeneous phases on the vertical boundaries ($n = i/2$, $i = 1, 2$) can be read from Fig. 4 and Table I. On the horizontal boundaries the PS states from both neighboring regions have equal energies and they coexist. Moreover, at infinitesimally $T > 0$ the diagrams do not change and the PS states still occur.

III. LOW DIMENSIONAL SYSTEMS

So far we have discussed the mean-field solutions of the model, which is an exact theory in high dimensions (formally $d \rightarrow +\infty$, $z_n \rightarrow +\infty$) [54–56]. In this section we discuss the qualitative behavior of lower dimension systems, which fulfill the four-sublattice restriction. In particular, we consider the 1D chain, 2D square (SQ) lattice, and 3D base-centered cubic (BCC) lattice. For the 3D one we choose the BCC lattice because (unlike simple cubic or face-centered cubic lattices) it can be divided into four equivalent sublattices.

A set of four sublattice concentrations $(n_A n_B n_C n_D)$ defines an elementary block. These blocks can be grouped in types. All blocks of a given type can be obtained by a cyclic change of sublattice indices, e.g., the
block alignment in $d = 2$. Note that the FNO block at the interface between the NO and CBO phases emerge (shadow, dotted line). For $W_2/|W_1| < 0$ the FNO block does not yield the minimal energy.

The FCBO type consists of four different elementary blocks, namely $[(2010), (0201), (1020), (0102)]$. Any elementary block of a ground state configuration must be among those that yield the minimal energy when extended periodically [40, 57–60]. In other words, in a construction those that yield the minimal energy when extended periodically must be among $(2010), (0201), (1020), (0102)$. Any elementary block of these phases are respectively $00$ and $11$. In Fig. 6 we show that if such blocks would be aligned next to each other the region with block $01$ would always be created that does not yield the minimal energy. In such a case even though both phases possess equal energies the ground state cannot be built of the composition of them, but it must “choose” one of the solutions. Then a coexistence of the phases can be realized only on a macroscopic level and only if

(i) **Nonmixing case.** In this case on the boundaries between two phases the state of the system can be constructed by periodical repetition of only one type of elementary block. In other words each elementary block of one type cannot be aligned next to a block of a different type. As an example of such a situation let us consider the NO–CBO boundary. The elementary blocks of these phases are respectively $00$ and $11$. In Fig. 6 we show that if such blocks would be aligned next to each other the region with block $01$ would always be created that does not yield the minimal energy. In such a case even though both phases possess equal energies the ground state cannot be built of the composition of them, but it must “choose” one of the solutions. Then a coexistence of the phases can be realized only on a macroscopic level and only if

(ii) **Partial mixing.** In Figs. 2 and 4 dashed-lines denote boundaries at which elementary blocks of different types can be aligned next to each other, but not arbitrarily (at $d = 2$). Some restrictions on a block’s configuration remains. An example of this type of the boundary occurs between the CBO$_1$ and STO$_1$ phases (see Fig. 7). We notice that if $\frac{1}{0}$ and $\frac{1}{1}$ blocks are aligned next to each other (in a given direction) we cannot find any region built of elementary blocks which does not belong to one of the phases with minimal energy (CBO$_1$ or STO$_1$). Specifically, it means that every column (or row) of blocks has to be purely built of one type of elementary blocks, whereas blocks can be freely aligned in rows (or columns). We note that opposed to non-mixing regime here we get microscopical mixing of each phase, but some macroscopic ordering remains as rows (or columns) are build of one type of elementary blocks. At such boundaries degeneracy $\Gamma$ of the system is infinite but not macroscopic (modulo spin), i.e., it increases with size of the system (i.e., with $L$) lower than $bA^L$ (where $b$ and $A$ are some fixed numbers; $0 < A < 3$) (entropy per site in the thermodynamical limit $s = \lim_{L \to +\infty} \frac{1}{L} \ln \Gamma$ is zero). Such boundaries at $d = 2$ are denoted by dashed lines in Figs. 2 and 4.

(iii) **Full mixing.** Solid lines in Fig. 2 denote boundaries at which elementary blocks of neighboring regions can be aligned freely without any restrictions for $d = 2$ (macroscopic degeneration). As an example one can consider the FCBO-CBO$_1$ boundary; see Fig. 8. In this case the system is micro-
For $d = 1$ the boundaries with infinite degeneration in Figs. 2 and 4 (dashed and solid lines) are macroscopically degenerated. In such a dimensionality of the system there is no partial-mixing at the boundaries.

Away from boundaries, in regions filled by the slantwise pattern in Fig. 2, two configurations of elementary blocks of the same phase can be mixed with each other, but arbitrarily. This situation is similar to a case of the partial mixing at phase boundaries. In low dimensions ($d = 1, 2$) mixing of the same type of elementary blocks but in different configurations (e.g. $\frac{2}{4}$ 0 and $\frac{1}{2}$ 0) leads to increased disorder in contrary to $d = 3$ case, where one configuration is present in whole system. Analogously to partial mixing, in the discussed cases every column (row) of blocks have to be purely built of elementary blocks in the same configurations, but blocks can vary from row to row (column to column), cf. Fig. 7. The ground state for $d = 2$ marked by the slantwise pattern in Fig. 2 has infinite degeneration, but it is not macroscopic (cf. Table I). For $d = 1$ the degeneracy in these regions is macroscopic.

To reach the situation, where in these regions a long-range charge-order would be present, an arbitrary weak interaction between third-nearest neighbors ($W_{3} \neq 0$) is sufficient. $W_{3} < 0$ gives long-range order of the four-sublattice type for SC and BCC lattices (for $W_{3} > 0$ 4 × 2 (eight-sublattice) orderings need to be considered) [61, 62]. In a case of 1D chain the long-range order appears for $W_{3} > 0$, whereas $W_{3} < 0$ stabilizes eight-sublattice orderings.

The phases with single-occupied sites are infinitely (macroscopically) degenerate with respect to spin degrees of freedom and thus the model considered does not exhibit any magnetic order in any dimension.

Similarly as the Ising model with short-range interactions, model (1) considered on one-dimensional lattice does not exhibit long-range order at any $T > 0$ for any model parameters [38, 48]. For the two-dimensional lattice the order above the ground state CBO, STO and FCBO, regions (i.e., nonfilled regions in Fig. 2) would occur for fixed $\bar{\mu}$ [40, 41, 63–66]. At incommensurate fillings one should expect the order at $T > 0$ also in the FCBO and FCOB regions as well as in regions where the PS states are stable at $T = 0$. For $d \geq 3$ the order should be present at small $T > 0$ for all model parameters (excluding those for which the NO phase occurs at $T = 0$).

IV. FINAL REMARKS

We considered the zero-bandwidth extended Hubbard model taking into account longer-range (NN and NNN) interactions. It was found that such correlations give rise to four-sublattice solutions for $W_{2} > 0$ at the mean-field level (with exact treatment of the on-site term). We indicated that these new phases emerge at a given magnitude of the on-site interactions $U$. It was shown that the FNO phase is present for arbitrary values of $U$, and the FSTO phase occurs only for repulsive $U$, while the FCBO phase is limited by the $0 < U < W_{1}$ condition. For fixed electron concentration the system is highly degenerated, but arbitrary small temperature ($T > 0$) removes this degeneracy. We also show that not all phase transitions occurring at $T = 0$ remain first-order at finite temperatures. They are second-order ones at $T > 0$.

We discussed the influence of the lattice dimensionality $d$ on the degeneracy of the ground state (for fixed $\mu$). For the $d = 3$ lattice the results are in an agreement with the mean-field findings and finite degeneracy is present for arbitrary model parameters. In a case of lower dimensionalities ($d = 1, 2$) the appearance of the partial and full mixing of the elementary blocks gives rise to infinite degeneracy. We showed also that four-sublattice long-range order in low dimensions is suppressed (in the FNO and FSTO phases), but in the FCBO phase the long-range order remains.

Finally, let us note that in this work we analyzed the system neglecting the influence of the electron hopping term. It is known that finite hopping induces additional magnetic orderings [8, 67–70]. The other aspect related to quantum fluctuations introduced by the hopping is a metal-insulator transition. Basing on the results obtained for two sublattice assumption (for $W_{2} = 0$) [6–9] one can expect that CBO and STO phases for $W_{2} \neq 0$ should survive in a presence of such fluctuations. It is an open question whether other orderings (i.e., FNO, FCBO, and FSTO) will also remain (in insulating or metallic states). Although our system is simplified for this point, the results obtained here are exact solutions.
Therefore, they can be used to inspect the validity of approximations used to the more general models including single-electron hopping.

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Appendix A: The equivalent models

One can show (cf. e.g. Refs. [40, 43]) that model (1) is equivalent with the classical Blume-Capel model with spin $S = 1$ [71–74] in the external magnetic field, which has the following form

$$\hat{H}_{BC} = \Delta \sum_i \left(\tilde{S}_i^z\right)^2 + \frac{1}{2} \sum_{i,j} J_{ij} \tilde{S}_i^z \tilde{S}_j^z - H \sum_i \tilde{S}_i^z + C, \quad (A1)$$

where $\Delta = \frac{1}{2} U + k_B T \ln(2)$ is temperature-dependent single-ion anisotropy, $J_{ij} = W_{ij}$, $H \equiv \tilde{\mu} = \mu - U/2 - \sum_n \tilde{\mu}_n W_n$, $C = L (k_B T \ln(2) + \tilde{\mu})$. For $U \to -\infty$ models (1) and (A1) are reduced to the standard $S = 1/2$ Ising model ($\tilde{S}_i^z = \pm 1$) [64–66, 75–77]. At $T = 0$ for $U = 0$ models (1) and (A1) are reduced to the $S = 1$ Ising model ($\tilde{S}_i^z = -1, 0, 1$). In Eq. (A1) we do not restrict the range of intersite interactions.

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