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Effects of Frustrating Hopping on Charge Ordered States in Itinerant Fermion Systems for Arbitrary Concentration in 2D Lattice

W.R. Czart*, P.R. Grzybowski, M. Nogala and S. Robaszkiewicz

Faculty of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

There is ongoing, intense, research in the field of electron charge orderings (CO) and charge density waves phenomena, due to experimental discovery of such phases in numerous important compounds. The aim of this work is to extend recent advances in the field by studying two simple effective paradigmatic models used to describe CO in narrow band materials i.e. (i) a model of correlated electrons: the so-called t–W model of spinless fermions with repulsive interaction W and (ii) the molecular crystal model with the coupling of electrons to intramolecular (crystal field) vibrations in the static limit. The finite temperature phase diagrams are evaluated at arbitrary carriers concentration for several representative cases. Our calculations are performed within the (broken symmetry) HFA for $d = 2$ square lattice and arbitrary carriers concentration. In this contribution we focus on the effects of next-nearest-neighbor hopping on the CO states in these systems and the problem of phase separations involving checkerboard CO with the nesting vector $\boldsymbol{Q} = (\pi, \pi)$. The results we show here are an extension of our previous work on the subject.

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1. Introduction

Charge orderings (CO) and charge density waves phenomena have been discovered experimentally in many important materials including manganites, cuprates, several nickel, vanadium and cobalt oxides, heavy fermion systems and numerous organic conductors (see e.g. [1–14] and references therein). The CO phenomena in narrow band materials can be explained on the bases of two main mechanisms: electron correlations and electron-lattice couplings. Here, as in our recent papers [12, 15, 16] we study this subject using the following two effective models: (i) model of correlated electrons — the so-called t–W model of spinless fermions with repulsive intersite interaction W [12, 16] and (ii) a model of electron-lattice interactions — the molecular crystal (MC) model in the static limit, with electrons coupled to intramolecular (crystal field) vibrations [15, 16].

So far our analysis has been mainly concentrated on the problem of phase separations (PS) involving checkerboard CO [12, 15] for arbitrary concentration and the exact half-filling case for MC and t–W models at the ground state.

In present work we analyze the finite temperature phase diagrams of these models for $d = 2$ square lattice. The calculations are performed within the (broken symmetry) HFA. In the study we take into consideration the effects of frustrating next-nearest-neighbor hopping t_2 on the charge ordered states in these systems at arbitrary concentration. We focus on the problem of homogeneous phases and PS(CO/NO) with the nesting vector $\boldsymbol{Q} = (\pi, \pi)$. The results we show are an extension of our previous work on the subject.

Here we present, for the first time, an overview of the effects of next-nearest-neighbor hopping t_2 on the finite temperature phase diagrams involving the CO states of the t–W and the MC models for $d = 2$ square lattice.

The model Hamiltonians have the following form: (i) the t–W model with intersite density interaction [12, 14, 16]:

$$\hat{H} = \sum_{ij} t_{ij} \hat{c}_i^+ \hat{c}_j + \frac{1}{2} \sum_{ij} W_{ij} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i,$$
$$n_s = \frac{N_s}{N} = \frac{1}{N} \sum_i \langle \hat{n}_i \rangle, \quad 0 < n_s < 1. \tag{1}$$

(ii) the MC model [14, 15, 16]:

$$\hat{H} = \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \frac{1}{\sqrt{N}} \sum_{iqv} A_{qv}^E \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_i} n_i \hat{\varphi}_{qv}$$
$$+ \sum_{qv} \Omega_{qv} \hat{b}_{qv}^+ \hat{b}_{qv} - (\mu - E) \sum_{i\sigma} \hat{n}_{i\sigma},$$
$$n_e = \frac{N_e}{N} = \frac{1}{N} \sum_{i\sigma} \langle \hat{n}_{i\sigma} \rangle, \quad 0 < n_e < 2. \tag{2}$$

In both models t_{ij} are the single particle hopping integrals (between the nearest neighbors t and the next nearest neighbors t_2), μ — the chemical potential.

* corresponding author; e-mail: czart@amu.edu.pl

In the model (1) $\hat{c}_i^+(\hat{c}_i)$ are the creation (annihilation) operators for spinless fermions on site i, $\hat{n}_i = \hat{c}_i^+\hat{c}_i$, W_{ij} are the intersite density–density interactions, assumed to be repulsive ($W_{ij} > 0$), and restricted to nearest neighbors.

In the model (2) $\hat{c}_{i\sigma}^+(\hat{c}_{i\sigma})$ are the creation (annihilation) operators for fermions on site i, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^+\hat{c}_{i\sigma}$, A_{qv}^E terms describe the coupling of electrons to various types of intramolecular (or cation — ligand) vibrations via modulation of the molecular (crystal field) energy E, Ω_{qv} are the phonon branches, arising from these intramolecular (cation–ligand) vibrations [14], $\hat{b}_{qv}^{(+)}$ are phonon operators of the v-th phonon branch, $\hat{\varphi}_{qv} = \hat{b}_{qv} + \hat{b}_{qv}^+$. We restrict considerations to the static limit and assume that the macroscopic distortions are caused by phonon modes with $\boldsymbol{q} = \boldsymbol{Q}$ ($\boldsymbol{Q}$ — half the smallest reciprocal lattice vector). Therefore we put [14]

$$\hat{b}_{qv}^{(+)} \to \langle \hat{b}_{qv}^{(+)} \rangle = \frac{1}{2}\sqrt{N}\langle\hat{\varphi}_{qv}\rangle\delta_{|\boldsymbol{q}|,\boldsymbol{Q}},$$
$$\hat{\varphi}_{qv} \to \sqrt{N}\varphi_{qv}\delta_{|\boldsymbol{q}|,\boldsymbol{Q}}, \tag{3}$$

neglecting all phonons with $\boldsymbol{q} \neq \boldsymbol{Q}$ and determining the classical field φ_{Qv} by minimizing of the free energy (for macroscopic distortion the phonon amplitudes may be treated classically i.e. the large quantum number correspondence-principle).

We have performed extensive studies of both models for arbitrary concentrations [17]. Below we only shortly summarize the main findings presenting selected finite temperature phase diagrams which have been evaluated at arbitrary concentration, by comparing the free energies of the homogeneous phases (CO, NO) and the PS states.

2. Results and discussion

We use the following notation (for $d = 2$ SQ lattice): $W_0 = 2dW/t$, for the model (1) and $G = \frac{G_{\boldsymbol{Q}}^E}{t}$, where $G_{\boldsymbol{Q}}^E = \sum_v \frac{4(A_{Qv}^E)^2}{\Omega_{Qv}}$, for the model (2), $b = t_2/t$.

In the model (1) the CO phases are characterized by the electron CO parameter:

$$\Delta_{\boldsymbol{Q}}^s = \frac{1}{N}\sum_i \langle\hat{n}_i\rangle \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i} \neq 0, \tag{4}$$

where $\boldsymbol{Q} = (\pi, \pi)$, whereas in the model (2) by:

$$\Delta_{\boldsymbol{Q}}^e = \frac{1}{N}\sum_{i\sigma} \langle\hat{n}_{i\sigma}\rangle \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i} \neq 0, \tag{5}$$

and simultaneously by the static internal distortions:

$$\varphi_{Qv} = -\frac{2A_{Qv}^E\Delta_{\boldsymbol{Q}}^e}{\Omega_{Qv}} \neq 0. \tag{6}$$

Obviously, the following relation also holds:

$$\Delta_{\boldsymbol{Q}}^e = -\sum_v 2A_{Qv}^E\varphi_{Qv}/G_{\boldsymbol{Q}}^E. \tag{7}$$

2.1. The phase diagrams in the absence of frustration ($t_2 = 0$)

In the absence of frustration ($t_2 = 0$) at half-filling (i.e. for $n_s = 0.5$ for the t–W model and $n_e = 1$ in case of the MC model) and considering the phase separation involving CO [12], the ground state (G S) of both models for $d \geq 2$ hypercubic lattices is homogeneous CO for any interaction strength W_0, $G > 0$ (see Figs. 1a,b and 2a,b in [16]), which is in agreement with the renormalization group results for $d \geq 2$ lattices [18].

At arbitrary concentration with increasing temperature the systems discussed can exhibit several different types of behavior. For the MC model one can observe either : (i) a sequence of two transitions PS(CO/NO) → CO → NO, or (ii) a single 1st order transition PS → NO, or (iii) a single 2nd order transition CO → NO at half-filling only. In Fig. 1b we show the T–n phase diagram of the MC model for $d = 2$ lattice and a representative value of G. The diagram is qualitatively different from the analogous diagram for the t–W model (Fig. 1a). On the diagram for the t–W model in definite ranges of n and W_0 one finds the reentrant charge-order phenomena: NO → CO → NO or NO → PS → CO → NO. On the diagram of the MC model the PS (CO/NO) state extends over much larger area of a phase space, preventing the reentrant CO transition.

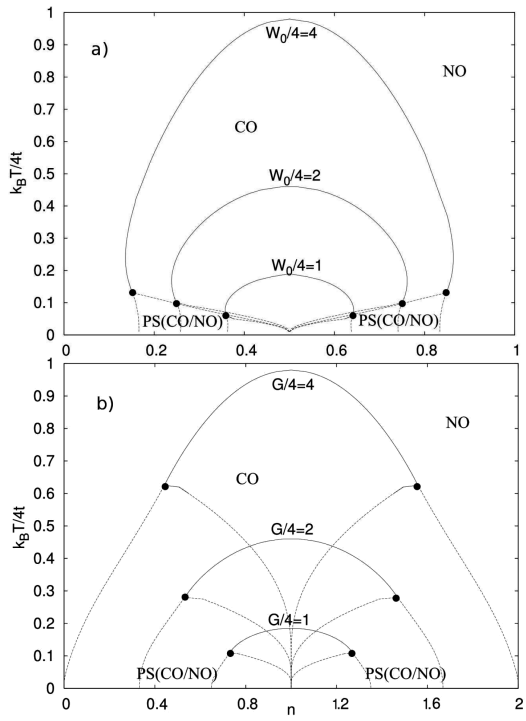

Fig. 1. Finite temperature phase diagram plotted for $d = 2$, $t_2 = 0$ and fixed interaction values: (a) t–W model, (b) MC model. Transitions between NO and PS(CO/NO) phases and between PS(CO/NO) and CO are of the first order; transition between NO and CO phases are of the second order. Filled dots denote the tricritical points (TCP).

2.2. The effects of frustration ($t_2 \neq 0$)

The next-nearest-neighbor hopping t_2 breaks the electron-hole symmetry of the systems considered and it can substantially change the structure of the phase diagrams (compare Fig. 1 with Fig. 2).

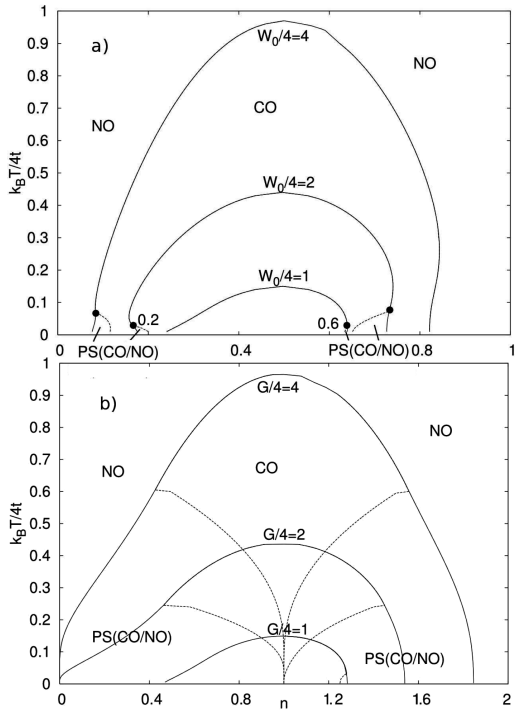

Fig. 2. Finite temperature phase diagrams for $b = -0.45$, $d = 2$ and a few fixed interaction values. TCP — the point where the second order transition line (above TCP) and the first order transition lines (below TCP) meet. (a) t–W model, (b) MC model.

For both models the frustration introduced by t_2 at half-filling suppresses the perfect nesting instability towards CO phases at weak interactions strength W_0 (or G).

In the presence of large frustration the GS phase diagrams are considerably changed when compared to the case $t_2 = 0$ (see Ref. [15]).

For $T > 0$ and $t_2 \neq 0$ in the t–W model one can observe several different sequences of transitions with increasing T depending on carrier concentration:

(i) at half filling, a single second order transition: CO $\rightarrow$ NO. It occurs if the ground state is CO,

(ii) a sequence of two transitions: PS $\rightarrow$ CO $\rightarrow$ NO,

(iii) a single 1st order transition PS $\rightarrow$ NO,

(iv) the reentrant charge-order phenomena NO $\rightarrow$ CO $\rightarrow$ NO or NO $\rightarrow$ PS $\rightarrow$ CO $\rightarrow$ NO.

Similar features are also found for the MC model but the latter model does not show the reentrant charge-order phenomena.

3. Conclusions

We have presented results for the t–W spinless model with repulsive intersite interaction W and the MC model in the static limit considering two homogenous phases (NO, CO) and the PS(CO/NO) states, for $d = 2$ SQ, non-frustrated ($t_2 = 0$) and frustrated ($t_2 \neq 0$) lattices, at arbitrary fillings at the ground state and finite temperatures. We have restricted our study to the two-sublattice CO case. We have found various first and second order phase transitions, possible sequences of transitions and critical points.

We compared results for the MC model with the analogous results for the t–W model. Generally we may conclude that for both models, the increasing interaction parameters increase critical temperature and extend the regions of CO phases stability on the phase diagrams. For both models phase transitions to the PS states are of the first order, while phase transitions to homogeneous CO phase are continuous, of the second order. In the absence of frustration the diagrams are symmetrical against the line of half filling. At the case of half filling below critical temperature analyzed systems are at homogeneous CO state both with and without frustration for considered frustration strength $b = -0.45$. For all shown cases there are the tricritical points where the studied phases meet.

In spite of many similarities the diagrams for both models show also lots of differences.

The PS(CO/NO) states are favored by the MC model and they are stable in much more extended ranges of n and T than in the case of the t–W model, as it is clearly seen on corresponding phase diagrams.

In a definite range of W_0 and n the t–W model can exhibit the reentrant charge-order phenomena (the transitions: NO $\rightarrow$ CO $\rightarrow$ NO or NO $\rightarrow$ PS $\rightarrow$ CO $\rightarrow$ NO with increasing T) (cf. Figs. 1a and 2a), and this feature is absent in the MC model.

More detailed discussion of the case of PS involving not only two-sublattice CO but also collinear CO for arbitrary concentration and $T \neq 0$ will be given elsewhere [17].

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