Phase diagram regions deduced for strongly correlated systems 
via unitary transformation

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Abstract

From known phase diagram regions of different model Hamiltonians describing strongly correlated systems we deduced new domains of the ground state phase diagram of the same model by an unitary transformation. Different types of extended Hubbard Hamiltonians were used for the starting point and the existence of new stable spin-density wave, charge-density wave, ferromagnetic state and a paramagnetic insulator is demonstrated. The used procedure itself is dimension independent.
I. INTRODUCTION

Because of their interesting properties, the strongly correlated systems polarized a huge effort in last decades given in specially by developments in high critical temperature superconductivity (Degiorgi 1999), heavy-fermion systems (Mathur et al. 1998), metal-insulator transition and layered materials (de Boer et al. 1999). The rigorous results obtained in this field are related mainly to one dimensional case being deduced by Bethe anzats and exact result for \( D > 1 \) are extremely rare. Generated by these state of facts, in this paper an interesting procedure is presented that allows the construction of new exact ground states (GS) in arbitrary dimensions for strongly correlated systems starting from known domains of the phase diagram of a given model in the same dimension. The essence of the method is simple. Given an examined Hamiltonian \((H)\) together with its ground state \(\psi_g\) valid in a restricted region of the phase diagram \(R\), based on an unitary transformation \(UU^\dagger = 1\) we obtain \(H' = UHU^\dagger, \psi'_g = U\psi_g\). The eigenvalues being unmodified by an unitary transformation, \(\psi'_g\) represents the GS wave function for \(H'\). For a class of analysed Hamiltonians, \(H\) can be given however with a coupling constant set \(\{g_i\}\) and an operatorial terms set \(\{O_i\}\) as \(H = \sum_i g_i O_i\). Taking \(U\) in such a way to transform the components \(O_i\) within the \(\{O_i\}\) set (i.e. \(UO_{i_1} = O_{i_2}\)), the unitary transformation change in fact \(\{g_i\}\) to \(\{g'_i\}\). Based on this observation, from \(R\), the transformed \(R'\) region can be deduced, \(R'\) being the parameter space region where \(\psi'_g\) is valid.

In this paper we are using an explicitely given \(U\) unitary transformation that transforms a spin density wave (SDW) into a charge density wave (CDW) wave function, a superconductor into a ferromagnet, a phase separation in spin into a phase separation in charge, and vice versa. The \(\{O_i\}\) operatorial set is so fixed to preserve the analysed model in the class of extended Hubbard models. The concretely analysed cases are connected to the model used by de Boer at al. (1995 a, b) and Montorsi and Campbell (1996) describeing superconducting properties, and Strack and Vollhardt (1993) and Aligia et al. (1995) studying different density wave phases. Our results underline the presence of new ferromagnetic, SDW and
insulating GS wave functions in the phase diagram of the enumerated models.

The remaining part of the paper is constructed as follows: in Chapter II. we describe the family of the model Hamiltonians that we analyse and define our unitary transformation $U$ used during the paper. Chapter III. contains the study of different concrete Hamiltonians and the results obtained. In Chapter IV. we present the summary, and Appendices containing the mathematical details close the paper.

II. THE SYSTEM AND METHOD USED

For the starting point we are introducing below a class of model Hamiltonians that are used in the remaining part of the paper for the exemplification of the used procedure.

A. The studied class of models.

We are developing here our study in a class of extended Hubbard models that generically can be given in the following form

$$\hat{H} = -t\hat{t} + U\hat{U} + X\hat{X} + V\hat{V} + J_z\hat{J}_z + \frac{J_{xy}}{2}\hat{J}_{xy} + Y\hat{Y} + R\hat{R}$$
$$+ P\hat{P} + Q\hat{Q} + \mu \sum_{j=1}^{N} n_j + \hbar \sum_{j=1}^{N} \left( n_{j\uparrow} - n_{j\downarrow} \right).$$

(1)

In this expression a general $A\hat{A}$ term represent the contribution of the $\hat{A}$ operator in the extended Hubbard Hamiltonian $H$, taken into account with the coupling constant $A$. The terms taken into consideration, in order, are the following.

The kinetic energy contribution has the form

$$\hat{t} = \sum_{<j,i>,\sigma} \left( c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{j\sigma} \right),$$

(2)

where $c_{i\sigma}$ are canonical Fermi operators which describe electrons on a d-dimensional lattice, $<j,i>$ denoting nearest-neighbor sites. The Hubbard on-site interaction is taken as

$$U\hat{U} = U \sum_{j=1}^{N} \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{j\downarrow} - \frac{1}{2} \right),$$

(3)
where $U$ represents the Hubbard coupling and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ denotes the particle number operator for electrons with spin $\sigma$ on site $i$. The bond-charge interaction is taken as

$$\hat{X} = \sum_{<i,j>,\sigma} \left( c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{j\sigma} \right) \left( n_{j,-\sigma} + n_{i,-\sigma} \right).$$

(4)

For a density-density type interaction we have taken into account the

$$\hat{V} = \sum_{<j,i>} \left( n_j - 1 \right) \left( n_i - 1 \right),$$

(5)

contribution that describes a nearest-neighbor Coulomb interaction.

Heisenberg type spin-spin interactions follow written for spin densities. These interactions have been taken anisotropic and are represented by

$$\hat{J}_z = \sum_{<j,i>} S_j^z S_i^z$$

(6)

$$\hat{J}_{xy} = \sum_{<j,i>} \left( S_j^+ S_i^- + S_j^- S_i^+ \right).$$

(7)

The spin operators in this expression are standard, namely $S_j^z = 1/2 (n_{j\uparrow} - n_{j\downarrow})$, $S_j^+ = c_{j\uparrow}^\dagger c_{j\downarrow}$, $S_j^- = c_{j\downarrow}^\dagger c_{j\uparrow}$.

A pair hopping term follows given by the Hamiltonian term

$$\hat{Y} = \sum_{<j,i>} \left( c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \right).$$

(8)

After this step three-particle interactions are taken into consideration. A correlated hopping term testing the opposite spin occupancy along the bond of the hopping is represented by

$$\hat{R} = \sum_{<j,i>,\sigma} \left( c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{j\sigma} \right) n_{j,-\sigma} n_{i,-\sigma}.$$  

(9)

Correlation effects produced by an empty site or a double occupancy are described by

$$\hat{P} = \sum_{<j,i>} \left[ \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{j\downarrow} - \frac{1}{2} \right) \left( n_i - 1 \right) + \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) \left( n_j - 1 \right) \right].$$

(10)

Finally, a four-particle interaction takes into consideration a double occupancy - double occupancy type correlation effect along different bonds

$$\hat{Q} = \sum_{<j,i>} \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{j\downarrow} - \frac{1}{2} \right) \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right).$$

(11)
Furthermore, in the starting Hamiltonian given in Eq.(1), $\mu$ represents the chemical potential, and $h$ is the external magnetic field applied in $z$ direction.

Concerning the notations from the Hamiltonian $\hat{H}$ we mention some limiting cases that emerges during the presentation. When the Heisenberg type interaction Eq.(7) becomes isotropic, the notation of the coupling constant becomes $W = J_z = J_{xy}$ and the corresponding Hamiltonian term is denoted by

$$\hat{W} = \sum_{<j,k>} \vec{S}_j \cdot \vec{S}_k,$$

where we have $\vec{S}_j \cdot \vec{S}_k = S_j^z S_k^z + 1/2 ( S_j^+ S_k^- + S_j^- S_k^+ )$. Furthermore, in case of $V = Y$, the common notation of the $V\hat{V} + Y\hat{Y}$ interactions becomes $S\hat{S}$ where

$$\hat{S} = \sum_{<j,k>} \vec{S}_j \cdot \vec{S}_k = \sum_{<j,k>} \left[ S_j^z S_k^z + \frac{1}{2} \left( S_j^+ S_k^- + S_j^- S_k^+ \right) \right],$$

where $S_j^z = \frac{1}{2} ( n_{j\uparrow} + n_{j\downarrow} - 1 )$, $S_j^+ = c_{j\uparrow} \dagger c_{j\downarrow}$, $S_j^- = c_{j\downarrow} c_{j\uparrow}$.

In the following paragraph we are presenting some basic wave functions that emerge during the paper.

**B. The applied wave functions.**

We are presenting in this Section the ground state wave functions used during the paper.

The superconductor state is considered in the form of an $\eta$-pairing state as follows

$$| \Psi_\eta \rangle = \left( S_+ \right)^{N_\eta} | 0 \rangle,$$

where $| 0 \rangle$ is the bare vacuum with no fermions present, and

$$S_+ = \sum_{i=1}^N e^{iP_i} c_{i\uparrow} \dagger c_{i\downarrow} \dagger,$$

creates the $\eta$-pairs within the system. Here $N$ represents the number of lattice sites, and $N_\eta$ the number of $\eta$-pairs present.

The ferromagnetic wave-function is taken as
\[ |\Psi_F\rangle = \prod_{i \in B} \prod_{j \in B'} c^\dagger_i c^\dagger_j |0\rangle, \]  

(16)

where \( B \) and \( B' \) are arbitrary disjoint sets of lattice points, which together build up the whole lattice. The number of components in \( B \) and \( B' \) is considered different.

The density wave functions considered are the following. The spin-density-wave (SDW) state is given by

\[ |\Psi_S\rangle = \prod_{i \in A} \prod_{j \in A'} c^\dagger_i c^\dagger_j |0\rangle, \]  

(17)

where \( A \) and \( A' \) represent sublattices of a given lattice. We mention that during the paper, in case of density waves we are working on bipartite lattice with odd and even sublattices.

In case of charge-density wave (CDW) we have

\[ |\Psi_C\rangle = \prod_{i \in A} c^\dagger_i c^\dagger_i |0\rangle, \]  

(18)

where the \( A \) has the meaning of a sublattice.

C. The unitary transformation used

The unitary transformation that we analysed during the paper has the form

\[ U = \prod_{i=1}^{N} (e^{iP_i} c^\dagger_{i\dagger} + c_{i\dagger}). \]  

(19)

As presented in Appendix 1, \( U \) given in Eq. (19) represents indeed an unitary transformation. It transforms the presented wave functions (see Appendix 2. for details) as follows

\[ U |\Psi_\eta\rangle = |\Psi_F\rangle, \]

\[ U |\Psi_S\rangle = |\Psi_C\rangle. \]  

(20)

Based on Eq. (19) the Hamiltonian from Eq. (1) can be unitary transformed. This procedure may be started with the transformation of the creator and annihilator operators (details presented in Appendix 3.).
\[ U_{c\uparrow} U^\dagger = (-1)^N c_{i\uparrow}, \]
\[ U_{c\downarrow} U^\dagger = (-1)^N c_{i\downarrow}, \]
\[ U_{c\downarrow} U^\dagger = (-1)^{N-1} e^{i\Pi_i} c_{i\downarrow}, \]
\[ U_{c\uparrow} U^\dagger = (-1)^{N-1} e^{-i\Pi_i} c_{i\uparrow}. \]  

(21)

Based on Eq. (21) the transformation of the particle number operators can be given. As presented in Appendix 4., the following results are obtained

\[ U n_{i\uparrow} U^\dagger = n_{i\uparrow}, \]
\[ U n_{i\downarrow} U^\dagger = 1 - n_{i\downarrow}. \]  

(22)

Using Eqs. (21,22) the complete Hamiltonian presented in Eq. (1) can be unitary transformed based on \( U \). For example in the case \( t = X, P = R = 0, \) and \( e^{i\Pi_i} = 1 \) for all \( i \), we obtain the following final result (see Appendix 5.)

\[ H' = -\tilde{t} \hat{t} + \tilde{U} \hat{U} + \tilde{X} \hat{X} + \tilde{V} \hat{V} + \tilde{J}_z \hat{J}_z + \frac{\tilde{J}_{xy}}{2} \hat{J}_{xy} + \tilde{Y} \hat{Y} + \tilde{Q} \hat{Q} + \tilde{\mu} \sum_{j=1}^{N} n_j \ + \tilde{h} \sum_{j=1}^{N} (n_{j\uparrow} - n_{j\downarrow}) + C. \]  

(23)

In this relation the renormalized coupling constants obtained after the transformation are denoted with a tilde superscript their values being

\[ \tilde{t} = -t, \quad \tilde{Y} = \frac{1}{2} J_{xy}, \]
\[ \tilde{X} = -X, \quad \tilde{Q} = Q, \]
\[ \tilde{U} = -U, \quad \tilde{\mu} = \mu, \]
\[ \tilde{V} = \frac{J_z}{4}, \quad \tilde{h} = h, \]
\[ \tilde{J}_z = 4V, \quad C = (\mu - h) N, \]
\[ \tilde{J}_{xy} = 2Y. \]  

(24)
III. THE OBTAINED RESULTS

Based on the results presented in Chapter II. we are analysing different concrete cases as follows.

A. Ferromagnetic states

De Boer et al (1995 a) in the study of the \( \eta \)-pairing ground state in the extended Hubbard model used the following model Hamiltonian

\[
\hat{H}_1 = -t \hat{\mathbf{i}} + U \hat{\mathbf{U}} + X \hat{\mathbf{X}} + V \hat{\mathbf{V}} + J_z \hat{\mathbf{J}_z} + \frac{J_{xy}}{2} \hat{\mathbf{J}_{xy}} + Y \hat{\mathbf{Y}} + R \hat{\mathbf{R}}
\]

\[
+ P \hat{\mathbf{P}} + Q \hat{\mathbf{Q}} + \mu \sum_{j=1}^{N} n_j + \hbar \sum_{j=1}^{N} (n_{j\uparrow} - n_{j\downarrow}),
\]

obtaining a superconducting \( \eta \)-pairing ground state at \( R = 0, \ P = 0 \), in the following parameter space region

\[
V \leq 0,
\]

\[
2V = Y,
\]

\[
t = X,
\]

\[
-\frac{U}{z} \leq \max \left[ V - \frac{J_z}{4} + \frac{2|h|}{z} ; V + \frac{J_z}{4} + \frac{J_{xy}}{2} \right] ;
\]

\[
2 \frac{|h|}{z} + \frac{Q}{4} + 2V + 2|t|,
\]

the ground state energy obtained being

\[
E_N = \frac{UN}{4} + \frac{ZN}{2} \left( V - \frac{P}{2} + \frac{Q}{16} \right) + N_e \left( 2\mu + \frac{PZ}{2} \right),
\]

where \( N_e \) represents the number of electrons within the system.

Based on this result, taking into consideration that from Eq.(20) the unitary transformed \( \eta \)-pairing state represents a ferromagnetic state, using Eqs.(23,24) we obtain a ferromagnetic ground state in the same model in the parameter space region \( P = R = 0 \) and
\( J_z \leq 0 \),
\( J_z = 2 J_{xy} \),
\( t = X \),
\[
\frac{U}{z} \leq \max \left[ \frac{J_z}{4} - V + \frac{2}{z} |\mu|; \frac{J_z}{4} + V + |Y|; \right.
\]
\[
\frac{2}{z} |\mu| + \frac{Q}{4} + \frac{J_z}{2} + 2 |t|
\]  \hspace{1cm} (28)

The ground state energy of this ferromagnetic state is given by

\[
\tilde{E}_N = -\frac{\bar{U} N}{4} + \frac{ZN}{2} \left( \frac{\bar{J}_z}{4} + \frac{\bar{Q}}{16} \right) + 2 N_e \tilde{\hbar} \]  \hspace{1cm} (29)

The position of the obtained ferromagnetic ground state in the \( T = 0 \) phase diagram of the model relative to the \( \eta \)-pairing state is illustrated in Fig. 1.

The second Hamiltonian that we analyse concretely here has been studied by Montorsi and Campbell (1996). The authors being interested in the emergence possibilities of \( \eta \)-pairing superconductivity, used the Hamiltonian

\[
H_2 = -t \hat{\mathbf{t}} + U \sum_{j=1}^{N} n_{j\uparrow} n_{j\downarrow} + X \hat{X}
\]
\[
+ 2 \bar{V} \sum_{<j,k>} S_{jz}^z S_{kz}^z - W \hat{W} - S \sum_{<j,k>} \vec{S}_{j} \vec{S}_{k} + C. \]  \hspace{1cm} (30)

This Hamiltonian has been studied by Montorsi and Campbell (1996) obtaining \( \eta \)-pairing superconducting ground state for \( \bar{V} = 0 \) in the domain

\[
U \leq -A, \]
\[
S \geq 0, \]  \hspace{1cm} (31)

where \( A = Z \left( 4 |X| + \frac{3}{2} |W| \right) \), \( Z \) representing the number of nearest neighbours.

In Appendix 6, we convert the Hubbard term from Eq.(30) into the form it has in (3). The unitary transformation presented in Chapter II then gives a ferromagnetic ground state for \( H_2 \) in the region

\[
U \leq A', \]  \hspace{1cm} (32)
\[
W \geq 0, \]  \hspace{1cm} (33)
where $A' = Z\left(4\, |X| + \frac{3}{2}\, |S| \right)$, and $V = 0$, $t = X$. The position of the ferromagnetic domain in the phase diagram of the model is presented in Fig. 2.

**B. Density wave states**

We are analysing now model Hamiltonians giving density wave states. We start the presentation of our results with the Hamiltonian used by Strack and Vollhardt (1993)

$$
H_3 = -t\hat{t} + U\hat{U} + X\hat{X} + V\sum_{<j,i>,\sigma,\sigma'} n_{j\sigma} n_{i\sigma'}.
$$

The last term from $H_3$ can be easily transformed into the form used in Eq.(3) (see Appendix 7.). For the model from Eq.(34) a paramagnetic insulator has been deduced in the phase diagram domain

$$
t = X, \\
\frac{U}{Z} - 4t - V \geq 0,
$$

and a charge density wave region has been obtained in the region (Strack and Vollhardt, 1993):

$$
t = X, \\
\frac{U}{Z} + 4t - V \leq 0.
$$

By the unitary transformation presented above we obtain instead of the phase from Eq.(35) an other paramagnetic insulator phase present in the region

$$
t = X, \\
-\frac{U}{Z} + 4t + V^+ \geq 0, \\
-\frac{U}{Z} + 4t + V^- \geq 0,
$$

and a spin density wave phase instead of the domain Eq.(36) in the region
\[ t = X, \]
\[ \frac{U}{Z} + 4t + V^+ \geq 0, \]
\[ -\frac{U}{Z} - 4t + V^- \leq 0. \]  

(38)

The results from Eqs. (37, 38) are valid in a model similar to Eq. (34) in which however the density-density type coupling has been replaced with \( V^+ \dot{V}^+ = V^+ \sum_{<j,i>,\sigma} n_{j\sigma} n_{i\sigma} \), and \( V^- \dot{V}^- = \sum_{<j,i>,\sigma} n_{j\sigma} n_{i,-\sigma} \), see Appendix 7. The results connected to the Hamiltonian \( H_3 \) are summarised in Fig. 3.

The next Hamiltonian that we analysed is connected to an extended Hubbard model studied by de Boer et al. (1995 b)

\[ H_4 = -t \hat{t} + U \hat{U} + X \hat{X} + V \hat{V} + J_z \hat{J}_z + \frac{J_{xy}}{2} \hat{J}_{xy} + Y \hat{Y} + \mu \sum_{j=1}^{N} n_j. \]  

(39)

Based on this Hamiltonian, de Boer et al. (1995 b.) proved the existence of a SDW ground state in the following region of the parameter space

\[ J_z \geq 0, \]
\[ J_{xy} = 0, \]
\[ t = X, \]
\[ \frac{U}{\hat{z}} \geq \max(\frac{J_z}{4} - V; 2|t| - \frac{J_z}{2}; V + |Y| - \frac{J_z}{4}). \]  

(40)

Using the presented unitary transformation, from Eq. (40) we obtain a CDW ground state in the following region of the phase diagram of the same model

\[ V \geq 0, \]
\[ Y = 0, \]
\[ t = X, \]
\[ -\frac{U}{\hat{z}} \geq \max(\frac{J_z}{4} - \frac{V}{16}; 2|t| - 2|V|; \frac{J_z}{2} + \frac{J_{xy}}{2} - V). \]  

(41)

de Boer and Schadschneider (1995 b.) obtained also a fully polarized ferromagnetic state in the following region
\[ J_z \geq |J_{xy}|, \]
\[ \frac{U}{z} \geq \max \left( 2|t| - \frac{J_z}{2}, \frac{J_z}{4} - V; V + Y + \frac{J_z}{4}; V - Y + \frac{J_z}{4} \right). \] (42)

Interestingly, from the phase presented in Eq.(42) our unitary transformation gives an insulating ground state in the domain
\[ \frac{V}{4} \geq |2Y|, \]
\[ -\frac{U}{z} \geq \max \left( 2|t| + \frac{V}{8}; \frac{V}{16} - \frac{J_z}{4}; \frac{J_z}{4} + \frac{J_{xy}}{2} + \frac{V}{16} \right). \] (43)

The obtained results related to the phase diagram of the Hamiltonian \( H_4 \) are summarized in Fig. 4.

Another extended Hubbard Hamiltonian containing in it's ground state phase diagram density waves has been analysed by Aligia et al. (1995)

\[ H_5 = +U \sum_{j=1}^{N} n_{j\uparrow} n_{j\downarrow} + V \sum_{<j,i>,\sigma\sigma'} n_{i\sigma} n_{j\sigma'} + \sum_{<j,i>,\sigma} \left( c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{j\sigma} \right) \left[ t_{AA} \left( 1 - n_{i,-\sigma} \right) \left( 1 - n_{j,-\sigma} \right) + t_{BB} n_{i,-\sigma} n_{j,-\sigma} \right]. \] (44)

They found a region of parameters in the phase diagram where a CDW phase is the ground state of the system in the domain \( V > V_c \), where
\[ V_c = 0, \text{ if } U \leq -2Zt, \]
\[ V_c = \frac{U}{2Z} + t, \text{ if } -2Zt \leq U \leq 2Zt, \]
\[ V_c = \frac{U}{Z}, \text{ if } U \geq 2Zt. \] (45)

Based on this result, using the presented unitary transformation (see Appendix 8.) we have obtained a SDW ground state in the domain \( V^+ > V_c, \ V^- < V_c \), where
\[ V_c = 0, \text{ if } -U \leq -2Zt, \]
\[ V_c = \frac{-U}{2Z} + t \text{ if } -2Zt \leq -U \leq 2Zt, \]
\[ V_c = \frac{-U}{Z} \text{ if } -U \geq 2Zt. \] (46)

In Eq.(46) we have \( t = |t_{AA}| = |t_{BB}| \) The position of the deduced CDW phase in the phase diagram of the model is presented in Fig. 5.
IV. SUMMARY

In this paper, we have presented a procedure that based on an explicitly given unitary transformation allows the rigorous deduction of new phase diagram domains starting from known ground state solutions of a given model. The method is not model-dependent and can be applied for arbitrary dimensions. We have applied this method to find new stable spin-density wave, charge-density wave, ferromagnetic and a paramagnetic insulator domains of different extended Hubbard type models.
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FIGURES

Fig.1. Phase diagram regions in the coupling constant space connected to Hamiltonian $H_1$. a) the superconducting state deduced by De Boer et al. (1995 a.); b) the ferromagnetic ground state obtained in this paper.

Fig.2. Ground-state phase diagrams for the Hamiltonian $H_2$. a) the superconducting state of Montorsi and Campbell (1996), b) the ferromagnetic ground state deduced in this paper.

Fig.3. Phase diagram regions in the coupling constant space connected to Hamiltonian $H_3$. a) the ground states deduced by Strack and Vollhardt (1993), densely dotted phase is CDW state, thinly dotted domain is paramagnetic insulator; b) ground states deduced in this paper: the densely dotted phase represents an SDW state and the thinly dotted region is an other paramagnetic insulator region.

Fig.4. Ground-state phase diagrams for the Hamiltonian $H_4$. a) the SDW state obtained by de Boer et al. (1995 b.), b) the CDW phase obtained in this paper.

Fig.5. Phase diagram regions in the coupling constant space for the Hamiltonian $H_5$. a) the CDW phase deduced by Aligia et al. (1995), b) the SDW ground state deduced in this paper.
V. APPENDICES

In this Chapter dedicated to Appendices we are presenting the mathematical details of the calculation.

A. Appendix 1.

This appendix prove the unitary nature of the operator $U$. We must deduce $U U^\dagger = 1$, where $U^\dagger$ is the adjoint of $U$. Indeed, $U$ can be written as

$$U = \prod_{i=1}^{N} z_i = z_1 z_2 ... z_N,$$

(47)

where $z_i^+ = (e^{-iP_i} c_{i\downarrow} + c_{i\uparrow}^+)$. With this notation we have $U^\dagger = z_N^+ ... z_1^+$, where $z_i^+ = (e^{-iP_i} c_{i\downarrow} + c_{i\uparrow}^+)$. Then we find $U U^\dagger = z_1 ... z_N z_N^+ ... z_1^+$. Since

$$(e^{iP_i} c_{i\downarrow}^+ + c_{i\uparrow}) (e^{-iP_i} c_{i\downarrow} + c_{i\uparrow}^+) = c_{i\downarrow}^+ c_{i\downarrow} + c_{i\downarrow} c_{i\downarrow}^+ = c_{i\downarrow}^+ c_{i\downarrow} + 1 - c_{i\uparrow}^+ c_{i\downarrow} = 1,$$

(48)

we obtain $z_i z_i^+ = 1$ for all $i$. As a consequence $U U^\dagger = 1$, so $U$ is indeed an unitary transformation.

B. Appendix 2

In this appendix the effect of $U$ on the wave-functions is presented. Let consider first the unitary transformation of the superconducting ($\eta$-pairing) wave-functions. If we consider a single doubly occupied state present in the wave function at site $i$, the effect of the operator $z_i$ on this state is to transform it in a single occupied state with spin up as follows

$$z_i |0, \ldots, \uparrow\downarrow_i, 0, \ldots, 0\rangle = |0, \ldots, \uparrow_i, 0, \ldots, 0\rangle.$$

(49)

The effect of $z_j$ on the same state for $i \neq j$ becomes

$$z_j |0, \ldots, 0_j, \ldots, \uparrow\downarrow_i, 0, \ldots, 0\rangle = e^{iP_j} |0, \ldots, \downarrow_j, \ldots, \uparrow\downarrow_i, 0, \ldots, 0\rangle.$$

(50)
From these equations it can be seen that the effect of $U$ on empty sites is to introduce a single occupancy with spin down on these sites. However, in case of doubly occupied sites containing an $\eta$-pair, the effect of $U$ is to transform these states in single occupied states with spin up. Based on these relations, for a general wave function containing $N_\eta$ $\eta$-pairs distributed on different sites we obtain

$$U | 0, \ldots, 0, \uparrow_{i1}, 0, \ldots, 0, \downarrow_{iN_\eta}, 0, \ldots, 0 \rangle = \frac{\prod_{j=1}^{N_\eta} e^{iP_j} | \uparrow, \uparrow, \ldots, \downarrow_{i1}, \uparrow, \ldots, \downarrow_{iN_\eta}, \ldots \uparrow \rangle}{\prod_{k=1}^{N_\eta} e^{iP_k} | \uparrow, \uparrow, \ldots, \downarrow_{i1}, \uparrow, \ldots, \downarrow_{iN_\eta}, \ldots \uparrow \rangle}. \quad (51)$$

Apart from a phase factor, this is a ferromagnetic state, if $N_\eta \neq N/2$, where $N$ represents the number of lattice sites.

The study of density waves starts from the observation that $z_i$ transforms differentially the single occupied states with up and down spin. Indeed, for an up spin single occupied state we have

$$z_i | \ldots, \uparrow_i, \ldots \rangle = e^{iP_i} | \ldots, \uparrow_{i-1}, \uparrow_{i+1}, \ldots \rangle, \quad (52)$$

but for the spin down counterpart we obtain

$$z_i | \ldots, \downarrow_i, \ldots \rangle = | \ldots, 0_i, \ldots \rangle. \quad (53)$$

Using this property, starting from a spin-density wave state, using $U$ we find

$$U | \downarrow, \uparrow, \downarrow, \uparrow, \ldots \rangle = \prod_{i=1}^{N/2} e^{iP(2i)} | 0, \uparrow \downarrow, 0, \uparrow \downarrow, \ldots \rangle. \quad (54)$$

The obtained state is a charge-density state.

C. Appendix 3

The transformation under $z_i$ of the creation and annihilation operators is presented in this Appendix. Starting with annihilation operators, we have for the spin up case

$$z_i c_{i\uparrow} = (e^{iP_i} c_{i\downarrow}^\dagger + c_{i\downarrow}) c_{i\uparrow} = e^{iP_i} c_{i\downarrow}^\dagger c_{i\uparrow} + c_{i\downarrow} c_{i\uparrow} = -e^{iP_i} c_{i\uparrow} c_{i\downarrow}^\dagger - c_{i\uparrow}^\dagger c_{i\downarrow}, \quad (55)$$
from where

\[ z_i c_i^\dagger z_i^+ = ( - e^{i\Pi_i} c_i^\dagger c_i^\dagger - c_i^\dagger c_i^\dagger ) ( e^{-i\Pi_i} c_i^\dagger + c_i^\dagger ) \]
\[ = - c_i^\dagger c_i^\dagger c_i^\dagger c_i^\dagger = - c_i^\dagger \]  

arise. For different indices \( i \neq j \) we find \( z_j c_{i,\uparrow}^+ z_j^+ = - c_{i,\uparrow}. \) Similarly, for the opposite spin direction and different indices we obtain \( z_j c_{i,\downarrow}^+ z_j^+ = - c_{i,\downarrow} \), and for \( i = j \) one have

\[ z_i c_i^\dagger = ( e^{i\Pi_i} c_i^\dagger + c_i^\dagger ) c_i^\dagger = e^{i\Pi_i} c_i^\dagger c_i^\dagger, \]
\[ (56) \]

\[ z_i c_i^\dagger z_i^+ = e^{i\Pi_i} c_i^\dagger c_i^\dagger ( e^{-i\Pi_i} c_i^\dagger + c_i^\dagger ) = e^{i\Pi_i} c_i^\dagger c_i^\dagger c_i^\dagger c_i^\dagger = e^{i\Pi_i} c_i^\dagger \]
\[ (57) \]

\[ z_i c_i^\dagger z_i^+ = e^{i\Pi_i} c_i^\dagger c_i^\dagger ( e^{-i\Pi_i} c_i^\dagger + c_i^\dagger ) = e^{i\Pi_i} c_i^\dagger c_i^\dagger c_i^\dagger c_i^\dagger = e^{i\Pi_i} c_i^\dagger \]
\[ (58) \]

In the case of creation operators, for up spin, independent on indices we have \( z_j c_{i,\uparrow}^+ z_j^+ = - c_{i,\uparrow}^\dagger \). For down spin, in case of different indices we obtain \( z_j c_{i,\downarrow}^+ z_j^+ = - c_{i,\downarrow}^\dagger \). However, in case of \( i = j \) the transformation gives

\[ z_i c_i^\dagger = ( e^{i\Pi_i} c_i^\dagger + c_i^\dagger ) c_i^\dagger = c_i^\dagger c_i^\dagger, \]
\[ (59) \]

\[ z_i c_i^\dagger z_i^+ = c_i^\dagger c_i^\dagger ( e^{-i\Pi_i} c_i^\dagger + c_i^\dagger ) = e^{-i\Pi_i} c_i^\dagger c_i^\dagger c_i^\dagger c_i^\dagger = e^{-i\Pi_i} c_i^\dagger \]
\[ (60) \]

¿From the presented results the transformation formulas from Eqs.(21) arise.

### D. Appendix 4

The unitary transformation generated by \( U \) of the particle number operators is presented below. We have

\[ U c_i^\dagger c_i^\dagger U^\dagger = U c_i^\dagger U U c_i^\dagger U^\dagger = ( - 1 )^N c_i^\dagger ( - 1 )^N c_i^\dagger = c_i^\dagger c_i^\dagger = n_i^\dagger, \]
\[ (61) \]

\[ U c_i^\dagger c_i^\dagger U^\dagger = U c_i^\dagger U U c_i^\dagger U^\dagger = ( - 1 )^{N-1} e^{-i\Pi_i} c_i^\dagger ( - 1 )^{N-1} e^{i\Pi_i} c_i^\dagger = c_i^\dagger c_i^\dagger = 1 - c_i^\dagger c_i^\dagger = 1 - n_i^\dagger. \]
\[ (62) \]

¿From Eq.(62) \( n_{i,\uparrow} \) remains unchanged, while \( n_{i,\downarrow} \) is transformed in \( (1 - n_{i,\downarrow}) \) under \( U \).
In this Appendix we are presenting the unitary transformation of different terms from the Hamiltonian. We start the presentation with the Hubbard on-site interaction

\[ U \left( n_{j\uparrow} - 1/2 \right) \left( n_{j\downarrow} - 1/2 \right) U^\dagger = \left( n_{j\uparrow} - 1/2 \right) \left( 1 - n_{j\downarrow} - 1/2 \right) = \left( n_{j\uparrow} - 1/2 \right) \left( 1/2 - n_{j\downarrow} \right). \]  

(63)

It can be seen that the Hubbard interaction term changes the sign under the unitary transformation used.

Concerning the hopping term, the following results are obtained

\[ U \hat{T}_{ij} U^\dagger = \hat{T}_{ij} \]

\[ U \hat{T}_{ij} U^\dagger = -U \left( c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \right) U^\dagger = \]

\[ - \left[ \left( -1 \right)^{N-1} e^{-iPj} \left( -1 \right)^{N-1} e^{iPi} c_{j\downarrow}^\dagger c_{i\downarrow} + \left( -1 \right)^{N-1} e^{-iPi} \left( -1 \right)^{N-1} e^{iPj} c_{i\downarrow}^\dagger c_{j\downarrow} \right] = -e^{iP(j-i)} \hat{T}. \]

(64)

The transformation of the \( \hat{X} \) operator yields

\[ U \hat{X}_{ij} U^\dagger = U \left( c_{j\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{j\uparrow} \right) \left( n_{j\downarrow} + n_{i\downarrow} \right) U^\dagger = \]

\[ = \left( c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \right) \left( 1 - n_{j\downarrow} + 1 - n_{i\downarrow} \right) = -\hat{X}_{ij} - 2 \hat{T}_{ji}. \]

\[ U \hat{X}_{ij} U^\dagger = \left( e^{i(Pj-Pi)} c_{j\downarrow}^\dagger c_{i\downarrow} + e^{i(Pi-Pj)} c_{i\downarrow}^\dagger c_{j\downarrow} \right) \left( n_{j\uparrow} + n_{i\uparrow} \right) = -e^{iP(j-i)} \hat{X}_{ij}. \]

(65)

We consider now the \( \hat{J}_z \) and \( \hat{V} \) operatorial terms

\[ U \hat{J}_z U^\dagger = \frac{1}{4} U \left( n_{j\uparrow} - n_{j\downarrow} \right) \left( n_{i\uparrow} - n_{i\downarrow} \right) U^\dagger \]

\[ = \frac{1}{4} \left( n_{j\uparrow} - 1 + n_{j\downarrow} \right) \left( n_{i\uparrow} - 1 + n_{i\downarrow} \right) = \]

\[ \frac{1}{4} \left( n_j - 1 \right) \left( n_i - 1 \right) = \frac{1}{4} \hat{V}. \]

\[ U \hat{V} U^\dagger = U \left( n_j - 1 \right) \left( n_i - 1 \right) U^\dagger = U \left( n_{j\uparrow} + n_{j\downarrow} - 1 \right) \left( n_{i\uparrow} + n_{i\downarrow} - 1 \right) U^\dagger \]

\[ = \left( n_{j\uparrow} - n_{j\downarrow} \right) \left( n_{i\uparrow} - n_{i\downarrow} \right) = 4 \hat{J}_z. \]

(66)
From Eq. (66) the $\hat{J}_z$ and $\hat{V}$ operators transform into each other.

The following terms analysed are $\hat{J}_{xy}$ and $\hat{Y}$. We obtain

$$U \hat{J}_{xyij} U^\dagger = U \frac{1}{2} \left( (S_j^+ S_i^- + S_j^- S_i^+) \right) U^\dagger =$$

$$U \frac{1}{2} \left( c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \right) U^\dagger =$$

$$\frac{1}{2} \left( c_{j\uparrow}^\dagger e^{ip_j} c_{j\downarrow}^\dagger e^{-ip_i} c_{i\uparrow}^\dagger + e^{-ip_j} c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger e^{ip_i} c_{i\downarrow}^\dagger \right) =$$

$$\frac{1}{2} \left( e^{i(p_j-p_i)} c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + e^{i(p_i-p_j)} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \right) = \frac{1}{2} e^{i(p_j-p_i)} \hat{Y} .$$

$$U \hat{Y}_{ij} U^\dagger = U \left( c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \right) U^\dagger =$$

$$e^{i(p_i-p_j)} c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + e^{i(p_i-p_j)} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger = 2 e^{i(p_j-p_i)} \hat{J}_{xyij} .$$

From Eq. (67), the $\hat{J}_{xy}$ and $\hat{Y}$ operators transform into each other if the phase factor $Pi = 0$ is considered. Because of this result and Eq. (66), the $\hat{W}$ and $\hat{S}$ operators transform into each other as well. Indeed,

$$U S_j^z S_i^z U^\dagger = S_j^z S_i^z ,$$

$$U S_j^+ S_i^- U^\dagger = e^{i(p_j-p_i)} S_j^+ S_i^- ,$$

$$U S_j^- S_i^+ U^\dagger = e^{i(p_j-p_i)} S_j^- S_i^+ ,$$

and

$$U S_j^z S_i^z U^\dagger = S_j^z S_i^z ,$$

$$U S_j^+ S_i^- U^\dagger = e^{i(p_j-p_i)} S_j^+ S_i^- ,$$

$$U S_j^- S_i^+ U^\dagger = e^{i(p_j-p_i)} S_j^- S_i^+ .$$

We consider now the transformation of the $\hat{R}$ operator

$$U \hat{R}_{ji}^\dagger U^\dagger = U \left( c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger + c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger \right) n_{ji}^\dagger n_{i\downarrow}^\dagger U^\dagger =$$

$$\left( c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger + c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger \right) \left( 1 - n_{ji} \right) \left( 1 - n_{i\downarrow} \right) =$$

$$\hat{R}_{ji}^\dagger - \left( c_{j\uparrow}^\dagger c_{i\uparrow}^\dagger + c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger \right) \left( n_{ji} + n_{i\downarrow} \right) =$$

$$\hat{R}_{ji}^\dagger - \hat{T}_{ji}^\dagger - \hat{X}_{ji} .$$
$U \hat{R}_{ji}^\dagger U^\dagger = U \left( (c_{j\downarrow}^{\dagger} c_{i\downarrow} + c_{i\uparrow}^{\dagger} c_{j\uparrow}) n_{j\uparrow} n_{i\uparrow} U^\dagger =
( e^{i(P_i-P_j)} c_{j\downarrow}^{\dagger} c_{i\downarrow} + e^{i(P_i-P_j)} c_{i\uparrow}^{\dagger} c_{j\uparrow}) n_{j\uparrow} n_{i\uparrow} =
\right) e^{i(P_i-P_j)} \hat{R}_{ji}^\dagger. \tag{70}$

We consider now the operator $\hat{P}$. This operator is build up from a sum of $\hat{P}_{ij}$ terms whose expression is given by

$$\hat{P}_{ij} = (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_{i\uparrow} + n_{i\downarrow} - \frac{1}{2} - \frac{1}{2}) +
(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})(n_{j\uparrow} - \frac{1}{2} + n_{j\downarrow} - \frac{1}{2}). \tag{71}$$

This operator can be decomposed in the following components

$$\hat{P}^+_{ij} = (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) +
(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})(n_{j\uparrow} - \frac{1}{2}) = \hat{P}^+_{ij},$$

$$\hat{P}^-_{ij} = (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_{i\uparrow} - \frac{1}{2}) +
(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})(n_{j\uparrow} - \frac{1}{2}). \tag{72}$$

The unitary transformation of $\hat{P}^+$ and $\hat{P}^-$ operators gives the following results

$$U \hat{P}^+_{ij} U^\dagger = (n_{j\uparrow} - \frac{1}{2})(-n_{j\downarrow} + \frac{1}{2})(-n_{i\downarrow} + \frac{1}{2}) +
(n_{i\uparrow} - \frac{1}{2})(-n_{i\downarrow} - \frac{1}{2})(n_{j\uparrow} + \frac{1}{2}) = \hat{P}^+_{ij}.$$

$$U \hat{P}^-_{ij} U^\dagger = (n_{j\uparrow} - \frac{1}{2})(-n_{j\downarrow} + \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) +
(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} + \frac{1}{2})(n_{j\uparrow} + \frac{1}{2}) = -\hat{P}^-_{ij}. \tag{73}$$

Based on these results one can see, that $\hat{P}^+_{ij}$ remains unaltered, while $\hat{P}^-_{ij}$ changes the sign under the unitary transformation used.

The following operatorial term transformed is $\hat{Q}$. We have

$$U \hat{Q}_{ij} U^\dagger = U \left( (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2})(n_{i\uparrow} - \frac{1}{2}) (n_{i\downarrow} - \frac{1}{2}) U^\dagger =
(n_{j\uparrow} - \frac{1}{2})(-n_{j\downarrow} + \frac{1}{2})(n_{i\uparrow} - \frac{1}{2})(-n_{i\downarrow} + \frac{1}{2}) = \hat{Q}_{ij}. \tag{74}$$

As a consequence, the operator $\hat{Q}$ transform into itself under the unitary transformation generated by $U$. 21
We consider now the chemical potential \( \mu \) and external field \( h \). Introducing the notations \( \mu_j = n_{j\uparrow} + n_{j\downarrow} \) and \( h_j = n_{j\uparrow} - n_{j\downarrow} \), we obtain
\[
U \mu_j U^\dagger = n_{j\uparrow} + 1 - n_{j\downarrow} = h_j + 1 , \\
U h_j U^\dagger = n_{j\uparrow} - 1 + n_{j\downarrow} = \mu_j - 1 .
\]
(75)

We mention that after transforming all terms of the Hamiltonian, driven by the aim to remain in the same class of model, we consider the transformed Hamiltonian identical with the original. This will be realized if for all lattice sites we have \( e^{\hat{P}_i} = 1 \), and \( \hat{X}^\dagger = \hat{X}^\downarrow \), \( \hat{t}^\dagger = \hat{t}^\downarrow \), \( \hat{P}^+ = \hat{P}^- \). Since \( \hat{X}^\dagger = -X - R \) and \( \hat{X}^\downarrow = -X \), from Eq.(70) we get the condition \( R = 0 \). Besides, as \( \hat{t}^\dagger = t - 2X \) and \( \hat{t}^\downarrow = -t \) we get \( t = X \). We also mention that during this paper \( Pi = 0 \) has been used.

F. Appendix 6

In this Appendix we are presenting the relation that connects the form of the Hubbard interaction analysed in Appendix 4. and the standard form of the on-site interaction expressed via a \( \sum_i n_{i\uparrow}n_{i\downarrow} \) product. We have
\[
\sum_i ( n_{i\uparrow} - \frac{1}{2} ) ( n_{i\downarrow} - \frac{1}{2} ) = \sum_i ( n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} ( n_{i\uparrow} + n_{i\downarrow} ) + \frac{1}{4} ) \\
= \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} \sum_{i\sigma} n_{i\sigma} + \frac{1}{4} \sum_i 1 = \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} N_e + \frac{1}{4} N ,
\]
(76)
where \( N_e \) represents the number of electrons within the system and \( N \) is the number of lattice sites. Denoting \( N/4 - N_e/2 = C \), we obtain
\[
U \sum_{j=1}^N n_{j\uparrow} n_{j\downarrow} = U \sum_i ( n_{i\uparrow} - \frac{1}{2} ) ( n_{i\downarrow} - \frac{1}{2} ) + U C .
\]
(77)

The result obtained in Eq.(77) is used for the study of the Hamiltonian \( H_2 \) presented in Eq.(30). Using Eq.(77), the Hamiltonian \( H_2 \) becomes
\[
H' = -t \hat{t} + U \sum_{j=1}^N ( n_{j\uparrow} - \frac{1}{2} ) ( n_{j\downarrow} - \frac{1}{2} ) + X \hat{X} \\
+ 2V \sum_{\langle j,k \rangle} S_j^{z} S_k^{z} - W \hat{W} - S \sum_{\langle j,k \rangle} \vec{S}_j \vec{S}_k + C' .
\]
(78)
This Appendix presents in detail the transformation of the Hamiltonian $H_3$ from Eq.(34) in a form more convenient for our study. We have converted the last term of $H_3$ with the help of the following identity:

$$
\sum_{<j,i>,\sigma,\sigma'} (n_{j\sigma} - \frac{1}{2}) (n_{i\sigma'} - \frac{1}{2}) = \sum_{<j,i>,\sigma} (n_{j\sigma} n_{i,-\sigma} - \frac{1}{2} n_{i\sigma} - \frac{1}{2} n_{j,-\sigma} + \frac{1}{4}) + \\
(n_{j\sigma} n_{i\sigma} - \frac{1}{2} n_{i\sigma} - \frac{1}{2} n_{j\sigma} + \frac{1}{4}) = \\
\sum_{<j,i>,\sigma} n_{i\sigma} n_{j\sigma} - \frac{1}{2} \sum_{<j,i>,\sigma} (n_{i\sigma} + n_{j,-\sigma} + n_{i\sigma} + n_{j\sigma}) + 4 \frac{1}{4} = \\
\sum_{<j,i>,\sigma,\sigma'} n_{i\sigma'} n_{j\sigma} - \sum_{<j,i>,\sigma} n_{i\sigma} - \frac{1}{2} \sum_{<j,i>} (n_{j\uparrow} + n_{j\downarrow} + n_{j\uparrow} + n_{j\downarrow}) + 1 = \\
\sum_{<j,i>,\sigma,\sigma'} n_{i\sigma'} n_{j\sigma} - 2 N_e + 1. \quad (79)
$$

Based on Eq.(79) we have

$$
\sum_{<j,i>,\sigma,\sigma'} n_{i\sigma'} n_{j\sigma} = \sum_{<j,i>,\sigma,\sigma'} (n_{j\sigma} - \frac{1}{2}) (n_{i\sigma'} - \frac{1}{2}) + \text{const.} \quad (80)
$$

Using Eq.(80), the Hamiltonian $H_3$ becomes

$$
H = -t \hat{t} + U \hat{U} + X \hat{X} + V \hat{V} + \text{const.} \quad (81)
$$

Using the form presented in Eq.(81) different terms of the Hamiltonian can be unitary transformed. The transformation of the operatorial terms presented in Eq.(80) gives

$$
U \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{i\uparrow} - \frac{1}{2} \right) U^\dagger = \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{i\uparrow} - \frac{1}{2} \right), \\
U \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) U^\dagger = \left( n_{j\uparrow} - \frac{1}{2} \right) \left( \frac{1}{2} - n_{i\downarrow} \right), \\
U \left( n_{j\downarrow} - \frac{1}{2} \right) \left( n_{i\uparrow} - \frac{1}{2} \right) U^\dagger = \left( \frac{1}{2} - n_{j\downarrow} \right) \left( n_{i\uparrow} - \frac{1}{2} \right), \\
U \left( n_{j\downarrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) U^\dagger = \left( \frac{1}{2} - n_{j\downarrow} \right) \left( \frac{1}{2} - n_{i\downarrow} \right). \quad (82)
$$

Decomposing the contribution presented in Eq.(80) is spin dependent terms, new notation has to be introduced
The unitary transformation of the operatorial components from Eq. (83) gives $UV^+U^\dagger = V^+$, and $UV^-U^\dagger = -V^-$. 

H. Appendix 8

The unitary transformation of the Hamiltonian $H_5$ from Eq. (44) is presented in this Appendix. Before starting the unitary transformation we mention that the first two terms of $H_5$ may be rewritten based on Eqs. (77, 80). For the third term of $H_5$ we are using the expression

$$
\sum_{<i,j>} (c_{j\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{j\uparrow}) [t AA_{i\downarrow} n_{j\downarrow} + t BB (1 - n_{i\downarrow}) (1 - n_{j\downarrow})] + \\
\sum_{<i,j>} (c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) [((-1) t AA (1 - n_{i\uparrow}) (1 - n_{j\uparrow}) + \\
( -1) t BB n_{i\uparrow} n_{j\uparrow}].
$$

The unitary transformation of the new operatorial terms not encountered up to this moment are

$$
U (c_{j\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{j\uparrow}) U^\dagger = (c_{j\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{j\uparrow}) \\
U (1 - n_{i\downarrow}) (1 - n_{j\downarrow}) U^\dagger = n_{i\downarrow} n_{j\downarrow} \\
U n_{i\downarrow} n_{j\downarrow} U^\dagger = (1 - n_{i\downarrow}) (1 - n_{j\downarrow}) \\
U (c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) U^\dagger = -(c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) \\
U (1 - n_{i\uparrow}) (1 - n_{j\uparrow}) U^\dagger = (1 - n_{i\uparrow}) (1 - n_{j\uparrow}) \\
U n_{i\uparrow} n_{j\uparrow} U^\dagger = n_{i\uparrow} n_{j\uparrow}
$$

We mention that during the paper we assumed $t_{AA} = -t_{BB}$, and the following notation has been used

$$t = |t_{AA}| = |t_{BB}| = |\tilde{t}_{AA}| = |\tilde{t}_{BB}|. $$
\[ \frac{J_{xy}}{J_z} \]

\[ \frac{V}{J_z} \]

\[ \frac{Y}{J_z} \]

\[ \text{a) } \]

\[ \text{b) } \]

1
