Exact solutions for the periodic Anderson model in 2D: A Non-Fermi liquid state in normal phase.

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Abstract

Presenting exact solutions for the two dimensional periodic Anderson model with finite and nonzero on-site interaction $U > 0$, we are describing a rigorous non-Fermi liquid phase in normal phase and 2D. This new state emerges in multi-band interacting Fermi systems above half filling, being generated by a flat band effect. The momentum distribution function $n_{\vec{k}}$ together with its derivatives of any order is continuous. The state possesses a well defined Fermi energy ($e_F$), but the Fermi momentum concept is not definable, so the Fermi surface in $\vec{k}$-space is missing. The state emerges in the vicinity of a Mott insulating phase when lattice distortions are present, is highly degenerated and paramagnetic. A gap is present at high $U$ in the density of low lying excitations. During low lying excitations, quasi-particles are not created above the Fermi level, only the number of particles at $e_F$ increases.

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I. INTRODUCTION

The topic of non-Fermi liquid (NFL) behavior in $D > 1$ dimensions and normal (non-symmetry broken) phase (NP) is currently of great interest. This is mainly due to the large amount of experimental results, obtained in principle in the last decade, showing NFL behavior in the NP of a variety of materials, including $D > 1$ dimensional systems of great interest. Examples are: high $T_c$ superconductors, heavy-fermions, layered systems, quasi-one dimensional conductors, doped semiconductors, systems with impurities, materials presenting proximity to metal-insulator transitions, etc. These results changed considerably our understanding of interacting Fermi systems. Indeed, until recently, Fermi-liquid (FL) theory seemed universally applicable to all sufficiently pure interacting Fermi systems, and its main features even to dirty systems, provided that their NP is not destroyed by a symmetry breaking process. This “dogma” has been based on high precision experimental verifications in liquid $He_3$ and simple metals. The concept of FL itself has been introduced by Landau many decades ago (for a thorough discussion see), and in principle has the meaning that in spite of the interactions, the low energy behavior can be well described within a picture of almost noninteracting quasi-particles. Formulated in rigorous terms, in a normal FL we have a one-to-one correspondence between the non-interacting and interacting single-particle states (determined e.g., by a perturbation theory convergent up to infinite orders). Furthermore, a quasi-particle pole is present in the single-particle propagator that gives rise to a step-like discontinuity of the momentum distribution function $n_{\vec{k}}$ at the Fermi surface, whose position is specified by a sharp Fermi momentum value $\vec{k}_F$. The observation of NFL behavior in the materials presented above polarized a huge intellectual effort in the last decade for the understanding of this new fermionic state. In this field the theoretical interpretations are often based on multi-band models, the presence of a some kind of gap in the NP being clearly established in many cases and subject of intensive experimental and theoretical studies. However, despite the great number of papers published in the field (see for example the references cited in or), and the fact that the observed most
interesting and important normal NFL properties emerge in two spatial dimensions (2D), (for example the normal phase of the high \( T_c \) superconductors), on the theoretical side, for pure systems, the existence of a NFL state in a NP has been proved exactly only in one dimensions (i.e. Luttinger liquid\(^1\)). The extension possibility of NFL-NP properties to 2D has not been demonstrated rigorously up today. In fact, a rigorous theory of a NFL normal state in higher than one dimensions is missing.

Driven by these state of facts, we started to focus our attention on possible NFL states using exact methods which are applicable in higher than one dimensions as well\(^2\). Based on the obtained results and a conjecture made by us\(^3\), in this paper we are reporting the first rigorously derived NFL state in 2D. We deduced for this reason exact solutions for a real space version of the periodic Anderson model (PAM) in 2D. The model is analyzed on a two dimensional square lattice, in case of non-vanishing and finite Hubbard on-site repulsion \( U \). In the paper in fact two qualitatively different solutions are described: a completely localized and a non-localized one, which represents the first exact results reported for PAM in 2D and finite \( U \). The solutions are valid on two surfaces of the parameter space, i.e. on restricted, but continuous and infinite regions of the \( T = 0 \) phase diagram, extended from the low \( U \) to the high \( U \) regions up to \( U = \infty \) at \( U > 0 \).

The derived non-Fermi liquid state is given by a flat band effect in multi-band systems with more than half filling. The obtained properties are extremely peculiar: the system in case of the described solution possesses a well defined Fermi energy \( e_F \) in conditions in which the \( \vec{k}_F \) Fermi momentum cannot be defined, and the \( n_{\vec{k}} \) momentum distribution function is continuous together with its derivatives of any order. The system has also a natural built in gap, which is clearly present in the density of low lying excitations at high \( U \). The state is paramagnetic and non-insulating. The gap symmetry is a possible symmetry allowed by the described 2D lattice, and depends on the starting parameters of the system. The state emerges in the proximity of a Mott insulating phase when lattice distortions in the unit cell are present. During low lying excitations quasi-particles are not created above the Fermi level, only the number of particles increases at \( e_F \).
Concerning the flat band features (FBF), we mention that such characteristics have been clearly observed in different systems where strong electron interactions and strong correlation effects play a main role. On numerical side, FBF are present for example in results connected to 2D Hubbard model\textsuperscript{17–19}, or 2D $t-J$ model\textsuperscript{20}. Experimentally FBF are seen in angle-resolved photo-emission (ARPES) data of high $T_c$ cuprates\textsuperscript{21,22}. For layered systems ARPES often shows main bands without any sharp characteristics in $n_\vec{k}$\textsuperscript{23}, or give results interpreted via FBF assumptions\textsuperscript{24}. Band structure calculations for these systems often reflects a Fermi level positioned exactly at the bottom of a conduction band with large effective mass around its minimum, below which a gap is present\textsuperscript{4}. We further wish to mention that connections between superconductivity and FBF were also clearly pointed out by Imada et al.\textsuperscript{25}, and FBF can be seen as well in experiments related to heavy-fermion materials\textsuperscript{26}. On the technological side, for example Lammert et al.\textsuperscript{27} have shown that squashing carbon nanotubes, FBF can be achieved around $e_F$, where a mismatch of nearly isoenergetic $\vec{k}$ states may have unexpected application possibilities.

The remaining part of the paper is constructed as follows: Section II. presents in detail the analyzed model and the general form of the deduced ground-state wave-functions. Section III. characterizes the obtained solutions from the point of view of the $\vec{k}$ - space representation of the Hamiltonian and wave-vectors described, and Section IV. analyzes magnetic properties of the system in the studied ground-states. Section V. describes a completely localized insulating solution, Section VI. presents the new non-Fermi liquid state in normal phase and 2D, Section VII. summarizes the paper, and the Appendix, containing mathematical details, closes the presentation.

**II. THE MODEL AND GROUND STATES DEDUCED**

We are describing in this Section the model we use and the ground-states detected for it in restricted domains of the phase diagram.
A. The model

We are considering in this paper a 2D square lattice described by a two-band model whose Hamiltonian for the start is given in direct space, containing on-site repulsive interaction in one band. The starting point will be sufficiently general in order to give us the possibility to characterize in detail the state we are presenting. However, the model contains also restrictions. Based on physical considerations, and denoting by \( \vec{d}_n \) the positions of the \( n \)th neighbors of a given but arbitrary lattice site, we are taking into consideration in this paper only the \( n \leq 2 \) (i.e. nearest, and next-nearest neighbor) contributions in the Hamiltonian. With these considerations, our starting Hamiltonian can be given as

\[
\hat{H} = \hat{H}_0 + \hat{U}, \quad \hat{H}_0 = \hat{T}_c + \hat{T}_f + \hat{V} + \hat{E}_f,
\]

where the non-interacting terms have been denoted together by \( \hat{H}_0 \). With \( \vec{r}_i \) denoting an arbitrary 2D lattice site position \( \vec{r}_i \), the contributing terms in Eq.\( (1) \) can be explicitly written as follows

\[
\begin{align*}
\hat{T}_c & = \sum_{j,\sigma} \left( t_{c,\sigma} \hat{c}^\dagger_{j,\sigma} \hat{c}_{j+x,\sigma} + h.c. \right) + \sum_{j,\sigma} \left( t_{c,\sigma} \hat{c}^\dagger_{j,\sigma} \hat{c}_{j+y,\sigma} + h.c. \right) + \\
& \sum_{j,\sigma} \left( t_{c,\sigma} \hat{c}^\dagger_{j,\sigma} \hat{c}_{j+(x+y),\sigma} + h.c. \right) + \sum_{j,\sigma} \left( t_{c,\sigma} \hat{c}^\dagger_{j,\sigma} \hat{c}_{j+2\sigma} + h.c. \right), \\
\hat{T}_f & = \sum_{j,\sigma} \left( t_{f,\sigma} \hat{f}^\dagger_{j,\sigma} \hat{f}_{j+x,\sigma} + h.c. \right) + \sum_{j,\sigma} \left( t_{f,\sigma} \hat{f}^\dagger_{j,\sigma} \hat{f}_{j+y,\sigma} + h.c. \right) + \\
& \sum_{j,\sigma} \left( t_{f,\sigma} \hat{f}^\dagger_{j,\sigma} \hat{f}_{j+(x+y),\sigma} + h.c. \right) + \sum_{j,\sigma} \left( t_{f,\sigma} \hat{f}^\dagger_{j,\sigma} \hat{f}_{j+2\sigma} + h.c. \right), \\
\hat{V}_1 & = \sum_{j,\sigma} \left( V^c_{1,x} \hat{c}^\dagger_{j,\sigma} \hat{f}_{j+x,\sigma} + h.c. \right) + \sum_{j,\sigma} \left( V^c_{1,y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+y,\sigma} + h.c. \right) + \\
& \sum_{j,\sigma} \left( V^c_{1,y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+(x+y),\sigma} + h.c. \right) + \sum_{j,\sigma} \left( V^{f\sigma}_{1,y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+y,\sigma} + h.c. \right), \\
\hat{V}_2 & = \sum_{j,\sigma} \left( V^c_{2,x+y} \hat{c}^\dagger_{j,\sigma} \hat{f}_{j+(x+y),\sigma} + h.c. \right) + \sum_{j,\sigma} \left( V^c_{2,x+y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+(x+y),\sigma} + h.c. \right) + \\
& \sum_{j,\sigma} \left( V^c_{2,x+y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+2\sigma} + h.c. \right) + \sum_{j,\sigma} \left( V^{f\sigma}_{2,x+y} \hat{f}^\dagger_{j,\sigma} \hat{c}_{j+y,\sigma} + h.c. \right),
\end{align*}
\]
\[ \hat{V}_0 = \sum_{j,\sigma} \left( V_0 c_{j,\sigma}^\dagger f_{j,\sigma} + h.c. \right), \quad \hat{E}_f = E_f \sum_{j,\sigma} f_{j,\sigma}^\dagger f_{j,\sigma}, \quad \hat{U} = U \sum_i \hat{n}_{f_i,\uparrow} \hat{n}_{f_i,\downarrow}. \] (6)

In these expressions \( x \) (\( y \)) represent elementary displacements along a single bond of length equal with the lattice constant \( a \) in \( \vec{x} \) (\( \vec{y} \)) direction, respectively. Taking into account different couplings along different lattice directions, we allow in fact the study of the system with distorted unit cell as well. The interaction term \( \hat{U} \) is the usual Hubbard interaction, where \( \hat{n}_{f_i,\sigma} = f_{i,\sigma}^\dagger f_{i,\sigma} \) is the particle number operator for \( f_{i,\sigma} \) electrons.

Our starting \( \hat{H} \) from Eq.(1) represents a prototype of an interacting two band system in 2D. It describes a square lattice containing fermions distributed in two bands \( b = c, f \). The kinetic energy term is in fact \( \hat{T} = \sum_{n=1}^{2} \sum_{\langle n; i, j \rangle, b, \sigma} \left( t_{b,\vec{d}_n} \hat{b}_{i,\sigma}^\dagger \hat{b}_{j,\sigma} + h.c. \right) \), where \( t_{b,\vec{d}_n} \) are hopping amplitudes, \( \sigma \) is the spin index, and \( \langle n; i, j \rangle \) has the meaning of a sum over bonds connecting \( n \)th neighbors, every bond being taken into account once. The hybridization between the bands is composed from on-site \( \hat{V}_0 \) and \( n \)th neighboring sites hybridizations \( \hat{V} = \sum_{n=1,2} \hat{V}_n \). As can be seen, in Eq.(1) the non-local hybridization \( \hat{V} = \hat{V}_1 + \hat{V}_2 \) contains the nearest-neighbor (\( \hat{V}_1 \)) and the next-nearest-neighbor (\( \hat{V}_2 \)) contributions only, the \( \hat{V}_n, n \geq 3 \) long-range terms being considered negligibly small. The on-site energy \( E_f \) for the second band fixes the relative position of the two bands, and finally, \( U \) represents in fact the on-site Coulomb repulsion in the second band \( b = f \), making the model interacting (\( U > 0 \)). We mention that \( U \) is present on all lattice sites. In order to help the reader in a better understanding of the notations, we are presenting in Fig.1. the hopping amplitudes for \( c \)-electrons (A), and hybridization matrix elements for \( c_{i}^\dagger f_{j} \) type transfers (B). The hopping amplitudes for \( f \)-electrons, and the hybridization matrix elements for \( f_{i}^\dagger c_{j} \) type transfers are similar. For them, only the index \( c \) has to be changed in \( f \) in Fig.1.A., and the superscript \( cf \) has to be replaced with \( fc \) in Fig.1.B. As given above, our Hamiltonian \( \hat{H} \) can be considered as a 2D - PAM given in a direct space version, or a 2D two-band Hubbard model containing the contribution of the Hubbard \( U \) only in one band, the other band being non-interacting.

We concentrate in this paper on a specific region of the phase diagram of the model \( \mathcal{P}_{\hat{H}} \). This region \( \mathcal{P}_{\hat{H}} \) can be defined as the domain of the parameter space where \( \hat{H} \) can
be expressed through elementary plaquette contributions in the form $\hat{A}^\dagger_{I,\sigma} \hat{A}_{I,\sigma}$. Here, the plaquette operator $\hat{A}_{I,\sigma}$ is build up from a linear combination of the starting $\hat{b}$ annihilation fermionic operators acting on the elementary plaquette $I$. We are denoting the four positions available on a plaquette by $j = 1, 2, 3, 4$, starting from the down-left corner and counting anti-clockwise (see the notation of sites from Fig.1.). The $I$th plaquette operator for a fixed spin $\sigma$ can be generally expressed as $\hat{A}_{I,\sigma} = \sum_{j,b} a_{j(I),b} \hat{b}_{j(I),\sigma}$, where, because of the translation invariance, $a_{j(I),b} = a_{j,b}$ plaquette independence will be considered for the emerging eight coefficients present in $\hat{A}_{I,\sigma}$, that have to be deduced. Taking the translational invariance explicitly into account, the plaquette operator acting on four corners of an elementary square plaquette $I$ becomes

$$\hat{A}_{I,\sigma} = a_{1,f} \hat{f}_1 + a_{2,f} \hat{f}_2 + a_{3,f} \hat{f}_3 + a_{4,f} \hat{f}_4$$

$$+ a_{1,c} \hat{c}_1 + a_{2,c} \hat{c}_2 + a_{3,c} \hat{c}_3 + a_{4,c} \hat{c}_4 .$$

(7)

Starting from Eq. (7), and taking into consideration periodic boundary conditions, the product $\hat{A}^\dagger_{I,\sigma} \hat{A}_{I,\sigma}$ summed over plaquettes for a fixed spin index $\sigma$ can be written as

$$\sum_{I} \hat{A}^\dagger_{I,\sigma} \hat{A}_{I,\sigma} = \left( \sum_{i=1}^{4} |a_{i,c}|^2 \right) \left( \sum_{j=1}^{N_{\Lambda}} \hat{c}^\dagger_{j,\sigma} \hat{c}_{j,\sigma} \right) + \left( \sum_{i=1}^{4} |a_{i,f}|^2 \right) \left( \sum_{j=1}^{N_{\Lambda}} \hat{f}^\dagger_{j,\sigma} \hat{f}_{j,\sigma} \right) +$$

$$\sum_{j=1}^{N_{\Lambda}} \left\{ \left[ (a^*_{1,c} a_{2,c} + a^*_{4,c} a_{3,c}) \hat{c}^\dagger_{j,\sigma} \hat{c}_{j+x,\sigma} + h.c. \right] + \left[ (a^*_{1,f} a_{2,f} + a^*_{4,f} a_{3,f}) \hat{f}^\dagger_{j,\sigma} \hat{f}_{j+x,\sigma} + h.c. \right] + \right.$$
In the expression of $\hat{s}$ consider the Hubbard term $\hat{\Lambda}$.

Based on Eq.(7), it can be observed that $\hat{\Lambda}$ is transformed as

$$\Lambda = \left( \sum_{i=1}^{N} \frac{a_i^* a_i}{\Lambda} \right) \left( \sum_{j=1}^{N} \frac{c_j^* \hat{f}_j}{\Lambda} \right) + h.c.$$

In Eq.(8), $N_\Lambda$ denotes the number of lattice sites. A comparison of Eq.(1) and Eq.(8) shows that $\hat{H}_0$ can be expressed via the $\hat{A}_{I,\sigma}$ operators as

$$\hat{H}_0 = -\sum_{I,\sigma} \hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} + K \hat{N},$$

if the following conditions are satisfied

$$-t_{c,x} = a_{1,c}^* a_{2,c} + a_{4,c}^* a_{3,c}, \quad -t_{c,y} = a_{1,c}^* a_{4,c} + a_{2,c}^* a_{3,c},$$

$$-t_{f,x} = a_{1,f}^* a_{2,f} + a_{4,f}^* a_{3,f}, \quad -t_{f,y} = a_{1,f}^* a_{4,f} + a_{2,f}^* a_{3,f},$$

$$-t_{c,x+y} = a_{1,c}^* a_{3,c}, \quad -t_{c,y-x} = a_{2,c}^* a_{4,c}, \quad -t_{f,x+y} = a_{1,f}^* a_{3,f}, \quad -t_{f,y-x} = a_{2,f}^* a_{4,f},$$

$$-V_{1,x}^{c} = a_{1,c}^* a_{2,c} + a_{4,c}^* a_{3,c}, \quad -V_{1,x}^{f} = a_{1,f}^* a_{2,c} + a_{4,f}^* a_{3,c},$$

$$-V_{1,y}^{c} = a_{1,c}^* a_{4,c} + a_{2,c}^* a_{3,c}, \quad -V_{1,y}^{f} = a_{1,f}^* a_{4,c} + a_{2,f}^* a_{3,c},$$

$$-V_{2,x+y}^{c} = a_{1,c}^* a_{3,c}, \quad -V_{2,x+y}^{f} = a_{1,f}^* a_{3,c},$$

$$-V_{2,y-x}^{c} = a_{2,c}^* a_{4,c}, \quad -V_{2,y-x}^{f} = a_{2,f}^* a_{4,c},$$

$$-V_0 = \sum_{i=1}^{4} a_{i,c}^* a_{i,f}, \quad K = \sum_{i=1}^{4} |a_{i,c}|^2,$$

$$E_f = K - \sum_{i=1}^{4} |a_{i,f}|^2.$$

In the expression of $\hat{H}_0$ the operator $\hat{N} = \sum_{i,k,\sigma} \hat{n}_{i,\sigma}^k$ represents the total particle number operator. Based on Eq.(7), it can be observed that $\hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} + \hat{A}_{I,\sigma} \hat{A}_{I,\sigma}^\dagger = \sum_{i=1}^{4} [ |a_{i,c}|^2 + |a_{i,f}|^2 ] = 2K - E_f$, so the Hamiltonian $\hat{H}_0$ can be written as

$$\hat{H}_0 = \sum_{I,\sigma} \hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} + K \hat{N} - 2 \left[ 2K - E_f \right] N_\Lambda.$$

In the presence of the interaction, besides $\hat{H}_0$ from Eq.(11), we have to take into consideration the Hubbard term $\hat{U}$ as well. However, we may observe that $\hat{U}$ can be exactly transformed as
\[
\hat{U} = U \hat{P}' + U \sum_{i,\sigma} \hat{n}_{i,\sigma}^f - U N_{\Lambda},
\]

where \( \hat{P}' = \sum_i \hat{P}'_i \) and \( \hat{P}'_i = (1 - \hat{n}_{i,2,\uparrow} - \hat{n}_{i,2,\downarrow} + \hat{n}_{i,1,\uparrow} \hat{n}_{i,1,\downarrow}) \). In the decomposition presented in Eq.(12) the \( \hat{P}' \) operator is a positive semidefinite operator. The reason for this is simple. \( \hat{P}'_i \) applied to a wave function gives one if on the \( i \) site there are no \( f \) electrons present, and gives zero, if on the site \( i \) there is at least one \( f \) electron present. As a consequence, \( \hat{P}' \) representing a sum of non-negative numbers, it is a positive semidefinite operator.

We have further to observe that in Eq.(12) the \( U \sum_{i,\sigma} \hat{n}_{i,\sigma}^f \) term simply renormalizes the \( E_f \) contribution from the Hamiltonian. Keeping this information, introducing the notations \( \tilde{E}_f = E_f + U \), and \( \tilde{G} = \sum_{I,\sigma} \hat{A}_{I,\sigma} \hat{A}_{I,\sigma}^\dagger \), the starting Hamiltonian from Eq.(1) can be written as

\[
\hat{H} = [ \tilde{G} + U \hat{P}' ] - [ U N_{\Lambda} + 2 ( 2 K - \tilde{E}_f ) N_{\Lambda} - K \hat{N} ].
\]

The decomposition presented in Eq.(13) is valid if the conditions presented in Eq.(9) are satisfied, and in Eq.(10) the \( E_f \) value is replaced by \( \tilde{E}_f \), where

\[
\tilde{E}_f = K - \sum_{i=1}^{4} |a_{i,f}|^2.
\]

We mention that from mathematical point of view, the parameter space region \( \mathcal{P}_{\hat{H}} \) is given by the solutions of the system of equations Eqs.(9,14). If this system of equations admits solutions for the coefficients \( a_{i,b} \) from Eq.(7), we are situated inside \( \mathcal{P}_{\hat{H}} \).

From Eq.(13) can be seen that in conditions presented by Eqs.(9,14), the analyzed Hamiltonian from Eq.(1) can be written as

\[
\hat{H} = \hat{P} + E^U_0,
\]

where the positive semidefinite operator \( \hat{P} \) and the constant number \( E^U_0 \) are given by \( \hat{P} = \tilde{G} + U \hat{P}' \), and

\[
E^U_0 = K N + ( U + 2 E_f - 4 K ) N_{\Lambda},
\]

where \( N \) being the eigenvalue of \( \hat{N} \), represents the number of particles within the system.
B. The detected ground-states

For the Hamiltonian from Eq.(15), $\hat{P}$ being a positive semidefinite operator, the ground-state energy is $E^U_g = E^U_0$, and the ground-state wave function is that $| \Psi^U_g \rangle$, for which we have $\hat{P} | \Psi^U_g \rangle = 0$. The interesting aspect from the mathematical side of the problem is that $| \Psi^U_g \rangle$ can be explicitly expressed in the concentration range situated at and above $3/4$ filling, obtained in this way a many-body, fully quantum mechanical solution in the interacting case and 2D. For this, we have to take into consideration that starting from the definition presented in Eq.(7), for plaquette operators we have $\hat{A}_{I,\sigma}^\dagger \hat{A}_{I',\sigma'}^\dagger + \hat{A}_{I',\sigma'}^\dagger \hat{A}_{I,\sigma}^\dagger = 0$. Furthermore, the number of elementary plaquettes $I$ from the system is equal with the number of lattice sites, and the product $\hat{F}^{(3)} = \prod_I \hat{F}_{1,f}^\dagger$ based on the operator (see also Eq.(20))

$$\hat{F}_{1,f} = \left( \alpha_{i,\uparrow} \hat{f}_{i,\uparrow} + \alpha_{i,\downarrow} \hat{f}_{i,\downarrow} \right)$$

containing arbitrary $\alpha_{i,\sigma}$ constants, creates an $f$ electron on every site of the lattice. As a consequences, for example at $3/4$ filling (i.e. $N = 3N_\Lambda$), the ground-state (not normalized) wave function $| \Psi^U_g \rangle$ becomes the ordered product

$$| \Psi^U_g \rangle = \prod_{\beta=1}^3 \hat{F}^{(3)} | 0 \rangle,$$

where

$$\hat{F}^{(1)} = \prod_I \hat{A}_{I,\uparrow}^\dagger, \quad \hat{F}^{(2)} = \prod_I \hat{A}_{I,\downarrow}^\dagger,$$

and $|0\rangle$ being the bare vacuum with no fermions present. Indeed, because of the $\hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma}^\dagger = 0$ property, we have $\hat{G} | \Psi^U_g \rangle = 0$ given by the $\hat{F}^{(1)} \hat{F}^{(2)}$ product in Eq.(18), while $\hat{F}^{(3)}$ introducing on every lattice site one electron, obliges $| \Psi^U_g \rangle$ to have at least one $f$ particle on each site, preserving $\hat{P}' | \Psi^U_g \rangle = 0$ as explained below Eq.(12).

We would like to underline here that the $\alpha_{i,\sigma}$ coefficients in Eq.(17) are completely arbitrary, so the most general form of the ground-state is in fact a linear combination of
components present in Eq. (18) taken over all possible combinations of all possible \( \alpha_{i,\sigma} \) values. This means that in the most general case, the \( \hat{F}_{i,f} \) operator (see Eq. (17)) contained in \( \hat{F}^{(3)} \), has the form

\[
\hat{F}_{i,f} = \sum_{\{\alpha_i,\sigma\}} g_{\{\alpha_i,\sigma\}} \left( \alpha_{i,\uparrow} \hat{f}_{i,\uparrow} + \alpha_{i,\downarrow} \hat{f}_{i,\downarrow} \right),
\]

(20)

where \( g_{\{\alpha_i,\sigma\}} \) represents numerical coefficients (connected to fixed \( \{\alpha_i,\sigma\} \) sets) restricted only by the normalization to unity of the whole wave function.

The solution for the ground-state can be also written for the system doped above \( \frac{3}{4} \) filling with arbitrary \( 1 \leq n_r < N_A \) number of electrons. For this reason we must define the operator

\[
\hat{F}^{(4)} = \epsilon_\uparrow \left( \hat{f}_{i,\uparrow}^\dagger + e^{i\phi_c} \hat{c}_{i,\uparrow}^\dagger \right) + \epsilon_\downarrow \left( \hat{f}_{i,\downarrow}^\dagger + e^{i\phi_c} \hat{c}_{i,\downarrow}^\dagger \right),
\]

(21)

which allows us to introduce randomly \( n_r \) additional electrons in the system above \( 3 N_A \) via

\[
\hat{F}^{(4)} = \sum_{\{i\}} C_{\{i\}} \prod_{i}^{n_r} \hat{F}^{(4)}_i.
\]

(22)

In Eq. (22), \( \prod_{i}^{n_r} \) represents an ordered product containing \( n_r \) arbitrary chosen lattice sites taken as a possible combination of \( n_r \) sites from \( N_A \) possibilities, and \( C_{\{i\}} \) are numerical coefficients. As a consequence, in the doped case with \( 1 \leq n_r < N_A \), the ground-state wave function becomes

\[
| \Psi_{g,d}^{U} \rangle = \prod_{\beta=1}^{4} \hat{F}^\beta | 0 \rangle.
\]

(23)

We mention that along this paper we will restrict our study to the \( N \geq 3 N_A \) (i.e. \( n_r \geq 0 \)) case.

It is extremely important to mention that the presented ground-state wave functions in Eqs. (18, 23) are valid only in interacting (\( U > 0 \)) case, and cannot be perturbatively obtained from the \( U = 0 \) noninteracting limit. The reason for this is that at \( U = 0 \), as explained below Eq. (19), the \( \hat{P} | \Psi_g^{U=0} \rangle = 0 \) property is entirely given by the \( \hat{F}^{(1)} \hat{F}^{(2)} \) product, the \( \hat{F}^{(3)} \) operator being completely arbitrary. In the noninteracting case the operator \( \hat{P} \)
reduces to $\hat{G}$, so we obtain inside $\mathcal{P}_{\hat{H}}$ at $U = 0$ the equality $\hat{G} \left| \Psi^0_g \right\rangle = 0$ with the ground-state wave function

$$\left| \Psi^0_g \right\rangle = \left[ \prod_{\beta=1}^{2} \hat{F}^\beta \right] \hat{Q} \left| 0 \right\rangle,$$

where $\hat{Q}$ is an arbitrary operator. As it can be seen, the concrete expression of the $\hat{F}^{(3)}$ operator is determined exactly by the nonzero $U > 0$ value of the interaction (see below Eq.(19)). Based on these characteristics mentioned, we would like to underline that is no way to re-obtain (together with all expectation values that it gives) $| \Psi^U_g \rangle$ from $| \Psi^0_g \rangle$ (or vice versa) in the $U \to 0$ limit.

The remaining part of the paper is devoted to the study of the physical properties of the $| \Psi^U_g \rangle$ wave function. We stress that depending on different solutions allowed by the system of equations Eqs.(14), the ground-state wave function given mathematically in Eq.(18) describes from physical point of view even qualitatively different ground-states, which will be analyzed below.

III. THE $K$-SPACE REPRESENTATIONS

First of all, we would like to understand the physical background of the Hamiltonian form presented in Eq.(13). We remember, that $\hat{H}$ from Eq.(13) represents an exact representation of the starting Hamiltonian from Eq.(1) in conditions in which Eqs.(9, 14) are valid (and admit solutions).

A. The Fourier transform for $\hat{H}$

In order to answer this question, let us transform the starting Hamiltonian from Eq.(1) in $\vec{k}$-space. In order to do this systematically, let us first concentrate on $\hat{H}_0$. Denoting by $\vec{k}$ the two-dimensional reciprocal space vector, and using for the operators the $b = c, f$ notation together with the Fourier sum $\hat{b}_j = \sum_{\vec{k}} \hat{b}_{\vec{k}} \exp \left[ -i \vec{k} \cdot \vec{r}_j \right]$, the kinetic energy terms becomes $\hat{T}_b = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}, \sigma} \hat{b}_{\vec{k}, \sigma} \hat{b}_{\vec{k}, \sigma}^\dagger$, where
$\hat{\varepsilon}_{k,\sigma}^h = \left( t_{b,x} e^{-i \vec{k} \cdot \vec{x}} + t_{b,x}^* e^{i \vec{k} \cdot \vec{x}} \right) + \left( t_{b,y} e^{-i \vec{k} \cdot \vec{y}} + t_{b,y}^* e^{i \vec{k} \cdot \vec{y}} \right) + \left( t_{b,x+y} e^{-i \vec{k} \cdot (\vec{x}+\vec{y})} + t_{b,x+y}^* e^{i \vec{k} \cdot (\vec{x}+\vec{y})} \right) + \left( t_{b,y-x} e^{-i \vec{k} \cdot (\vec{y}-\vec{x})} + t_{b,y-x}^* e^{i \vec{k} \cdot (\vec{y}-\vec{x})} \right).$ (25)

Concerning the notations, we mention that using $\vec{d}_n$ introduced at the beginning of Sec. II., defining $t_{b,d_n} = |t_{b,d_n}| \exp(i \phi_{t,b,d_n})$, we simply have $\varepsilon_{k,\sigma}^h = 2 \sum_{d_n} |t_{b,d_n}| \cos(\phi_{t,b,d_n} - \vec{k} \cdot \vec{d}_n)$.

For the on-site energy at the $f$ level we simply obtain $\hat{E}_f = E_f \sum_{k,\sigma} \hat{f}_{k,\sigma}^+ \hat{f}_{k,\sigma}$. Introducing the notation $\hat{T}_f = \hat{T}_c + \hat{T}_h$ together with the definitions $\varepsilon_{k,\sigma}^c = \varepsilon_{k,\sigma}^f$, $\varepsilon_{k,\sigma}^f = E_f + \varepsilon_{k,\sigma}^f$, we simply have at the level of Fourier transforms $\hat{T}_c + \hat{T}_h = \sum_{b,k,\sigma} \hat{b}_{k,\sigma}^\dagger \hat{b}_{k,\sigma}$ (note the difference between $\varepsilon_{k,\sigma}^c$ and $\varepsilon_{k,\sigma}^f$).

In the case of the hybridization, the on-site term becomes $\hat{V}_0 = \sum_{k,\sigma} (V_{0 \cdot k} \hat{c}_{k,\sigma}^\dagger \hat{f}_{k,\sigma} + h.c.)$. For the non-local hybridization $\hat{V}$, as shown in Sec.II., we have $\hat{V} = \hat{V}_1 + \hat{V}_2$, where, for $n = 1, 2$ we obtain $\hat{V}_n = \sum_{k,\sigma} \left( V_{n \cdot k} \hat{c}_{k,\sigma}^\dagger \hat{f}_{k,\sigma} + h.c. \right)$. The hybridization matrix elements in these expressions for $n = 1, 2$, are given by

$$V_{1,k} = \left( V_{1,1}^{cf} e^{-i \vec{k} \cdot \vec{x}} + V_{1,1}^{fe} e^{i \vec{k} \cdot \vec{x}} \right) + \left( V_{1,1}^{cf} e^{-i \vec{k} \cdot \vec{y}} + V_{1,1}^{fe} e^{i \vec{k} \cdot \vec{y}} \right) + \left( V_{1,1}^{cf} e^{-i \vec{k} \cdot (\vec{x}+\vec{y})} + V_{1,1}^{fe} e^{i \vec{k} \cdot (\vec{x}+\vec{y})} \right) + \left( V_{1,1}^{cf} e^{-i \vec{k} \cdot (\vec{y}-\vec{x})} + V_{1,1}^{fe} e^{i \vec{k} \cdot (\vec{y}-\vec{x})} \right).$$

$$V_{2,k} = \left( V_{2,2}^{cf} e^{-i \vec{k} \cdot \vec{x}} + V_{2,2}^{fe} e^{i \vec{k} \cdot \vec{x}} \right) + \left( V_{2,2}^{cf} e^{-i \vec{k} \cdot (\vec{y}-\vec{x})} + V_{2,2}^{fe} e^{i \vec{k} \cdot (\vec{y}-\vec{x})} \right).$$

Introducing the notation $V_{\vec{k}} = V_0 + V_{1,\vec{k}} + V_{2,\vec{k}}$, the total hybridization can be given as $\hat{V}_0 + \hat{V} = \sum_{\vec{k},\sigma} \left( V_{\vec{k}} \hat{c}_{\vec{k},\sigma}^\dagger \hat{f}_{\vec{k},\sigma} + h.c. \right)$, and for $\hat{H}_0$ we get

$$\hat{H}_0 = \sum_{\vec{k},\sigma} \left[ \varepsilon_{\vec{k},\sigma}^c \hat{c}_{\vec{k},\sigma}^\dagger \hat{c}_{\vec{k},\sigma} + \varepsilon_{\vec{k},\sigma}^f \hat{f}_{\vec{k},\sigma}^\dagger \hat{f}_{\vec{k},\sigma} + \left( V_{\vec{k}} \hat{c}_{\vec{k},\sigma}^\dagger \hat{f}_{\vec{k},\sigma} + h.c. \right) \right].$$ (27)

The diagonalization of $\hat{H}_0$ can now be simply done. For this reason we have to introduce the row vector $W_{\vec{k},\sigma}^\dagger = ( \hat{c}_{\vec{k},\sigma}^\dagger, \hat{f}_{\vec{k},\sigma}^\dagger )$, and the $(2 \times 2)$ matrix $\tilde{M}$ with components $M_{1,1} = \varepsilon_{\vec{k}}^c$, $M_{1,2} = V_{\vec{k}}$, $M_{2,1} = \varepsilon_{\vec{k}}^f$, $M_{2,2} = V_{\vec{k}}^*$. The $\hat{H}_0$ from Eq.(27) will contain under the sum over $\vec{k}$ the expression $( W_{\vec{k}}^\dagger \tilde{M} W_{\vec{k}} )$. The diagonalization of $\hat{H}_0$ in $\vec{k}$-space reduces to the secular equation written for the matrix $\tilde{M}$. We obtain from this $\left( \varepsilon_{\vec{k}}^c - E_{\vec{k}} \right) \left( \varepsilon_{\vec{k}}^f - E_{\vec{k}} \right) - |V_{\vec{k}}|^2 = 0,$ from where, as expected, two bands arise ($i = 1, 2$)

$$E_{\vec{k},i} = \frac{1}{2} \left[ \varepsilon_{\vec{k}}^c + \varepsilon_{\vec{k}}^f \pm T_{\vec{k}} \right].$$ (28)
The expression of $T_{\vec{k}}$ in Eq. (28) is given by $T_{\vec{k}} = \sqrt{(\epsilon_{k}^{c} - \epsilon_{k}^{f})^2 + 4|V_{\vec{k}}|^2}$. If we are using now Eqs. (9,10) in the expressions given for $\epsilon_{k}^{c}$, $\epsilon_{k}^{f}$, and $V_{\vec{k}}$ in terms of the starting Hamiltonian parameters in Eqs. (25,26), we realize that the following equality holds

$$|V_{\vec{k}}|^2 = (K - \epsilon_{k}^{c})(K - \epsilon_{k}^{f}).$$

(29)

This is a lengthy but straightforward calculation which in fact, easily can be done. Using now Eq. (29) for $T_{\vec{k}}$, we find $T_{\vec{k}}^2 = (\epsilon_{k}^{c} + \epsilon_{k}^{f} - 2K)^2$, so the band structure given by Eq. (28) becomes

$$E_{k,1} = K = \text{constant}, \quad E_{k,2} = \epsilon_{k}^{c} + \epsilon_{k}^{f} - K.$$  

(30)

From Eq. (30) we can see that $K \geq 0$, since $K$ is positive definite. Furthermore, we have $K \geq \epsilon_{k}^{c}$ as well. Indeed, using Eqs. (1,23) we obtain

$$K - \epsilon_{k}^{c} = \sum_{i=1}^{4} a_{i,c} |^2 + \left[ (a_{1,c} a_{2,c} + a_{4,c} a_{3,c}) e^{-i k_x} + c.c. \right] + \left[ (a_{1,c} a_{4,c} + a_{2,c} a_{3,c}) \times e^{-i k_y} + c.c. \right] + \left[ a_{1,c} a_{3,c} e^{-i (k_x + k_y)} + c.c. \right] + \left[ a_{2,c} a_{4,c} e^{-i (k_y - k_x)} + c.c. \right].$$

(31)

Introducing now the notations

$$a_{1,c}' = a_{1,c} e^{i \frac{k_x + k_y}{2}}, \quad a_{2,c}' = a_{2,c} e^{-i \frac{k_x - k_y}{2}},$$

$$a_{3,c}' = a_{3,c} e^{-i \frac{k_x + k_y}{2}}, \quad a_{4,c}' = a_{4,c} e^{i \frac{k_x - k_y}{2}},$$

(32)

the exponential factors disappear from Eq. (31), and for $K - \epsilon_{k}^{c}$ we find (see also Eq. (41))

$$K - \epsilon_{k}^{c} = (a_{1,c}' + a_{2,c}' + a_{3,c}' + a_{4,c}')(a_{1,c}' + a_{2,c}' + a_{3,c}' + a_{4,c}') = |a_{1,c}' + a_{2,c}' + a_{3,c}' + a_{4,c}'|^2.$$  

(33)

However, $K \geq \epsilon_{k}^{c}$ via Eq. (29) means $K \geq \epsilon_{k}^{f}$ as well, since $|V_{\vec{k}}|^2$ is a non-negative number. As a consequence, the band structure obtained in Eq. (30) contains an upper band that is completely flat ($E_{k,1} = E_1 = K$), and a lower, normal, $\vec{k}$-dependent band ($E_{k,2}$) with dispersion. The $\vec{k}$ dependent gap between these two bands is given by $\Delta_{\vec{k}} = E_1 - E_{\vec{k},2} = 2K - (\epsilon_{k}^{c} + \epsilon_{k}^{f})$, and based on Eqs. (29,31) $\Delta_{\vec{k}} \geq 0$ holds. Introducing
\( \Delta = \text{Min} [\Delta_{\vec{k}}] \), we have \( \Delta \geq 0 \). Being important below, at this point we mention that \( \Pi_{\vec{k}} \Delta_{\vec{k}} > 0 \) means \( \Delta > 0 \) as well. From physical point of view, \( \Delta \geq 0 \) means that the diagonalized bands from Eq.\((30)\) are never intersecting. In case of \( \Delta = 0 \), \( E_{\vec{k},1} \) and \( E_{\vec{k},2} \) touch each other, while for \( \Delta > 0 \) the diagonalized bands are completely separated.

From Eq.\((30)\) it can be observed, that the conditions from Eqs.\((9,10)\) that allows the transformation of the starting Hamiltonian Eq.\((1)\), into \( \hat{H} \) from Eq.\((15)\), are exactly the conditions that give a band structure containing a completely flat (i.e. dispersion-less) upper band seen in Eq.\((30)\).

When the system is interacting and the \( U > 0 \) Hubbard term is present, the Hamiltonian becomes \( \hat{H} \) given in Eq.\((13)\). In the ground-state, because of \( \hat{P} [\Psi_U] = 0 \), the effective Hamiltonian has in fact exactly the form of \( \hat{H}_0 \)\[28\], excepting that \( E_f \) is renormalized as \( \tilde{E}_f = E_f + U \) (i.e. the condition from Eq.\((10)\) has to be changed to that given in Eq.\((14)\)), and the energy scale, as seen from Eq.\((10)\), is shifted with \( U N_{\Lambda} \). As a consequence, effectuating the band structure calculation as presented above, using instead of \( E_f \) the \( \tilde{E}_f \) value, we re-obtain (shifted with \( U N_{\Lambda} \)) for the ground-state the structure presented in Eq.\((30)\). The same holds for excited states which give \( \hat{P} [\Psi] = 0 \) as well.

It is interesting to mention at this point, that a two - band system with a band structure as given in Eq.\((30)\), above half filling (i.e. with more than two electrons per lattice site), has a well defined Fermi energy positioned at \( e_F = E_1 = K \) (where \( K \) is a \( \vec{k} \) independent constant), but the Fermi momentum \( \vec{k}_F \) is not definable. A such type of system has no Fermi surface in \( \vec{k} \)-space, so for this case, the Luttinger theorem is without meaning.

Another aspect that has to be accentuatedly underlined, is the fact that the Hubbard interaction gives effectively its contribution in the flattening of the upper diagonalized band \( E_{\vec{k},1} \) in the case in which the here reported solutions are valid. In order to understand this, first let as mention that for \( U = 0 \), as seen from Eq.\((24)\), the solutions from Eqs.\((18,23)\) are not applicable. Let turn then to the \( U \neq 0 \) case, and analyze a concrete pedagogical example. Consider for example the Hamiltonian parameters \( t_{c,x} = t_{c,y} = 12 \), \( t_{c,x+y} = t_{c,y-x} = -4 \), \( t_{f,x} = t_{f,y} = 3 \), \( t_{f,x+y} = t_{f,y-x} = -1 \), \( V_0 = 18 \), \( V_{1,x} = V_{1,y} = -6 \), \( V_{2,x+y} = V_{2,y-x} = 2 \), and
$E_f = 2$. The written numbers are expressed in $|t_{f,x+y}|$ units. This particular case describes an isotropic situation, with $V^{cf} = V^{fc} = V$, which has been chosen only to be easy for the reader to follow, without diminishing the general physical content of the behavior reflected by Eq.(30). The $E_{\vec{k},1}$ band from Eq.(28) with $U = 0$ and parameters given above, is presented in the upper plot of Fig. 2. (the $k_x$ and $k_y$ values cover the first Brillouin-zone, i.e. $[-\pi, +\pi]$ in units of the lattice constant). As can be seen, for this non-interacting case we have a normal $\vec{k}$ dependent band, the system is metallic, and the system of equations Eqs.(9,10) has no solutions (i.e. at $U = 0$ we are situated outside of $\mathcal{P}_H$). However, turning the interaction on (note that for $U \neq 0$ we have $\tilde{E}_f$ instead of $E_f$ in Eq.(28), and Eq.(10) has to be changed with Eq.(14)), the presence of the interaction starts to flatten the $E_{\vec{k},1}$ band. Indeed, as seen from Fig. 2. (middle plot: $U = 10$, bottom: $U = 20$), the $E_{\vec{k},1}$ surface starts to flatten with increasing $U$ values. The completely flat $E_{\vec{k},1}$ case given in Eq.(30) is obtained for $U = 25$, which at the level of the system of equations Eqs.(11,14) is represented by the solution $a_{1,c} = 3 + \sqrt{5}$, $a_{2,c} = -2$, $a_{3,c} = 3 - \sqrt{5}$, $a_{4,c} = -2$, $a_{1,f} = -(\sqrt{5} + 3)/2$, $a_{2,f} = 1$, $a_{3,f} = (\sqrt{5} - 3)/2$, $a_{4,f} = 1$. When this solution emerges at $U = 25$, the Hubbard interaction has pushed the system inside $\mathcal{P}_H$, so its role is fully active in obtaining the interacting ground-states described here.

### B. Decomposition into composite operators

We have to mention that obtaining the diagonalized band picture for $\hat{H}$ presented in Eq.(30), the mathematical description can be given in $\vec{k}$-space in term of new (composite) fermionic operators, which creates composite fermions in the upper and lower band. To see this, we note that the following relation holds

$$
eq K \hat{C}_{\vec{k},1,\sigma}^{\dagger} \hat{C}_{\vec{k},1,\sigma} + ( \epsilon_{\vec{k},\sigma}^c + \epsilon_{\vec{k},\sigma}^f - K ) \hat{C}_{\vec{k},2,\sigma}^{\dagger} \hat{C}_{\vec{k},2,\sigma},$$

where for $j = 1, 2$ the operators $\hat{C}_{\vec{k},j,\sigma}$ are defined as
\[ \hat{C}_{k,j,\sigma} = \frac{(-1)^j}{\sqrt{\Delta_k}} \left( \sqrt{K - \epsilon_k^c} \hat{f}_{k,\sigma} - (-1)^j e^{(-1)^j i \phi_V} \sqrt{K - \epsilon_k^f} \hat{c}_{k,\sigma} \right) e^{+i \theta_j}. \] (35)

From Eq.(34) it can be seen that \( \phi_V \) represents the argumentum of \( V_k \), i.e. \( V_k = |V_k| e^{i \phi_V} \).

Furthermore, \( \theta_1 \) and \( \theta_2 \) represent two arbitrary, independent, and \( \vec{k} \) independent phases.

Using Eqs.(30,34), the operator \( \hat{H}_0 \) can be written now in a simple form

\[ \hat{H}_0 = \sum_{k,\sigma} \left( E_{k,1} \hat{C}_{k,1,\sigma}^\dagger \hat{C}_{k,1,\sigma} + E_{k,2} \hat{C}_{k,2,\sigma}^\dagger \hat{C}_{k,2,\sigma} \right). \] (36)

The expression presented in Eq.(36) shows that the operators defined in Eq.(35) annihilate (their adjoint create) particles from (into) the ,,diagonalized bands” \( j = 1 \) (upper flat band), and \( j = 2 \) (lower band with dispersion), respectively. Since \( \{ \hat{C}_{k,j,\sigma}, \hat{C}_{k',j',\sigma'} \} = \delta_{k,k'} \delta_{j,j'} \delta_{\sigma,\sigma'} \), \( \{ \hat{C}_{k,j,\sigma}, \hat{C}_{k',j',\sigma'}^\dagger \} = \{ \hat{C}_{k,j,\sigma}^\dagger, \hat{C}_{k',j',\sigma'} \} = 0 \) , the \( \hat{C}_{k,j,\sigma} \) operators represent new, rigorous, canonical and anti-commuting Fermionic operators.

The transformation into Eq.(36) physically is more deep as seems to be at first view. In order to see this, we have to analyze the Fourier transform of the plaquette operators \( \hat{A}_{I,\sigma} \).

Starting from Eq.(37), the Fourier transform of \( \hat{A}_{I,\sigma}^\dagger \) can be written as

\[ \hat{A}_{I,\sigma}^\dagger = \sum_k e^{i \vec{k} \cdot \vec{x}} \left[ X_c(\vec{k}) \hat{c}_{k,\sigma}^\dagger + X_f(\vec{k}) \hat{f}_{k,\sigma}^\dagger \right], \] (37)

where, for \( b = c, f \) we have

\[ X_b(\vec{k}) = a_{1,b}^* + a_{2,b}^* e^{i \vec{k} \cdot \vec{x}} + a_{3,b}^* e^{i \vec{k} \cdot (\vec{x} + \vec{y})} + a_{4,b}^* e^{i \vec{k} \cdot \vec{y}}. \] (38)

Effectuating the product over the ordered plaquette index \( I \) in \( \prod_I \hat{A}_{I,\sigma}^\dagger \) (such a product emerges in the ground-state wave function from Eqs.(18,23)), given by the anti-commutation rules of the starting \( \hat{f}, \hat{c} \) operators, only a product containing different \( \vec{k} \) indices survives.

Introducing the notation \( Y = \sum_P (-1)^p \exp[i (\vec{r}_1 \cdot \vec{k}_{i_1} + \vec{r}_2 \cdot \vec{k}_{i_2} + \ldots + \vec{r}_{N,\Lambda} \cdot \vec{k}_{i_{N,\Lambda}})], \) where \( \sum_P \) denotes a sum over all possible permutations of \( (1, 2, \ldots, N,\Lambda) \) to \( (i_1, i_2, \ldots, i_{N,\Lambda}) \), and \( \bar{p} \) represents the number of pair permutations in a given \( P \), we obtain

\[ \prod_I \hat{A}_{I,\sigma}^\dagger = Y \prod_{\vec{k}} \left[ X_c(\vec{k}) \hat{c}_{k,\sigma}^\dagger + X_f(\vec{k}) \hat{f}_{k,\sigma}^\dagger \right]. \] (39)
As can be seen from Eq. (39), the contribution into the norm of the ground state wave function given by
\[ \prod I \hat{A}_I,\sigma \] is proportional to \( \mathcal{R} = \prod \mathcal{R}_k \) where \( \mathcal{R}_k = \left[ |X_c(k)|^2 + |X_f(k)|^2 \right] \). However, using Eq. (25) together with the definitions given in Sec.III. for \( \epsilon^b_\vec{k} \) and Eqs. (9, 38), we find
\[ |X_c(\vec{k})|^2 = K - \epsilon^c_\vec{k}, \quad |X_f(\vec{k})|^2 = K - \epsilon^f_\vec{k}, \quad X_c(\vec{k}) X^*_f(\vec{k}) = -V_\vec{k}. \] (40)

For example, in the case of the first relation from Eq. (40), we simply must use \( X^*_c(\vec{k}) \) from Eq. (38) and multiply it with \( \exp \left[ \frac{i}{2} (k_x + k_y) \right] \) in order to see the expression of \( (K - \epsilon^c_\vec{k}) \) presented in Eq. (33). The remaining two equalities can be similarly deduced.

From the first two relations of Eq. (40) we observe that the contribution of the operator \( \hat{F}^{(1)} \) (or \( \hat{F}^{(2)} \)) into the norm of the ground state wave function is determined via Eq. (39) by
\[ \mathcal{R}_k = \Delta_k = |X_c(\vec{k})|^2 + |X_f(\vec{k})|^2 = 2 K - (\epsilon^c_\vec{k} + \epsilon^f_\vec{k}). \] (41)

Let us now introduce instead of the initial plaquette operators \( \hat{A}_I,\sigma \), new plaquette operators „normalized to unity”, i.e. whose contribution under the \( \prod I \) product give unity into the norm of the wave function. In this case instead of \( \hat{A}_I,\sigma \) we must use
\[ \hat{B}_I,\sigma = \left( \frac{|Y|^{-1}}{\sqrt{\prod \Delta_k}} \right)^{\frac{1}{2}} \hat{A}_I,\sigma. \] (42)

In this case we have instead of \( \prod I \hat{A}_I,\sigma \), the product
\[ \prod I \hat{B}^I_{I,\sigma} = \prod \hat{B}^I_{k,\sigma} \left[ \frac{1}{\sqrt{\Delta_k}} \left( X_c(\vec{k}) \hat{c}^I_{k,\sigma} + X_f(\vec{k}) \hat{f}^I_{k,\sigma} \right) \right] = \prod \hat{B}^I_{k,2,\sigma}, \] (43)

where
\[ \hat{B}^I_{k,2,\sigma} = \frac{1}{\sqrt{\Delta_k}} \left( X_c(\vec{k}) \hat{c}^I_{k,\sigma} + X_f(\vec{k}) \hat{f}^I_{k,\sigma} \right). \] (44)

Now let us denote \( X_c(\vec{k}) = |X_c(\vec{k})| e^{i\phi_c}, \quad X_f(\vec{k}) = |X_f(\vec{k})| e^{i\phi_f}, \quad V_\vec{k} = |V_\vec{k}| e^{i\phi_V}. \) Using these notations, from Eq. (33) and first two equations from Eq. (40) we find \( \hat{C}^I_{k,2,\sigma} = \Delta_k^{-1/2} \left( |X_c(\vec{k})| \hat{c}^I_{k,\sigma} - e^{-i\phi_V} |X_f(\vec{k})| \hat{f}^I_{k,\sigma} \right). \) From Eq. (44) we have however \( \hat{B}^I_{k,2,\sigma} = \Delta_k^{-1/2} \left( |X_c(\vec{k})| \hat{c}^I_{k,\sigma} - e^{-i\phi_V} |X_f(\vec{k})| \hat{f}^I_{k,\sigma} \right). \)
\[ \Delta_k^{-1/2} (|X_c(\vec{k})| e^{i \phi_c} \hat{c}_{\vec{k},\sigma} + |X_f(\vec{k})| e^{i \phi_f} \hat{f}_{\vec{k},\sigma}^\dagger) = e^{i \phi_c} \Delta_k^{-1/2} (|X_c(\vec{k})| \hat{c}_{\vec{k},\sigma}^\dagger + |X_f(\vec{k})| e^{i (\phi_f - \phi_c)} \hat{f}_{\vec{k},\sigma}^\dagger). \]

From the third relation of Eq. (37) via Eqs. (29, 40) we obtain
\[ e^{i (\phi_f - \phi_c)} = - e^{i \phi_v}, \]
which means \[ e^{i (\phi_f - \phi_c)} = - e^{-i \phi_v}, \] and the expression of \( \hat{B}_{\vec{k},2,\sigma}^\dagger \) becomes
\[ \hat{B}_{\vec{k},2,\sigma}^\dagger = e^{i \phi_c} \hat{C}_{\vec{k},2,\sigma}^\dagger. \] (45)

This means that the Fourier transform of \( \hat{B}_{\vec{k},\sigma} \) (i.e. the normalized \( \hat{A}_{\vec{k},\sigma} \)), is in fact \( \hat{C}_{\vec{k},2,\sigma}^\dagger \) if we fix the phase \( \theta_2 \) from Eq. (35) to \( \theta_2 = - \phi_c \).

Similar to \( \hat{B}_{\vec{k},2,\sigma}^\dagger \), we can introduce the normalized \( \hat{B}_{\vec{k},1,\sigma}^\dagger = e^{-i \phi_c} \hat{C}_{\vec{k},1,\sigma}^\dagger \), which creates a particle in the upper band, by fixing the \( \theta_1 \) phase as \( \phi_c \). We obtain
\[ \hat{B}_{\vec{k},1,\sigma}^\dagger = \frac{1}{\sqrt{\Delta_k}} \left( X_{f}(\vec{k}) \hat{c}_{\vec{k},\sigma}^\dagger - X_{c}(\vec{k}) \hat{f}_{\vec{k},\sigma}^\dagger \right). \] (46)

Since in comparison with \( \hat{C}_{\vec{k},j,\sigma}^\dagger \), only a phase factor difference emerges, the canonical anti-commutation relations remain true for \( \hat{B}_{\vec{k},j,\sigma} \) operators as well. Using Eqs. (45, 46), the initial operators can be also expressed via
\[ \hat{f}_{\vec{k},\sigma} = \frac{X_{f}(\vec{k}) \hat{B}_{\vec{k},2,\sigma} - X_{c}(\vec{k}) \hat{B}_{\vec{k},1,\sigma}}{\sqrt{\Delta_k}}, \quad \hat{c}_{\vec{k},\sigma} = \frac{X_{c}(\vec{k}) \hat{B}_{\vec{k},2,\sigma} + X_{f}(\vec{k}) \hat{B}_{\vec{k},1,\sigma}}{\sqrt{\Delta_k}}. \] (47)

With the composite operators introduced, for the \( \hat{H}_0 \) operator we obtain
\[ \hat{H}_0 = \sum_{j=1,2} \sum_{\vec{k},\sigma} E_{\vec{k},j,\sigma} \hat{B}_{\vec{k},j,\sigma}^\dagger \hat{B}_{\vec{k},j,\sigma}, \] (48)
and the ground-state wave functions presented in Sec.II. becomes
\[ |\Psi_{g}^{U}\rangle = \prod_{\vec{k}} \left( \hat{B}_{\vec{k},2,\uparrow}^\dagger \hat{B}_{\vec{k},2,\downarrow}^\dagger \right) \hat{F}^{(3)} |0\rangle, \]
\[ |\Psi_{g,d}^{U}\rangle = \prod_{\vec{k}} \left( \hat{B}_{\vec{k},2,\uparrow}^\dagger \hat{B}_{\vec{k},2,\downarrow}^\dagger \right) \hat{F}^{(3)} \hat{F}^{(4)} |0\rangle, \] (49)
where the ordered product over \( \vec{k} \) has to be taken over the whole first Brillouin zone. The norm of the ground-state wave functions from Eq. (49) is entirely determined by \( \hat{F}^{(3)} \) with \( \beta = 3, 4 \).
We however stress, that the $\vec{k}$ representations for the deduced ground-state wave functions presented in Eqs.(49) are valid only if the initial ground-state wave functions from Eqs.(18,23) have nonzero norm. This is the case if $\Pi_{\vec{k}} \Delta_{\vec{k}} \neq 0$ holds (see Eq.(42)), i.e. the diagonalized bands $F_{\vec{k},j=1,2}$ are completely separated. In order to find such situations, mathematically is sufficient to have for all $\vec{k}$ values from the first Brillouin zone $|X_c(\vec{k})| > 0$.

IV. MAGNETIC PROPERTIES

Continuing the study of physical properties of the deduced ground-state, the following natural step is to analyze its magnetic properties. This is motivated by the existence of ferro-magnetism in some flat-band models\textsuperscript{29}. Because of this reason, we have to check if something similar is present for our solutions, or not. Starting from this motivation, we obtain however paramagnetic properties (i.e. large spin degeneracy) for the deduced ground states. The reason for this is the following one.

As can be seen from Eq.(20), the obtained ground-state wave functions have a large degeneracy. With this observation in mind, let us consider first the $N = 3N_\Lambda$ (i.e 3/4 filling) case. We have a $d_g = 2^{N_\Lambda}$ fold degeneracy in $|\Psi^U_g\rangle$ due to the up or down orientation possibilities of the $N/3 = N_\Lambda$ electrons from the system, since $2N_\Lambda$ particles fill up completely the lower band, so their contribution in the total spin is zero. From the point of view of the $\alpha_{i,\sigma}$ coefficients entering in $\hat{F}^{(3)}$ as given in Eq.(17), this means that it is possible for us to obtain $d_g$ linearly independent contributions in $|\Psi^U_g\rangle$, by choosing arbitrary $\alpha_{i,\uparrow}$ and $\alpha_{i,\downarrow}$ coefficients. The $S^z$ value of these states (S being the total spin) is situated between $[-N_\Lambda/2, +N_\Lambda/2]$. The contributions from these states with strictly $S^z = N_\Lambda/2$ can be obtained by choosing $\alpha_{i,\uparrow} = 1$ and $\alpha_{i,\downarrow} = 0$ for all $i$ sites. This maximal $S^z$ for the system can be achieved in an unique way, therefore there is an unique state (apart from the trivial $(2S + 1)$ fold degeneracy) among the linearly independent contributions in the ground-state, with $S = N_\Lambda/2$.

After finding this contribution in $|\Psi^U_g\rangle$ characterized by $S = N_\Lambda/2$ total spin, let us
chose one single lattice site $i_1$ with $\alpha_{i_1,\uparrow} = 0$ and $\alpha_{i_1,\downarrow} = 1$, the remaining sites $i \neq i_1$ being maintained with $\alpha_{i,\uparrow} = 1$, $\alpha_{i,\downarrow} = 0$. Moving the position of the $i_1$ site along the lattice, we obtain all contributions in the ground-state with $S^z = N_A/2 - 1$. Let us denote these states by $|\Psi_\beta\rangle$, where $\beta = 1, 2, \ldots N_A$. These states are linearly independent (see Appendix), and they span an $N_A$ dimensional subspace since a single particle spin can be flipped down independently on $N_A$ lattice sites. The mentioned $|\Psi_\beta\rangle$ states are also components of $|\Psi_g^U\rangle$. Since between the $|\Psi_\beta\rangle$ wave vectors it must be one term corresponding to the $(S^z = N_A/2 - 1, S = N_A/2)$ state, we have $N_A - 1$ linearly independent states with $S = N_A/2 - 1$. As a consequence, $|\Psi_g^U\rangle$ contains not only components with $S = N_A/2$, but also components with $S = N_A/2 - 1$. Continuing this procedure, one can see that every spin value $S$ is present among the ground state contributions $N!(2S+1)/[(N/2+S+1)!(N/2-S)!]$ times (and certainly everyone has $2S + 1$ components with different $S^z$ values). The $S = 0$ subspace has the greatest degeneracy, i.e. it has the greatest statistical weight. Therefore, in the thermodynamic limit the expectation value of the spin goes to zero, i.e. the system is paramagnetic.

In fact, since states with different $S$ can be obtained from $|\Psi_g^U\rangle$ simply by modifying the $\alpha_{i,\sigma}$ values in Eq.(17), it means that calculating the ground-state expectation value $\langle \hat{S}^2 \rangle$ based on Eqs.(17,18), we obtain an expression that depends on the arbitrary coefficients $\alpha_{i,\sigma}$. This means that for $|\Psi_g^U\rangle$, the value of the total spin is not fixed, it possesses a large spin degeneracy, i.e. is paramagnetic. This property will not be changed even if we take into consideration the $\hat{F}^{(4)}$ operator in the ground-state wave function (i.e. doped system), because we add in this case in the expression of $\langle \hat{S}^2 \rangle$, contributions depending on $\alpha_{i,\sigma}$ multiplied by arbitrary constants $C_{\{i\}}$ present in Eq.(22). As a consequence, the detected solutions describes paramagnetic phases.

Before closing this section, we have to mention that large spin degeneracy characteristics of the ground-states for strongly correlated systems have been also reported elsewhere. An interesting result on this line, is that described by Arita and Aoka [30]. These authors have found for $t-t'$ type Hubbard models ground-states holding simultaneously total spin $S = 0$
and \( S = S_{\text{max}} \) values in the thermodynamical limit. In their case, the singlet \( S = 0 \) component is created by a spiral spin state with a spin correlation length as large as the system size, which accompanies the fully polarized ferromagnetic state with total spin \( S_{\text{max}} \).

We have to underline, that our case differs semnificatively from that presented in Ref. 30. In contrast to Ref. 30, in the ground states from Eqs. (18,23), all total spin \( S \) values are present. As will be exemplified later on (see for example a concrete solution described in Eq.(57)), given by the arbitrary nature of the coefficients \( \alpha_{i,\sigma} \), a local spin periodicity presence in the ground-state is rather accidental, instead of a characteristic (or general) property.

V. THE INSULATING PHASE

Besides the fact that the states we obtained are non-magnetic, their physical properties still remain to be clarified. These properties depend in fact from the possible solutions of Eqs.(9,14). To have an insight in these possibilities, let us analyze Eq.(9). In this study we have to consider the coupling constants from the Hamiltonian \( \hat{H} \) known variables, and to try to deduce based on them the \( a_{i,b} \) parameters entering into \( \hat{A}_{I,\sigma} \) presented in Eq.(7). We may start solving this problem by introducing the parameters

\[
\begin{align*}
 p_1 &= \frac{V_{c}^{f}}{t_{f,x+y}} = \frac{a_{1,c}}{a_{1,f}}, & \quad p_2 &= \frac{V_{c}^{f}}{t_{f,x+y}} = \frac{a_{3,c}}{a_{3,f}}, \\
 q_1 &= \frac{V_{c}^{f}}{t_{f,y-x}} = \frac{a_{2,x}}{a_{2,f}}, & \quad q_2 &= \frac{V_{c}^{f}}{t_{f,y-x}} = \frac{a_{4,c}}{a_{4,f}}.
\end{align*}
\]

Comparing Eqs.(7,50), we can rewrite the plaquette operator \( \hat{A}_{I,\sigma} \) as follows

\[
\begin{align*}
 \hat{A}_{I,\sigma} &= a_{1,f} \left( \hat{f}_{1,\sigma} + p_1^* \hat{c}_{1,\sigma} \right) + a_{2,f} \left( \hat{f}_{2,\sigma} + q_1^* \hat{c}_{2,\sigma} \right) + \\
 & \quad \left( \hat{f}_{3,\sigma} + p_2 \hat{c}_{3,\sigma} + a_{3,f} \left( \hat{f}_{4,\sigma} + q_2 \hat{c}_{4,\sigma} \right). \right)
\end{align*}
\]

The physical nature of the ground-state is strongly influenced by the particle distribution created within the lattice by \( | \Psi_{U} > \) or \( | \Psi_{g,d} > \). Since \( \hat{F}^{(3)} \) introduces one electron on every lattice site, this particle distribution is essentially determined by the product \( \hat{F}^{(1)} \hat{F}^{(2)} \). But on a given lattice site we independently can introduce two electrons with opposite spin,
reason for which we focus on the behavior of $\hat{F}^{(1)}$. In order to have an image about these aspects, we are interested to analyze the situation in which the operator $\hat{F}^{(1)} = \prod_I \hat{A}_I^{\dagger}$ introduces two electrons (one $c$ and one $f$), at least on a lattice site. If a such situation emerges, $\hat{F}^{(1)}$ creates a non-uniform particle distribution within the lattice. This is because it introduces in the system $N_\Lambda$ particles on $N_\Lambda$ lattice sites creating somewhere a double occupancy, which must be followed by an empty site. Using Eq.(51) and multiplying two arbitrary neighboring plaquettes, for a site taking place in both plaquettes the following six type of nonzero products may emerge

$$
\begin{align*}
I_1 &= (f_{i,\sigma}^{\dagger} + p_1 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + q_1 \hat{c}_{i,\sigma}^{\dagger}), \\
I_2 &= (f_{i,\sigma}^{\dagger} + p_1 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + p_2 \hat{c}_{i,\sigma}^{\dagger}), \\
I_3 &= (f_{i,\sigma}^{\dagger} + p_1 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + q_2 \hat{c}_{i,\sigma}^{\dagger}), \\
I_4 &= (f_{i,\sigma}^{\dagger} + q_1 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + \hat{c}_{i,\sigma}^{\dagger}), \\
I_5 &= (f_{i,\sigma}^{\dagger} + q_1 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + q_2 \hat{c}_{i,\sigma}^{\dagger}), \\
I_6 &= (f_{i,\sigma}^{\dagger} + p_2 \hat{c}_{i,\sigma}^{\dagger}) \cdot (f_{i,\sigma}^{\dagger} + q_2 \hat{c}_{i,\sigma}^{\dagger}).
\end{align*}
$$

(52)

If at least one $I_j$ term from Eq.(52) is nonzero, we identified at least a site $i$, where $\prod_I \hat{A}_I^{\dagger}$ introduces two particles. Effectuating the products in Eq.(52) and taking into consideration the anti-commutation rules for the fermionic creation operators, for $I_j$ from Eq.(52) we find

$$
\begin{align*}
I_1 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (p_1 - q_1), \\
I_2 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (p_1 - p_2), \\
I_3 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (p_1 - q_2), \\
I_4 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (q_1 - p_2), \\
I_5 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (q_1 - q_2), \\
I_6 &= \hat{c}_{i,\sigma}^{\dagger} f_{i,\sigma}^{\dagger} (p_2 - q_2).
\end{align*}
$$

(53)

Usually for the hybridization matrix elements we have $V_{\chi}^{cf} = V_{\chi}^{fc} = V_{\chi}$ for an arbitrary element $\chi$, reason for which we focus in the remaining part of the paper to this case (the results presented up to the end of Sec.IV. remaining valid for the general $V_{\chi}^{cf} \neq V_{\chi}^{fc}$ situation as well). This means that we have in fact

$$
p = p_1 = p_2, \quad q = q_1 = q_2.
$$

(54)

Now if we consider only real coupling constants in the Hamiltonian $\hat{H}$, in Eq.(53) only the terms containing $\delta = (p - q)$ survives. From physical point of view, if $\delta = 0$, the wave function $|\Psi_g^U\rangle$ introduces on every lattice site the same number of electrons. Since hopping
matrix elements for a such type of state are all zero, the ground-state is completely localized, i.e. represents a Mott-insulator.

After this step, considering $p$ and $q$ pure real variables (i.e. all coupling constants from $\hat{H}$ are pure real), we have to check if the solutions allowed by Eqs.(9,14) gives $\delta = 0$ or not. For this reason two cases have to be enumerated.

A. The symmetric case

In the first step we analyze the $p = q$ situation, called symmetric case. Physically a such type of parameter region can be obtained, for example, when the lattice has a non-distorted unit cell. In these circumstances $t_{b,x+y} = t_{b,y-x}$ and $V_{2,x+y} = V_{2,y-x}$, i.e. $(p - q) = 0$, so all $I_j = 0$ from Eq.(53). (We underline that rigorously the condition $p = q$ means $V_{2,x+y} V_{2,y-x} = t_{f,x+y} t_{c,y-x}$, which exceeds in fact the non-distorted unit cell situation.). We mention here, that for $p = q$ the system of equations from Eq.(9) admits only solutions of the type $p = p^*$. In this case $\hat{A}_{I,\sigma}^+ = \sum_{i=1}^4 a_{i,f}^* (p \hat{c}_{i,\sigma}^\dagger + \hat{f}_{i,\sigma}^\dagger)$, and the product $\prod_I \hat{A}_{I,\sigma}^I$ from the ground-state wave function can be replaced by $\hat{F}_\sigma = \prod_I \hat{F}_{I,\sigma}$, where $\hat{F}_{I,\sigma} = (p \hat{c}_{I,\sigma}^1 + \hat{f}_{I,\sigma}^1)$. We note, that the product in $\hat{F}_\sigma$ is a product over lattice sites instead of plaquettes. The contribution into the norm of $\hat{F}_\sigma$ is well defined and equal with $(1 + p^2)^N\Lambda$. The ground-state wave function becomes for the insulating case

$$| \Psi^U_I \rangle = \prod_I \left[ \hat{F}_{i,\uparrow} \hat{F}_{i,\downarrow} \hat{F}_{i,f} \right] | 0 \rangle.$$  (55)

We mention that this ground-state is present only at $3/4$ filling, $p = q$, and real coupling constants in the Hamiltonian. It is interesting to note that for $p = q$ and real, the $\vec{k}$ representations for the ground-state wave functions from Eq.(19) have no meaning since (see Eq.(12,63)) we have $\prod_{\vec{k}} \Delta_{\vec{k}} = 0$ for this case. This means, that the norm of the initial $| \Psi^U_g \rangle$ wave function from Eq.(18) is not well defined (i.e. is zero) as expressed in the form of a product over plaquette operators in its $\hat{F}^{(1)} \hat{F}^{(2)}$ part. However, a re-structuration in the ground-state wave function by changing $\hat{A}_{I,\sigma}$ to $\hat{F}_{I,\sigma}$ eliminates from the wave vector the
source of the zero norm, and the ground-state from Eq. (55) becomes well defined, and its norm is finite.

From Eq. (55) we obtain \(|\Psi_f^U\rangle = \Pi_i \hat{F}_i^I |0\rangle\), where

\[
\hat{F}_i^I = [p^2 \alpha_{i\uparrow} \hat{c}_{i\uparrow}^{\dagger} \hat{f}_{i\uparrow} + p^2 \alpha_{i\downarrow} \hat{c}_{i\downarrow}^{\dagger} \hat{f}_{i\downarrow}^\dagger + p \alpha_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{c}_{i\uparrow} + p \alpha_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}] \quad (56)
\]

Introducing the notation \(|\alpha_i|^2 = |\alpha_{i\uparrow}|^2 + |\alpha_{i\downarrow}|^2\), and \(q_i = \left[ (1 + p^2) |\alpha_i|^2 \right]^{-1}\), all nonzero ground-state one-particle expectation values can be given as

\[
\langle \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \rangle = q_i \left[ p^2 |\alpha_{i\sigma}|^2 + |\alpha_i|^2 \right] \quad (57)
\]

Summing up over \(\sigma\) we obtain

\[
\sum_{\sigma} \langle \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \rangle = \frac{p^2 + 2}{p^2 + 1} \quad \sum_{\sigma} \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \rangle = \frac{2p^2 + 1}{p^2 + 1} \quad \sum_{\sigma} \langle \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \rangle = \frac{p}{p^2 + 1} \quad (58)
\]

Evidently, here \(\langle \ldots \rangle = \langle \Psi_f^U | \ldots | \Psi_f^U \rangle / \langle \Psi_f^U | \Psi_f^U \rangle\) holds. Based on Eq. (58) we re-obtain \(N = 3N_A\), and the ground-state expectation values of different Hamiltonian terms becomes

\[
\langle \hat{T}_c \rangle = 0 \quad \langle \hat{T}_f \rangle = 0 \quad \langle \hat{V} \rangle = 0 \quad \langle \hat{V}_0 \rangle = \frac{2p V_0 N_A}{1 + p^2} \quad (59)
\]

Summing up all contributions in Eq. (59) we obtain for the ground-state energy of the insulating phase

\[
\frac{E_0^I}{N_A} = \frac{1}{1 + p^2} \left[ U + E_f (p^2 + 2) + 2p V_0 \right] \quad (60)
\]

Introducing \(\langle \hat{R}_{loc} \rangle = \langle \hat{U} \rangle + \langle \hat{E}_f \rangle + \langle \hat{V}_0 \rangle\) as the contribution of the on-site (i.e. localized) Hamiltonian terms into the ground state energy, and \(\langle \hat{R}_{mov} \rangle = \langle \hat{T}_c \rangle + \langle \hat{T}_f \rangle + \langle \hat{V} \rangle\) as the contribution in the ground-state energy of the Hamiltonian terms connected to the movement of particles within the system, we find

\[
\langle \hat{R}_{loc} \rangle = E_0^I \quad \langle \hat{R}_{mov} \rangle = 0 \quad (61)
\]
which clearly shows that the system is completely localized.

In fact, from Eq.(60) we have \( E_0^I/N_\Lambda = -U + 2(U + E_f) + [2pV_0 - p^2(U + E_f)]/(1 + p^2) \), which becomes \( E_0^I/N_\Lambda = -U + 2(U + E_f) - K \) via

\[
K = p^2 \bar{S}, \quad V_0 = -p \bar{S}, \quad U + E_f = K - \bar{S}, \quad \bar{S} = \sum_{i=1}^{4} |a_{i,f}|^2. \tag{62}
\]

But, for \( p = q \) and all coupling constants real, Eqs.(62) can be directly obtained from the system of equations Eqs.(11,14). As can be seen, the ground-state energy obtained in Eq.(60) gives exactly back the value deduced in Eq.(16) at \( N = 3N_\Lambda \). Taking into account from Eq.(50), that \( p = V_{2,x+y}/t_{f,x+y} \), based on Eq.(62), we find the surface \( (U + E_f)/V_0 = (1 - p^2)/p \) in the \( \{U, E_f, V_0\} \) parameter space where the described solution emerges. The multiple conditions seen in Eq.(50) relating the hopping matrix elements and neighboring hybridizations to the \( p \) parameter can be achieved in the simplest way in the case of the non-distorted unit cell. As can be seen, \( \delta = 0 \) for \( p = q \) and \( p = p^* \), represents a possible physical solution for the analyzed problem.

Before continuing, some observations has to be made here. First of all, from Eq.(58) one can see that the sum over \( \sigma \) of the nonzero ground-state expectation values presented in Eq.(57) are independent on the \( \alpha_{1,\sigma} \) coefficients introduced by \( \hat{F}^{(3)} \) in Eq.(17). This implies that the results given in Eq.(59) are valid also for the most general form of the ground-state wave function expressed with \( \hat{F}^{(3)} \) constructed via Eq.(20) instead of Eq.(17). We underline that the independence on the \( \alpha_{1,\sigma} \) coefficients of the ground-state expectation values summed up over \( \sigma \) is a general property of the ground-state wave function, and is valid not only in the insulating case described here (see Appendix).

Secondly, we mention that doping the system, the properties described here will be destroyed. The reason for this is that introducing electrons above \( 3/4 \) filling, the number of particles per site will not be constant along the whole lattice, and as a consequence, the ground-state expectation values of the kinetic energy terms become to be nonzero.
B. The non-symmetric case

Both \( p \) and \( q \) being considered pure real, we concentrate now on the possibility of a \( p \neq q \) solution. We arrive to this inequality for example taking into account distorted unit cell, which gives usually the \( p \neq q \) condition. The \( \delta \) value introduced after Eq. (54) is nonzero, so the state we are analyzing is clearly a non-localized state. Solving however for this case Eq. (9), and calculating the norm of the ground state wave function \( |\Psi_g^U\rangle \) from Eq. (18), we obtain zero value.

Indeed, solving the system of equations Eqs. (9,10) for \( p \neq q \) and both real (see Eq. (33)), we finally obtain

\[
|X_c|^2 = K - \epsilon_c^\pm = 4p^2 |t_{f,x+y}| \left( C_{1,s,k} + \frac{sqr}{p} C_{2,s,k} \right)^2, \\
|X_f|^2 = K - \epsilon_f = 4 |t_{f,x+y}| \left( C_{1,s,k} + r s C_{2,s,k} \right)^2, \\
V_k = -4p |t_{f,x+y}| \left( C_{1,s,k} + \frac{sqr}{p} C_{2,s,k} \right) \cdot \left( C_{1,s,k} + r s C_{2,s,k} \right), \\
K = 2p^2 |t_{f,x+y}| \left( 1 + \frac{q^2r^2}{p^2} \right), \\
V_0 = -2p |t_{f,x+y}| \left( 1 + r^2 \frac{q}{p} \right),
\]

(63)

where \( s = t_{f,x}/t_{f,y}, r = t_{f,x}/(2t_{f,x+y}) \), and, for \( s > 0 \) we have \( C_{i,s,k} = \cos \left[ \frac{k}{2} \cdot (x + (-1)^i+1 y) \right] \) and for \( s < 0 \), \( C_{i,s,k} = \sin \left[ \frac{k}{2} \cdot (x + (-1)^i+1 y) \right] \), respectively. We mention that for the case of real coupling constants in the Hamiltonian and \( p = p_1 = p_2 \neq q = q_1 = q_2 \) presented here, the system of equations Eqs. (9,10) admits solutions only for \( -s t_{f,x+y} > 0 \), \( sign[t_{f,x+y}] = sign[t_{f,y-x}] \) and \( t_{f,x}^2 = t_{f,y}^2 \). From Eq. (63) it can be seen that there exist at least one \( k \) value, for which \( \Delta_k = 0 \) (for example, \( k_x = k_y = 0 \) for \( s < 0 \), or \( k_y = 0, k_x = \pi \) for \( s > 0 \)). So indeed, the norm of the ground-state wave function is vanishing, it is not possible to remove this property as in \( p = q \) case, and as a consequence, the solution is not proper for describing the presented situation.

As a conclusion, we can see that for pure real coupling constants in the Hamiltonian, the described solution at \( 3/4 \) filling represents a completely localized state. The part of the wave function \( |\Psi_g^U\rangle \) that gives nonzero norm introduces on every site of the lattice rigorously the same number of electrons. Given by this reason, a hopping \( \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}, \hat{f}_{i,\sigma}^\dagger \hat{f}_{j,\sigma}, \) or \( \hat{c}_{i,\sigma}^\dagger \hat{f}_{j,\sigma}, \) with...
\( i \neq j \) creates a state orthogonal to \( |\Psi_g^U\rangle \). As a consequence, all ground-state expectation values connected to the movement of particles within the system (i.e. kinetic energy terms and neighboring hybridizations) are zero. In this respect, the obtained state represents a paramagnetic Mott insulator, and the ground-state energy can be obtained as a sum of the ground-state expectation values of the on-site terms from the Hamiltonian.

Before continuing, we would like to underline the extreme sensitivity of the solutions contained in Eqs. (9, 14) to lattice distortions. In specially we stress, that in the case of the undistorted unit cell (i.e. \( t_{b,x} = t_{b,y}, t_{b,x+y} = t_{b,y-x}, V_{1,x} = V_{1,y}, V_{2,x+y} = V_{2,y-x} \)) the system of equations Eqs. (9, 14) admits only pure real solutions for \( p \) and \( q \), i.e. a completely localized ground-state.

VI. THE NON-LOCALIZED SOLUTION

In order to obtain another type of solution than that presented in the previous Section, we must consider the hybridization coupling constants imaginary, the Hamiltonian remaining hermitian. We further consider in this Section all hopping matrix elements real and \( V_\gamma^{cf} = V_\gamma^{fc} \) for all hybridization matrix elements \( \gamma \). Again, as in the case of the completely localized solution, two cases emerge, namely \(|p| \neq |q|\), and \(|p| = |q|\), which will be analyzed separately.

A. The possible solutions for imaginary \( p \) and \( q \)

We study now the solutions allowed by Eqs. (9, 14) in case of imaginary \( p \) and \( q \). The first group of solutions obtained, emerge at \(|p| \neq |q|\), case that will be denoted as non-symmetric below.

1. The non-symmetric case

Introducing the notations from Eq. (50) and being interested only in situations described by Eq. (54), for \(|p| \neq |q|\) the solutions allowed by Eqs. (9, 14) are characterized by five indepen-
dent and free starting parameters, namely $V_{2,x+y} = iV_{2,x+y}, V_{2,y-x} = iV_{2,y-x}, t_{f,x+y}, t_{f,y-x}$, and $U$, where $\tilde{V}_\gamma$ are pure real variables. Solutions are obtained for $|t_{f,x}| = |t_{f,y}| = 2\sqrt{t_{f,x+y} t_{f,y-x}}, \theta = -t_{f,x+y} t_{f,x}/t_{f,y} > 0$ and gives $V_{1,x} = (p+q^*)t_{f,x}/2, V_{1,y} = (p+q)t_{f,y}/2, V_0 = 0$. We obtain $a_{1,f} = \chi e^{i\phi}, a_{2,f} = 2\chi(t_{f,y-x}/t_{f,y}) e^{i\phi}, a_{3,f} = \chi(t_{f,x}/t_{f,y}) e^{i\phi}, a_{4,f} = 2\chi(t_{f,y-x}/t_{f,x}) e^{i\phi}$, where $\chi = \sqrt{\theta}$, and $\phi$ is an arbitrary phase. From this, $K = 2|\chi|^2(|p|^2 + |q|^2|2t_{f,y-x}/t_{f,y}|^2), K_f = K - \bar{E}_f = 2|\chi|^2(1 + |2t_{f,y-x}/t_{f,y}|^2)$. Introducing the notations $r = t_{f,x}/(2 t_{f,x+y}), s = t_{f,y}/t_{f,x},$ for $|X_c(\mathbf{k})|^2$ we obtain

$$
|X_c(\mathbf{k})|^2 = 4 |p|^2 |t_{f,x+y}| \left( C_{1,-s,k} + \frac{s q r}{p} C_{2,-s,k} \right),
$$

where $C_{i,s,k}$ has been introduced in Eq.(63). Since for a well defined non-zero norm we have to have $|X_c(\mathbf{k})|^2 > 0$ for all $\mathbf{k}$ (see for example Eq.(63), or the explication presented after Eq.(19)), Eq.(64) shows that the non-symmetric case described here fails to represent a proper physical solution.

2. The symmetric case

From mathematical point of view the symmetric $|p| = |q|$ solution is more complicated than the non-symmetric one. For this case two situations emerge, namely $p = q$, and $p = q^*$, respectively. These two situations are however physically equivalent, and can be obtained each from other by a rotation with $\pi/2$ of the system of coordinates. Because of this reason, we have to analyze in detail only one of them, namely the $p = q, p = -p^*$. As for the non-symmetric solutions, we have $V_\gamma = i \tilde{V}_\gamma$ for all hybridization matrix elements.

The $p = q$ solution emerge only for distorted unit cell. Five parameters can be independently chosen, namely $t_{f,x+y}, t_{f,y-x}, V_{2,x+y}, V_0,$ and $U$, so that $t_{f,x+y} \neq t_{f,y-x}$ and $\text{sign}(t_{f,x+y}) = \text{sign}(t_{f,y-x})$. The solution gives via the $p = V_{2,x+y}/t_{f,x+y}$ parameter the relations $t_{c,x+y} = p^2 t_{f,x+y}, t_{c,y-x} = p^2 t_{f,y-x}, t_{c,x} = |p|^2 t_{f,x}, t_{c,y} = -|p|^2 t_{f,y}, V_{1,x} = 0, V_{1,y} = p t_{f,y}, V_{2,y-x} = p t_{f,y-x}, t_{f,x}^2 = 4 t_{f,x+y} t_{f,y-x},$ and $t_{f,y} = -t_{f,x} \text{[sign}(t_{f,x+y}) \text{]} [1 + (\tilde{\theta})^2]^{1/2}$ so that $-t_{f,x} t_{f,y}/t_{f,x+y} > 0, -r t_{f,y} > 0,$ where
\[ r = \frac{t_{f,x}}{(2 t_{f,x+y})}, \bar{\theta} = \frac{V_0}{2 V_{2,x+y}} \left( t_{f,y-x} - t_{f,x+y} \right) \]. For the \( a_{i,f} \) coefficients we find \( |a_{1,f}|^2 = w - u, |a_{2,f}|^2 = -r^2 (w - u), |a_{3,f}|^2 = -w - u, |a_{4,f}|^2 = r^2 (w - u) \), where \( w = \frac{V_0}{2 p (r^2 - 1)} \) and \( u = \frac{t_{f,y}}{(2 r)} \). We have to consider \(|p|^2 > 1\) and \( r^2 \neq 1 \), the solution being present in the \( \{U, E_f, V_0\} \) parameter space on the surface

\[
U + E_f = \frac{|t_{f,y}|}{|r|} \left( |p|^2 - 1 \right) \left( r^2 + 1 \right).
\]

Introducing the notation \( s = -t_{f,x+y}/t_{f,x+y} \), for \( z = t_{f,x}/t_{f,y} \) we obtain \( z = s/\sqrt{1 + (\bar{\theta})^2} \), so \( 0 < |z| < 1 \) emerge. For \(|X_c(k)|^2\), using the notation \( D_k = (C_{1,s,k} + r s C_{2,s,k})^2 \), we find

\[
|X_c(k)|^2 = 4 |p|^2 |t_{f,x+y}| \left[ D_k + \frac{1 - |z|}{2|z|} \left( 1 + r^2 - 2 r \cos(k_y) \right) \right].
\]

For \(|r| \neq 1\) the expression from Eq.(66) is strictly positive, so the norm of the ground-state wave function is nonzero and well defined. In this case we obtain besides \(|X_c(k)|^2 > 0\) as well \( \Delta_k > 0 \), since \(|X_c(k)|^2\) and \(|X_f(k)|^2\) change their sign at the same \( k \) value. As explained in Sec. III., in the present case \( \Delta > 0 \), which physically means that the diagonalized bands from Eq.(34) are non-intersecting and completely separated.

From mathematical point of view, at the level of \(|X_c(k)|^2\), the main difference between the non-symmetric and symmetric case presented in this Section arises from the fact that for \( p \neq q \) we have \(|a_{1,c}| = |a_{3,c}|, |a_{2,c}| = |a_{4,c}|\), and the phase of \( a_{1,c}, a_{3,c}, (or a_{2,c}, a_{4,c}) \), differs only by \( 0 \) or \( \pi \). Such properties are not present for \( p = q \). In view of Eq.(32), this means that in the non-symmetric case, coupling together \((a'_{1,c}, a'_{3,c}), (or a'_{2,c}, a'_{4,c})\) in the expression of \(|X_c(k)|^2 = K - \epsilon^c_k\), the trigonometric factors \( C_{i,s,k} \) automatically arise, leading to Eq.(34). For the symmetric case, a such type of direct term grouping in \(|X_c(k)|^2\) is no more possible.

**B. Ground-state expectation values**

Once in conditions presented in Sec.VI.A.2. the norm of the ground-state wave function is well defined and \(|X_c(k)|^2 > 0, \Pi_k \Delta_k > 0\), we have find a completely different solution
in comparison with the ground-state presented in Sec. V. Being motivated by the interest to find the physical properties of the system in the analyzed case, we can start now the calculation of all ground-state expectation values of interest. Since the study can now be easier done in the $\vec{k}$ coordinates, we are presenting the calculations using the $\vec{k}$ representation of the ground-state wave function and Hamiltonian described in Sec.III.B.

The deduction of the main expectation values based on which the physical interpretations are made can be followed using the presented Appendix in their full generality in the case of arbitrary $\alpha_{1,\sigma}$ coefficients. However, in order to be easier for the reader to follow the main steps of the deduction, we are presenting below a simplified version of the calculation obtained in the case of site independent $\alpha_{1,\sigma}$ coefficients, which leads to the same results. In fact, the Appendix shows for example, that rigorously, in order to calculate ground-state expectation values of different Hamiltonian terms (i.e. expectation values summed over the spin index), is enough to consider site independence for the $\alpha_{1,\sigma}$ coefficients entering in the $\hat{F}^{(3)}$ operator present in the ground-state wave function. We mention, that from physical point of view, the difference between $\alpha_{1,\sigma} = \alpha_{\sigma}$, and site dependent $\alpha_{1,\sigma}$, is that the first case describes the maximal total spin $S$ part of the ground-state wave function only, and the second case takes into account the full expression of the ground-state wave function.

Introducing for the $\alpha_{1,\sigma} = \alpha_{\sigma}$ case the notation $|\alpha|^2 = \sum_{\sigma} |\alpha_{\sigma}|^2$, the $\hat{F}^{(3)}$ operator becomes $\hat{F}^{(3)} = \prod_i \hat{F}_i^{(3)\dagger}$ where

$$\hat{F}_i^{(3)\dagger} = |\alpha|^{-1} \left( \alpha_{\uparrow} \hat{f}_{i,\uparrow}^\dagger + \alpha_{\downarrow} \hat{f}_{i,\downarrow}^\dagger \right),$$

the coefficients $\alpha_{\sigma}$ being arbitrary. In the $\vec{k}$ space the contribution of $\hat{F}^{(3)}$ (taking into account normalized factors) becomes in this case $\hat{F}^{(3)} = \sum_{\vec{k}} \hat{F}_{\vec{k}}^{(3)}$, where

$$\hat{F}_{\vec{k}}^{(3)} = \sum_{\sigma} \frac{\alpha_{\sigma}}{|\alpha|} \hat{f}_{\vec{k},\sigma}^\dagger,$$

and for the norm of the ground-state wave function from Eq.(49) we obtain

$$\langle \Psi^U_g | \Psi^U_g \rangle = \prod_{\vec{k}} |X_c(\vec{k})|^2.$$
In the case of 3/4 filling, the desired expectation values becomes (we have here \( \langle ... \rangle = \langle \Psi^U_g | ... | \Psi^U_g \rangle / \langle \Psi^U_g | \Psi^U_g \rangle \))

\[
\langle \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} \rangle = \frac{|\alpha|^2|X_c(\vec{k})|^2 + |\alpha_\sigma|^2|X_f(\vec{k})|^2}{|\alpha|^2 \Delta_\vec{k}}, \quad \langle \hat{f}^\dagger_{k,\sigma} \hat{f}_{k,\sigma} \rangle = \frac{|\alpha|^2|X_f(\vec{k})|^2 + |\alpha_\sigma|^2|X_c(\vec{k})|^2}{|\alpha|^2 \Delta_\vec{k}},
\]

\[
\langle \hat{f}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} \rangle = -V_\vec{k} \frac{|\alpha_\sigma|^2}{|\alpha|^2 \Delta_\vec{k}}.
\]  

Effectuating the sum over the spin index in Eq.(70), as expected from the Appendix, the numerical coefficients \( \alpha_\sigma \) disappear from the expectation values

\[
\sum_\sigma \langle \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} \rangle = \frac{2}{\Delta_\vec{k}} |X_c(\vec{k})|^2 + |X_f(\vec{k})|^2, \quad \sum_\sigma \langle \hat{f}^\dagger_{k,\sigma} \hat{f}_{k,\sigma} \rangle = \frac{2}{\Delta_\vec{k}} |X_f(\vec{k})|^2 + |X_c(\vec{k})|^2,
\]

\[
\sum_\sigma \langle \hat{f}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} \rangle = -V_\vec{k} \frac{2}{\Delta_\vec{k}}.
\]  

Comparing with Eqs.(A12,A13), we see that the expectation values from Eq.(71) are true for arbitrary \( \alpha_{1,\sigma} \), so are correct also in the case of using the general Eq.(20) instead of Eq.(17) into \( \tilde{F}^{(3)} \). The ground-state expectation values of different Hamiltonian terms become

\[
\langle \hat{T}_c \rangle = \sum_\vec{k} \frac{\epsilon^c_\vec{k}}{\Delta_\vec{k}} (2 |X_c(\vec{k})|^2 + |X_f(\vec{k})|^2), \quad \langle \hat{T}_f \rangle = \sum_\vec{k} \frac{(\epsilon^f_\vec{k} - \tilde{E}_f)}{\Delta_\vec{k}} (2 |X_f(\vec{k})|^2 + |X_c(\vec{k})|^2),
\]

\[
\langle \hat{V} \rangle = -\sum_\vec{k} \frac{2 V_\vec{k}^2 - (V^*_\vec{k} V_0 + V_0^* V_\vec{k})}{\Delta_\vec{k}}, \quad \langle \hat{U} \rangle = U \sum_\vec{k} \frac{|X_f(\vec{k})|^2}{\Delta_\vec{k}},
\]

\[
\langle \hat{V}_0 \rangle = -\sum_\vec{k} \frac{V^*_\vec{k} V_0 + V_0^* V_\vec{k}}{\Delta_\vec{k}}, \quad \langle \hat{E}_f \rangle = E_f \sum_\vec{k} \frac{2 |X_f(\vec{k})|^2 + |X_c(\vec{k})|^2}{\Delta_\vec{k}}.
\]  

To have more insight about the physical behavior of the system, all ground-state expectation values at \( U > 0 \) relevant for our study can be explicitly expressed from Eq.(22). The analysis of the described state first of all shows that \( N = \sum_{\vec{k},\sigma} [ \langle (\hat{f}^\dagger_{\vec{k},\sigma} \hat{f}_{\vec{k},\sigma} + \hat{c}^\dagger_{\vec{k},\sigma} \hat{c}_{\vec{k},\sigma}) \rangle ] = 3 N_\Lambda \), as must be for 3/4 filling from Eq.(71). Secondly, summing up all contributions from Eq.(72), we obtain for the ground-state energy \( E_g = \sum_{\vec{k}} (\Delta^{-1}_{\vec{k}}) [ \epsilon^c_{\vec{k}} (2 |X_c(\vec{k})|^2 + |X_f(\vec{k})|^2) + \epsilon^f_{\vec{k}} (2 |X_f(\vec{k})|^2 + |X_c(\vec{k})|^2) - 2 |V_\vec{k}|^2 - U (|X_c(\vec{k})|^2 + |X_f(\vec{k})|^2) ] \). Taking into account from Eq.(10) \( \Delta_{\vec{k}} = (|X_c(\vec{k})|^2 + |X_f(\vec{k})|^2) \), this expression becomes \( E_g = 2 \sum_{\vec{k}} (\epsilon^c_{\vec{k}} + \epsilon^f_{\vec{k}}) - \sum_{\vec{k}} (\Delta^{-1}_{\vec{k}}) [ \epsilon^c_{\vec{k}} |X_f(\vec{k})|^2 + \epsilon^f_{\vec{k}} |X_c(\vec{k})|^2 - 2 |V_\vec{k}|^2 ] - U N_\Lambda \). The first sum in \( E_g \) gives \( 2 \tilde{E}_f N_\Lambda \) (we note at this step that at \( U \neq 0 \) we have \( \tilde{E}_f \) instead of \( E_f \) in the relation
\( \epsilon_{k,\sigma}^f = E_f + \varepsilon_{k,\sigma}^f \) following Eq. (23)). Using Eqs. (24, 40, 41), the second sum becomes \(-KN_\Lambda\).

As a consequence, the ground-state energy obtained from Eq. (72) is \( E_g/N_\Lambda = 2E_f + U - K \), which is exactly the value \( E_0^U/N_\Lambda \) given by Eq. (16) for \( N = 3N_\Lambda \).

Deducing now from Eq. (71) the total momentum distribution function \( n_{\vec{k}} = \sum_{b,\sigma} \langle \hat{n}_{\vec{k},\sigma}^b \rangle \), where \( b = c, f \), we obtain \( n_{\vec{k}} = 3 \), i.e. a completely uniform and continuous behavior for the whole \( \vec{k} \)-space. This value of \( n_{\vec{k}} \) contains however also the contribution of the lower band, which being completely filled up, is 2 for every \((\vec{k}, \sigma)\) state. This can be seen well from Eq. (A11) of the Appendix, taking into consideration that \( \hat{f}_{\vec{k},\sigma}^\dagger \hat{f}_{\vec{k},\sigma} + \hat{c}_{\vec{k},\sigma}^\dagger \hat{c}_{\vec{k},\sigma} = \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} + \hat{B}_{\vec{k},2,\sigma}^\dagger \hat{B}_{\vec{k},2,\sigma} \), writing the general ground state as \(|\Psi_g^U\rangle = \sum_{\sigma} a_{\sigma} |\Psi_{g,\sigma}^U\rangle \), where \( a_{\sigma} \) are arbitrary coefficients, taking into consideration that as shown in Eq. (45), \( \hat{B}_{\vec{k},1,\sigma}^\dagger \) creates a particle in the lower band, and obtaining \( \langle \sum_{\sigma} \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} \rangle = 2 \) independent on the \((\vec{k}, \sigma)\) indices. As a consequence, \( n_{\vec{k}} = 3 \) means in fact, that for the upper band (denoted by 1) we have \( n_{\vec{k}}^{(1)} = 1 \) independent on \( \vec{k} \). This information is also contained in Eq. (A10) of the Appendix, which gives \( \langle \sum_{\sigma} \hat{B}_{\vec{k},2,\sigma}^\dagger \hat{B}_{\vec{k},2,\sigma} \rangle = 1 \), where as shown through Eq. (16), \( \hat{B}_{\vec{k},2,\sigma}^\dagger \) creates a particle in the upper band. Using Eqs. (A11-A15) we have even \( \langle \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} \rangle = 1/2, \langle \hat{B}_{\vec{k},2,\sigma}^\dagger \hat{B}_{\vec{k},2,\sigma} \rangle = 1 \), which via Eq. (47) can be transformed into the \( n_{\vec{k}}^c \) and \( n_{\vec{k}}^f \) momentum distribution functions defined for the starting operators \( \hat{f} \) and \( \hat{c} \).

We note at this step, that even the simplified calculation presented in Eq. (70) gives back all essential features presented above since it leads to \( \langle \hat{B}_{\vec{k},2,\sigma}^\dagger \hat{B}_{\vec{k},2,\sigma} \rangle = 1, \langle \sum_{\sigma} \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} \rangle = 1, \langle \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} \rangle = \text{const} \). The same results are re-obtained in case of \( \vec{k} \) dependent \( \alpha_{\vec{k},\sigma} \) coefficients in Eq. (28).

Since \( \Delta_{\vec{k}} > 0 \) in the studied case, \( n_{\vec{k}} \) and all individual contributions in \( n_{\vec{k}} \) listed above are continuous together with their derivatives of any order in the whole momentum space. As a consequence, the system is in a non-Fermi liquid (NFL) state. From physical point of view, this property is clearly given by the presence at \( U > 0 \) of a partially filled completely flat upper band, which is not hybridized with the lower band that contains dispersion.

In order to further analyze the described state three integrals must be introduced
Using Eq. (73), from Eq. (72) we now find

\[
\langle \hat{\mathcal{E}} \rangle = -K I_0 + I_1, \quad \langle \hat{T}_f \rangle = -(K - E_f - U) N_A + (K - E_f - U) I_0 + I_1, \\
\langle \hat{V} \rangle = -2I_1 + (V_0^* I_2 + V_0 I_2^*), \quad \langle \hat{\mathcal{U}} \rangle = U I_0, \\
\langle \hat{V}_0 \rangle = -(V_0^* I_2 + V_0 I_2^*) , \quad \langle \hat{\mathcal{E}}_f \rangle = E_f N_A + E_f I_0 ,
\]

(74)

where, starting from Eq. (73) \( I_0 > 0, I_1 > 0, \) and based on Eqs. (3, 14) we have \( K > 0, \)

\( (K - E_f - U) > 0, \) respectively. Introducing as in Eq. (51) the contribution of the

on-site, and hopping-type Hamiltonian terms into the ground-state energy, we get \( \langle \hat{R}_{\text{loc}} \rangle = E_f N_A + \tilde{E}_f I_0 - (V_0^* I_2 + V_0 I_2^*), \) and \( \langle \hat{R}_{\text{mov}} \rangle = (\tilde{E}_f - K) N_A - \tilde{E}_f I_0 + (V_0^* I_2 + V_0 I_2^*) \)

from where, as expected, \( E_0^U = \langle \hat{R}_{\text{loc}} \rangle + \langle \hat{R}_{\text{mov}} \rangle = (2 E_f + U - K) N_A \) is re-obtained.

From here one can write

\[
\langle \hat{R}_{\text{loc}} \rangle = E_0^U + \mathcal{J}, \quad \langle \hat{R}_{\text{mov}} \rangle = -\mathcal{J}, \quad \mathcal{J} = (K - E_f - U) N_A + (E_f + U) I_0 - (V_0^* I_2 + V_0 I_2^*). 
\]

(75)

The study of \( \mathcal{J} \) shows that \( \mathcal{J} > 0 \) holds. In order to see this, via \( \Delta_k^2 = |X_c(k)|^2 + |X_f(k)|^2, \)

we obtain \( \mathcal{J} \) as \( \sum_k P_k/\Delta_k, \) where \( P_k = K (K - c_k^f) + (K - \tilde{E}_f) (K - c_k^c) - (V_0^* V_0 + c.c). \)

Using now Eq. (60), we get \( P_k = (K - \tilde{E}_f) |X_c(k)|^2 + K |X_f(k)|^2 + [X_c(k) X_f(k) V_0^* + c.c]. \)

Based on this relation, introducing the notations \( d_{i,c} = a_{i,c} X_f^*(k), d_{i,f} = a_{i,f} X_c^*(k), \) and

using Eqs. (59, 14) we find

\[
P_k = \sum_{i=1}^4 \left[ |d_{i,f}|^2 + |d_{i,c}|^2 - d_{i,c} d_{i,f}^* + d_{i,f} d_{i,c}^* \right] = \sum_{i=1}^4 |d_{i,c} - d_{i,f}|^2 \geq 0 .
\]

(76)

From Eq. (70), one can see that for all \( k, \) the value of \( P_k \) is non-negative, i.e. \( \mathcal{J} > 0. \) So we have

\[
\langle \hat{R}_{\text{loc}} \rangle > E_0^U, \quad \langle \hat{R}_{\text{mov}} \rangle < 0 .
\]

(77)

Taking into consideration Eq. (77), it can be seen that the ground-state energy cannot be expressed as a sum over expectation values of on-site contribution terms of the Hamiltonian.
We have \( \langle \hat{R}_{\text{loc}} \rangle > E^U_g \), and as a consequence, the system is not localized. From the other side, since \( \langle \hat{R}_{\text{mov}} \rangle < 0 \), the sum of the expectation values of Hamiltonian terms that preserve the movement of the particles within the system, is nonzero and negative. As a consequence, the ground-state energy is exactly \( E^U_g \), because in this way the system is maintaining its itinerant character that allows to reach the state with the minimum possible energy. In this conditions, the ground-state is a 2D normal state (i.e. non-symmetry broken) NFL, which is paramagnetic and non-insulating. The presented ground-state expectation values are correct only for \( U > 0 \), since for the noninteracting \( U = 0 \) case, the \( |\Psi^U_g\rangle \) contained in Eq.(18) represents only a negligible fraction from the linear combination of wave functions that build up the ground-state \( |\Psi^0_g\rangle \) defined at the end of Sec.II. via the arbitrary operator \( \hat{Q} \) instead of \( \hat{F}^{(3)} \). As a consequence, we can clearly state, that the interacting ground-state cannot be obtained perturbatively from the ground-state of the \( U = 0 \) case. This confirms the general belief, that a NFL emergence in normal phase and two dimensions has to be a completely non-perturbative effect, similar to 1D case\(^{33}\).

Doping the system above \( 3/4 \) filling, the ground-state wave function becomes \( |\Psi^U_{g,d}\rangle \) from Eq.(23). With the operator \( \hat{F}^{(4)} \) in \( |\Psi^U_{g,d}\rangle \), given by the product \( \prod_{\beta=1}^{3} \hat{F}^{(\beta)} \) present in the ground-state wave function, we further have \( [\hat{G} + U \hat{P}'] |\Psi^U_{g,d}\rangle = 0 \). The band remaining flat and being not possible to arrange the particles in such a way, to have the same number of electrons on every site of the lattice, the system is not localized, and remains a non-Fermi liquid as well.

C. Excited states

Starting from Eq.(43), it can be seen that excited states are obtained by removing \( \hat{B}^\dagger_{k,2,\sigma} \) operators from the first product of Eq.(43), changing their band index to 1 (i.e. removing particles from the completely filled lower band to the partially filled upper band), and leaving intact the \( F^{(3)} \) component of the wave function. For example, removing one \( \hat{B}^\dagger_{k,2,-\sigma} \), we obtain
\[ | \Psi_{k_1}^U \rangle = \left[ \prod_k \hat{B}_{k,2,\sigma}^\dagger \right] \left[ \prod_{k \neq k_1} \hat{B}_{k,2,-\sigma}^\dagger \right] (\hat{B}_{k_1,1,-\sigma}^\dagger) \hat{F}^{(3)} | 0 \rangle. \tag{78} \]

Since in Eq.\((\ref{78})\) the \(\hat{F}^{(3)}\) operator remains intact, it further preserves at least one \(f\)-electron on every site of the lattice, so \(\hat{P}^\dagger | \Psi_{k_1}^U \rangle = 0\) also in this case. Using Eq.\((\ref{48})\), the remaining part of the Hamiltonian besides \(\hat{P}^\dagger\) is essentially \(\sum_{\vec{k},\sigma} (E_{\vec{k},1} \hat{B}_{\vec{k},1,\sigma}^\dagger \hat{B}_{\vec{k},1,\sigma} + E_{\vec{k},2} \hat{B}_{\vec{k},2,\sigma}^\dagger \hat{B}_{\vec{k},2,\sigma})\), for which, the component of \( | \Psi_{k_1}^U \rangle \) from Eq.\((\ref{78})\) which is orthogonal to the ground-state represents an eigenstate. Other eigenstates of this type can be obtained removing more than one \(\hat{B}_{\vec{k},2,\sigma}^\dagger\) operator from the lower band and changing their band index to 1. A similar procedure can be applied also in the presence of doping. These excited states (for example, for one removed \(\hat{B}_{\vec{k},2,\sigma}^\dagger\), have energy \(E_{\vec{k},1}^{(1)}\) greater than the ground-state energy with a value of order \(\Delta = Min[\Delta_{\vec{k}}]\). Since in the analyzed case \(\Delta_{\vec{k}} > 0\), the obtained energy spectrum for Eq.\((\ref{78})\) is gaped.

The excited states of the type presented in Eq.\((\ref{78})\) were obtained by modifications in the first two operatorial components \(\hat{F}^{(1)}\) and \(\hat{F}^{(2)}\) of the ground-state wave function from Eq.\((\ref{18})\). In principle, is not possible to exclude excited states obtained by modifications made at the level of \(\hat{F}^{(3)}\) part of the wave function, by introducing in it a double occupancy - empty site pair in direct space (creating in fact a supplementary double occupied site at the level of \( | \Psi_{\vec{g}}^U \rangle \) from Eq.\((\ref{18})\)). In this case, the decompositions used for \(\hat{H}\) presented in Eqs.\((\ref{11}),\(\ref{12})\) are not usable, and even the band structure described by \(E_{\vec{k},i}, i = 1,2\) in Eq.\((\ref{30})\) is questionable at \(U \neq 0\). However, these excited states have energy greater than the ground-state energy with a value of order \(O(U)\), since a supplementary double occupied state has been introduced in the direct space on a given lattice site. Taking

\[ U >> \Delta, \tag{79} \]

the low lying excitation spectrum of the system will be clearly dominated by \(E_{\vec{k},1}^{(1)}\) given by the states presented in Eq.\((\ref{78})\). This means, that the low lying excitation spectrum will be gaped, so will be clearly visible in the physical properties of the system at \(T > 0\). The gap becomes \(\Delta_{\vec{k}}\) (i.e. \(\vec{k}\) dependent), its minimum value being \(\Delta\). The gap symmetry
is a possible symmetry allowed by the described 2D lattice and depends on the starting parameters of the system via Eqs. \((25,41)\).

\section*{VII. SUMMARY AND CONCLUSIONS}

In conditions in which even the exact solution for the 1D periodic Anderson model (PAM) is not known at finite \(U\), we present in this paper rigorous and exact solutions for 2D-PAM in the interacting case. The described solutions are present on two surfaces of the \(T = 0\) parameter space of the model. Both solutions describe the interacting \(U > 0\) model, and the deduced ground-state wave functions cannot be obtained perturbatively from the non-interacting case.

The first solution described in Sec.V emerges for pure real hybridization coupling constants at \(3/4\) filling and represents a paramagnetic Mott insulator, the ground-state being completely localized.

The second solution presented in Sec. VI represents a new non-Fermi liquid in 2D normal (non-symmetry broken) phase and emerges in case of pure imaginary hybridization coupling constants (the Hamiltonian remaining hermitian) at \(N/N_{\lambda} \geq 3/4\) filling. This phase presents an \(n_{\vec{k}}\) momentum distribution function which is continuous together with its derivatives of any order, has a well defined Fermi energy, but the Fermi momentum is not definable and the system has no Fermi surface in the \(\vec{k}\)-space. At high on-site repulsion \(U\), the described phase has a gap in the density of low lying excitations, and in the parameter space it emerges in the vicinity of a Mott insulating phase. The ground-state presents a large spin degeneracy and is paramagnetic. The behavior physically is given by a partially filled upper completely flat band situated above a normal band with dispersion. Low lying excitations do not give quasi-particles above the Fermi level, and have the effect to increase the number of particles at the Fermi energy. In this process particles are removed from the lower band and introduced into the upper flat band.

We have to underline that in the case of non-distorted unit cell, from the presented
ground-state solutions only the completely localized state emerges. Introducing distortions in the unit cell (maintaining however its translation invariance) we allow in fact the emergence of the described non-Fermi liquid state in the normal phase. In this way, the presented non-Fermi liquid phase is strongly related to the presence of lattice distortions.

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FIGURES CAPTIONS

Fig.1. The hopping amplitudes for c-electrons (A), and hybridization coupling constants for $c^\dagger f$ type hybridization terms (B) connecting the nearest and next-nearest neighbors lattice sites. The hopping amplitudes for f-electrons, and hybridization couplings for $f^\dagger c$ type hybridization terms are similar.

Fig.2. The effect of the Hubbard interaction $U$ in the flattening of the $E_{\vec{k},1,\sigma}$ band. The $U$ and $E_{\vec{k},1}$ values are in $|t_{f,x+y}|$ units, and $k_x$, $k_y$ cover the first Brillouin zone. For the values of the other Hamiltonian parameters see text.
APPENDIX A:

This Appendix contains the mathematical details related to the calculation of ground-state expectation values in case of arbitrary, and site dependent coefficients \( \alpha_{i,\sigma} \) introduced by the operator \( \hat{F}^{(3)} \) in Eq.(17). The calculations are presented for the non-doped case.

First of all, we compute the one-particle ground state expectation values of the form
\[
\hat{\Theta}_{b,b'} = \sum_{\sigma} \hat{b}^\dagger_{k,\sigma} \hat{b}^\sigma_{k,\sigma},
\]
where \( b, b' = c, f \), and we show that these are independent from the coefficients \( \alpha_{i,\sigma} \).

For shake of simplicity of the presentation we use the notation \( \sigma = (\sigma_i)_{i=1}^{N_\Lambda}, \sigma_i \in \{\uparrow, \downarrow\} \), and denote by \( \hat{F}^{(3)}_{\sigma} \) the \( \hat{F}^{(3)} \) operator containing a concrete set of values \( \alpha_{i,\uparrow} = \delta_{\sigma_i,\uparrow} \) and \( \alpha_{i,\downarrow} = \delta_{\sigma_i,\downarrow} \) (i.e. zero or one depending on \( \sigma \)). We prove that the set of vectors defined by all possible \( \sigma \) values (see also Eq.(49))
\[
|\Psi^U_{g,\sigma}\rangle = \hat{F}^{(1)} \hat{F}^{(2)} \hat{F}^{(3)}_{\sigma} |0\rangle \quad (A1)
\]
give the same expectation values for \( \hat{\Theta}_{b,b'} \) independent on \( \sigma \). We mention that the wave vectors presented in Eq.(A1) span the subspace of the ground state, they are non-orthogonal, but as seen below are linearly independent.

We express also the operator \( F^{(3)}_{\sigma} \) in terms of \( \hat{B}^\dagger_{k,j,\sigma} \). For this reason first the Fourier transforms of the original \( \hat{b}_{i,\sigma} \) operators, then the Eq.(47) must be used. Due to the first term in Eq.(A1) every \( \hat{B}^\dagger_{k,2,\sigma} \) from \( \hat{F}^{(3)}_{\sigma} \) cancels out and we find
\[
|\Psi^U_{g,\sigma}\rangle = \prod_k \left( \hat{B}^\dagger_{k,2,\uparrow} \hat{B}^\dagger_{k,2,\downarrow} \right) \prod_i \left( \sum_{\tilde{k}_i} e^{-ik_i \vec{r}_i} \frac{X_c(\tilde{k}_i)}{\sqrt{\Delta_{\tilde{k}_i}}} \right) |0\rangle \quad (A2)
\]

Here \( \vec{k} \) denotes a set of \( \vec{k} \) values whose first \( N_\uparrow \) elements (i.e. \( \vec{k}_i \) for spin-up states) and also the last \( N_\downarrow = N_\Lambda - N_\uparrow \) elements (i.e. \( \vec{k}_i \) for spin-down states) are ordered, but there is no any relation between spin-up and spin-down \( \vec{k} \) values. As a consequence \( \vec{k} = \{(\vec{k}_1 < \vec{k}_2 < \ldots < \vec{k}_{N_\uparrow}), (\vec{k}_{N_\uparrow+1} < \vec{k}_{N_\uparrow+2} < \ldots < \vec{k}_{N_\Lambda})\} \), and \( \sum_{\vec{k}} \) means a sum over all different \( \{\vec{k}\} \).
configurations allowed by $\sigma$ (i.e. $S^z(k) = (N_\uparrow - N_\downarrow) / 2$ and $S^z(\sigma) = \sum_i \frac{1}{2} (\delta_{\sigma_i,\uparrow} - \delta_{\sigma_i,\downarrow}$ are equal). Denoting $N_\uparrow = N_\Lambda / 2 + S^z(k)$ we have

$$
\hat{F}_{k,1} = \prod_{j \leq \frac{N_\Lambda}{2} + S^z(k)} \hat{B}_{k,j,1} \prod_{j > \frac{N_\Lambda}{2} + S^z(k)} \hat{B}_{k,j,1,\downarrow}, \quad Z(k) = \prod_{j=1}^{N_\Lambda} \frac{-X_c(\vec{k}_j)}{\sqrt{\Delta_{\vec{k}_j}}}, \quad (A3)
$$

$$
\hat{Y}(k, \sigma) = (-1)^{|Q|} \sum_{P \in G} (-1)^{|P|} \exp(i \sum_{j=1}^{N_\Lambda} \vec{k}_{P(j)} \cdot \vec{r}_{Q(j)}).
$$

In Eq. (A3) $|Q|$ is the parity of the permutation $Q$ producing the spin-up spin-down separation (i.e. $Q(\sigma) = (\sigma_{Q(i)})_{i=1}^{N_\Lambda} = \{\uparrow, \uparrow, \ldots, \uparrow, \downarrow, \downarrow, \ldots, \downarrow\}$), and $|P|$ is the parity of the permutation $P \in G = S_{\{1, \ldots, N_\uparrow\}} \times S_{\{N_\uparrow + 1, \ldots, N_\Lambda\}}$ which rearranges the $k$ subsets $\uparrow$ and $\downarrow$.

On the other hand, the Fourier transform of $\hat{F}_\sigma^{(3)} = \prod_i \hat{f}_{i,\sigma_i}$ gives

$$
\hat{F}_\sigma^{(3)} |0\rangle = \sum_{k} \delta_{S^z(k), S^z(\sigma)} Y(k, \sigma) \prod_{j \leq \frac{N_\Lambda}{2} + S^z(k)} \hat{f}_{k,j} \prod_{j > \frac{N_\Lambda}{2} + S^z(k)} \hat{f}_{k,j} \cdot |0\rangle,
$$

which excepting $Z(k)$ is exactly the second parentheses from Eq. (A2). Based on this observation it can be proved that the non-orthogonal set of ground-state wave-vectors from Eq. (A3) are linearly independent. In order to do this, we prove that there exists a dual basis (i.e., $|\Psi_{g,\sigma}\rangle$ are linearly independent). The dual basis has the form

$$
|\Psi_{g,\sigma}\rangle = \prod_{\vec{k}} \left( \begin{array}{c} \hat{B}_{\vec{k},2,\uparrow}^\dagger \\ \hat{B}_{\vec{k},2,\downarrow}^\dagger \end{array} \right) \sum_{k} \delta_{S^z(k), S^z(\sigma)} \frac{1}{Z^*(k)} Y(k, \sigma) \hat{F}_{k,1} |0\rangle,
$$

and the proof via Eq. (A3) is simple

$$
\langle \Psi_{g}^{U,\sigma'} | \Psi_{g}^{U,\sigma}\rangle = \sum_{k''} \sum_{k} \delta_{S^z(k''), S^z(\sigma')} \frac{1}{Z(k'')} Y^*(k'', \sigma') \delta_{S^z(k), S^z(\sigma)} Z(k) Y(k, \sigma) \langle 0 | \hat{F}_{k''}^\dagger \hat{F}_{k,1} |0\rangle = \sum_{k} \delta_{S^z(k), S^z(\sigma)} Y^*(k, \sigma') Y(k, \sigma) \times \langle 0 | \prod_{j \leq \frac{N_\Lambda}{2} + S^z(k')} \hat{f}_{k,j} \prod_{j > \frac{N_\Lambda}{2} + S^z(k')} \hat{f}_{k,j} \rangle \langle 0 | \prod_{j \leq \frac{N_\Lambda}{2} + S^z(k)} \hat{f}_{k,j} \prod_{j > \frac{N_\Lambda}{2} + S^z(k)} \hat{f}_{k,j} \rangle = \delta_{\sigma,\sigma'}
$$

(A7)
Due to the fact that all $\hat{F}_{k,1} | 0 \rangle$ are eigenvectors of the operator $\hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma}$ with the same eigenvalue than the $\prod_{j \leq \frac{N}{2} + S^z(k)} \prod_{j > \frac{N}{2} + S^z(k)} \hat{f}_{k_j,\uparrow}^\dagger | 0 \rangle$ eigenvectors of the operator $\hat{f}_{k,\sigma}^\dagger \hat{f}_{k,\sigma}$, similarly to Eq. $(A7)$ we find

$$
\langle \Psi_{g,\sigma'} | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle = \langle 0 | \hat{F}_{\sigma'}^3(3) \sum_{\sigma} \hat{f}_{k,\sigma}^\dagger \hat{f}_{k,\sigma} \hat{F}(3) | 0 \rangle = \frac{1}{N_A} \sum_{j, j'} e^{-i\hat{\mathbf{k}} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})} \sum_{\sigma} \langle 0 | \hat{F}_{\sigma'}^3(3) \hat{f}_{j,\sigma}^\dagger \hat{f}_{j,\sigma} \hat{F}(3) | 0 \rangle \frac{1}{N_A} \sum_{j, j'} e^{-i\hat{\mathbf{k}} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})} \sum_{\sigma} \delta_{\sigma, \sigma_j} \delta_{j, j'} \delta_{\sigma, \sigma'} = \delta_{\sigma, \sigma'} \tag{A8}
$$

The dual-basis to basis expectation value from Eq. $(A8)$ gives however

$$
\langle \Psi_{g,\sigma} | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle = \sum_{\sigma'} \langle \Psi_{g,\sigma} | \Psi_{g,\sigma'} \rangle \langle \Psi_{g,\sigma'}' | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle = \langle \Psi_{g,\sigma} | \Psi_{g,\sigma} \rangle \tag{A9}
$$

from where we find that independent from $\sigma$ we have

$$
\frac{\langle \Psi_{g,\sigma} | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle}{\langle \Psi_{g,\sigma} | \Psi_{g,\sigma} \rangle} = 1 \tag{A10}
$$

After this step, using the form of the ground state wave function from Eq. $(A4)$ we simply obtain for all $\sigma$ and $\sigma$

$$
\hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,2,\sigma} | \Psi_{g,\sigma} \rangle = | \Psi_{g,\sigma} \rangle, \quad \hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle = 0. \tag{A11}
$$

From Eq. $(A11)$, $\langle \Psi_{g,\sigma} | \hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,2,\sigma} | \Psi_{g,\sigma} \rangle / \langle \Psi_{g,\sigma} | \Psi_{g,\sigma} \rangle = 1$, and $\langle \Psi_{g,\sigma} | \hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma} \rangle = 0$ relations arise independent on $\sigma$ spin arrangement of the ground-state. Eq. $(A11)$ shows that in order to calculate from $\hat{\Theta}_{k,l}$ the desired expectation values $\langle \Psi_{g,\sigma} | \sum_{\sigma} \hat{b}_{k,\sigma}^\dagger \hat{b}_{k,\sigma} | \Psi_{g,\sigma} \rangle / \langle \Psi_{g,\sigma} | \Psi_{g,\sigma} \rangle$, first of all we may use Eq. $(A7)$ to transform the initial operators into $\hat{B}_{k,j,\sigma}^\dagger (j = 1, 2)$. After this step the non-diagonal $\hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,2,\sigma}$ terms cancel out based on Eq. $(A11)$, and the remaining parts of the expectation value can be deduced from Eq. $(A10)$ and first relation of Eq. $(A11)$. For example in the case of $\hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma}$ we find
\[
\frac{\langle \Psi_{g,\sigma}^U | \sum_{\sigma} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} | \Psi_{g,\sigma}^U \rangle}{\langle \Psi_{g,\sigma}^U | \Psi_{g,\sigma}^U \rangle} = \frac{\Delta_{\hat{k}} \left( \langle \Psi_{g,\sigma}^U | \sum_{\sigma} \left( X_c(\vec{k}) X_c(\vec{k}) \hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,2,\sigma} + X_f(\vec{k}) X_f(\vec{k}) \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} + X_c(\vec{k}) X_f(\vec{k}) \hat{B}_{k,2,\sigma}^\dagger \hat{B}_{k,1,\sigma} + X_c(\vec{k}) X_f(\vec{k}) \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,2,\sigma} \right) | \Psi_{g,\sigma}^U \rangle \right)}{2 | X_c(\vec{k}) |^2 + | X_f(\vec{k}) |^2} = 1 + \frac{\overline{K} - \epsilon_{\hat{k}}^e}{\overline{\Delta_{\hat{k}}}}, \quad (A12)
\]

where we used Eq.(III) and Eq.(IV). Similarly
\[
\frac{\langle \Psi_{g,\sigma}^U | \sum_{\sigma} \hat{f}_{k,\sigma}^\dagger \hat{f}_{k,\sigma} | \Psi_{g,\sigma}^U \rangle}{\langle \Psi_{g,\sigma}^U | \Psi_{g,\sigma}^U \rangle} = 1 + \frac{\overline{K} - \epsilon_{\hat{k}}^f}{\overline{\Delta_{\hat{k}}}}, \quad \frac{\langle \Psi_{g,\sigma}^U | \sum_{\sigma} \hat{f}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} | \Psi_{g,\sigma}^U \rangle}{\langle \Psi_{g,\sigma}^U | \Psi_{g,\sigma}^U \rangle} = -\frac{V_{\hat{k}}}{\overline{\Delta_{\hat{k}}}} \quad (A13)
\]

With Eqs. (A12,A13) the independence of the analyzed expectation values on \(\alpha_{1,\sigma}\) has been demonstrated.

We concentrate now on ground-state expectation values from operatorial terms not summed over the spin index \(\sigma\). In conditions in which \(\langle \Psi_{g,\sigma}^U \rangle\) build up a non-orthogonalized basis, the best way for this is to consider the \(T \to 0\) limit of temperature dependent expectation values. We have
\[
\lim_{T \to 0} \frac{\text{Tr} e^{-\beta H} \hat{A}}{\text{Tr} e^{-\beta H}} = \frac{\text{Tr}_{H_0} \hat{A}}{\text{Tr}_{H_0} 1} = \frac{\sum_{\sigma} \langle \Psi_{g,\sigma}^U | \hat{A} | \Psi_{g,\sigma}^U \rangle}{\sum_{\sigma} \langle \Psi_{g,\sigma}^U | \Psi_{g,\sigma}^U \rangle} = \frac{1}{2 N_{\Lambda}} \sum_{\sigma} \langle \Psi_{g,\sigma}^U | \hat{A} | \Psi_{g,\sigma}^U \rangle. \quad (A14)
\]

Based on Eq.(A14) the ground-state expectation value of \(\hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma}\) becomes
\[
\langle \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} \rangle = \frac{1}{2 N_{\Lambda}} \sum_{\sigma} \langle \Psi_{g,\sigma}^U | \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi_{g,\sigma}^U \rangle = \frac{1}{2 N_{\Lambda}} \sum_{\sigma} \langle 0 | \hat{F}_{\sigma}^{(3)\dagger} \hat{f}_{k,\sigma}^\dagger \hat{f}_{k,\sigma} \hat{F}_{\sigma}^{(3)} | 0 \rangle = \frac{1}{2 N_{\Lambda}} \frac{1}{N_{\Lambda}} \sum_{jj' \sigma} e^{-i\overline{k}(r_j-r_{j'})} \sum_{\sigma} \langle 0 | \hat{F}_{\sigma}^{(3)\dagger} \hat{f}_{j,\sigma}^\dagger \hat{f}_{j',\sigma} \hat{F}_{\sigma}^{(3)} | 0 \rangle = \frac{1}{N_{\Lambda}} \sum_{jj' \sigma} e^{-i\overline{k}(r_j-r_{j'})} \delta_{jj'} \frac{1}{2 N_{\Lambda}} \sum_{\sigma} \delta_{\sigma,\sigma_j} = \frac{1}{2} \quad (A15)
\]
where the validity of the second equality is preserved by the same argument as used for the first equality from Eq.(A8), and the last equality holds because half of the all $\sigma$ has $\sigma_j = \sigma$ value.

We mention, that the presented expectation values for $\hat{B}_{k,i,\sigma}^\dagger \hat{B}_{k,j,\sigma}$ operators are valid also for the complete ground-state wave function $|\Psi^U_g\rangle = \sum_{\sigma} \gamma_\sigma |\Psi^U_{g,\sigma}\rangle$, where $\gamma_\sigma$ are numerical coefficients. For the case of Eq.(A11) this is trivial, and in the case of Eq.(A14) automatically all contributions $|\Psi^U_{g,\sigma}\rangle$ are taken into account. For the the case of Eq.(A11), using Eq.(A8), we have

$$
\langle \Psi^U_g | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi^U_g \rangle = \\
\sum_{\sigma^1,\sigma^2,\sigma^3} \gamma^{\sigma^1}_\sigma \gamma^{\sigma^2}_\sigma \gamma^{\sigma^3}_\sigma \langle \Psi^U_{g,\sigma^1} | \Psi^U_{g,\sigma^3} \rangle \langle \Psi^U_{g,\sigma^3} | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi^U_{g,\sigma^2} \rangle = \\
\sum_{\sigma^1,\sigma^2,\sigma^3} \gamma^{\sigma_1}_\sigma \gamma^{\sigma_2}_\sigma \gamma^{\sigma^3}_\sigma \langle \Psi^U_{g,\sigma^1} | \Psi^U_{g,\sigma^3} \rangle \delta_{\sigma^3,\sigma^2} = \\
\sum_{\sigma^1,\sigma^2} \gamma^{\sigma_1}_\sigma \gamma^{\sigma_2}_\sigma \langle \Psi^U_{g,\sigma^1} | \Psi^U_{g,\sigma^2} \rangle = \langle \Psi^U_g | \Psi^U_g \rangle,
$$

(A16)

from where $\langle \Psi^U_g | \sum_{\sigma} \hat{B}_{k,1,\sigma}^\dagger \hat{B}_{k,1,\sigma} | \Psi^U_g \rangle / \langle \Psi^U_g | \Psi^U_g \rangle = 1$ arises.
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28. With mathematical rigorosity this means $\hat{H}|\Psi_g^{U}\rangle = \hat{H}_{0}^{eff}|\Psi_g^{U}\rangle$, where $\hat{H}_{0}^{eff}$ containing the $U$ parameter as well, has the functional form of $\hat{H}_0$.

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31. Eq.(B5) represents a continuous and infinite surface in the space of the normalized and
independent starting parameters of $\hat{H}$ from Eq.(1), crossing the phase diagram from the low $U$ to the high $U$ regions up to $U \to \infty$ at $U > 0$.

32 In the phase diagram we are situated now in conditions presented by Sec.VI.A.2., for which $P^*_k$ becomes

$$P^*_k = |X^*_c(\vec{k}) + pX^*_f(\vec{k})|^2(|a_{1,f}|^2 + |a_{2,f}|^2) + |X^*_c(\vec{k}) - pX^*_f(\vec{k})|^2(|a_{3,f}|^2 + |a_{4,f}|^2).$$

The $X_c(\vec{k})$ given in Eq.(60) is not identically zero, so clearly $\mathcal{J} > 0$ holds.

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