Exact Ground States of the Periodic Anderson Model

in \( D = 3 \) Dimensions

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Abstract

We construct a class of exact ground states of three-dimensional periodic Anderson models (PAMs) — including the conventional PAM — on regular Bravais lattices at and above \( 3/4 \) filling, and discuss their physical properties. In general, the \( f \) electrons can have a (weak) dispersion, and the hopping and the non-local hybridization of the \( d \) and \( f \) electrons extend over the unit cell. The construction is performed in two steps. First the Hamiltonian is cast into positive semi-definite form using composite operators in combination with coupled non-linear matching conditions. This may be achieved in several ways, thus leading to solutions in different regions of the phase diagram. In a second step, a non-local product wave function in position space is constructed which allows one to identify various stability regions corresponding to insulating and conducting states. The compressibility of the insulating state is shown to diverge at the boundary of its stability regime. The metallic phase is a non-Fermi liquid with one dispersing and one flat band. This state is also an exact ground state of the conventional PAM and has the following properties: (i) it is non-magnetic with spin-spin correlations disappearing in the thermodynamic limit, (ii) density-density correlations are short-ranged, and (iii) the momentum distributions of the interacting electrons are analytic functions, i.e., have no discontinuities even in their derivatives. The stability regions of the ground states extend through a large region of parameter space, e.g., from weak to strong on-site interaction \( U \). Exact itinerant, ferromagnetic ground states are found at and below \( 1/4 \) filling.

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I. INTRODUCTION

The periodic Anderson model (PAM) is the basic microscopic model for the investigation of compounds with heavy-fermion or intermediate valence properties such as cerium or uranium. The model describes $f$ electrons which interact via a strong on-site Coulomb repulsion $U$ and hybridize with noninteracting $d$ electrons. In the simplest case the $f$ electrons are assumed dispersionless, the hybridization purely local, and the $d$ electron hopping nonzero only between nearest neighbor sites. However, for real systems this is an oversimplification since there is experimental evidence for (i) a weak, but finite dispersion of the $f$ electrons, especially in uranium compounds, (ii) nonlocal contributions to the hybridization, and (iii) hopping of the $d$ electrons beyond nearest neighbors.

Recently the PAM was employed to study the dramatic volume collapse at the $\alpha \rightarrow \gamma$ transition in cerium compounds. These investigations called attention to the possibility of a Mott metal-insulator transition in the PAM. In fact, a remarkable similarity between the Hubbard model with nearest-neighbor hopping and the PAM with nearest neighbor hybridization and $d$ hopping was found. These results show that the range of the hopping and hybridization in the PAM are quite important but still poorly understood.

In this paper we not only present details of the construction and the physical properties of a class of exact ground states of three-dimensional ($D = 3$) periodic Anderson models reported in Ref.20, but extend the range of applicability of our approach substantially. In particular, we (i) demonstrate the uniqueness of the metallic and insulating solutions discovered at $3/4$ filling, (ii) explicitly present and analyze the non–linear matching conditions connecting the starting Hamiltonian to the transformed Hamiltonian, (iii) deduce the current operator and the sum rule for the charge conductivity, (iv) derive several local and global expectation values such as the magnetization of the system, (v) calculate correlation functions, (vi) extend the solutions to the conventional PAM case, and (vii) show that, by employing different procedures to cast the Hamiltonian into positive semi-definite form, one
arrives at exact ground states in different regions of the parameter space.

The paper is structured as follows. In Section II we present the Hamiltonian, discuss its transformation into positive semi-definite form, and construct a class of exact ground states. Section III describes the localized solution, and Section IV characterizes the metallic non-Fermi liquid state. In Section V the approach is generalized, leading to solutions in other regions of parameter space, and in Section VI the results are summarized. Technical details are discussed in Appendices A - E.

II. TRANSFORMATION OF THE HAMILTONIAN AND CONSTRUCTION OF EXACT GROUND STATES

A. General form of the periodic Anderson model

We consider a general form of the periodic Anderson model (PAM) describing non-interacting \(d\) electrons which hybridize with interacting \(f\) electrons. In contrast to the conventional PAM we do not assume the \(f\) electrons to be localized, i.e., the Hamiltonian is given by

\[
\hat{H} = \hat{H}_0 + \hat{H}_U, \tag{1.a}
\]

\[
\hat{H}_0 = \sum_{k,\sigma} [(\epsilon^d_k \hat{n}_k^d + \epsilon^f_k \hat{n}_k^f) + (V^d \hat{f}_k^\dagger \hat{d}_k + V^f \hat{d}_k^\dagger \hat{f}_k)], \tag{1.b}
\]

\[
\hat{H}_U = U \sum_i \hat{n}_i^f \hat{n}_i^f. \tag{1.c}
\]

We denote the two types of electrons by \(b = d, f\), i.e., \(\hat{b}_k^\dagger\) creates a \((d, f)\) electron with momentum \(k\) and spin \(\sigma\). The corresponding particle number operators are \(\hat{n}_k^b = \hat{b}_k^\dagger \hat{b}_k\), and the dispersion relations of the \(b\)-electrons are given by \(\epsilon_k^b\). Furthermore, the hybridization amplitude and the local (Hubbard) interaction are denoted by \(V^b\) and \(U\), respectively.

In real space the model is defined on a general Bravais lattice in \(D = 3\) dimensions, with a unit cell \(I\) defined by the primitive vectors \(\{x_\tau\}, \tau = 1, 2, 3\). The non-interacting part of the Hamiltonian, \(\hat{H}_0\), reads

\[
\hat{H}_0 = \sum_{i,\sigma} \left\{ \sum_r [(t^d_r \hat{d}_{i+r,\sigma}^\dagger \hat{d}_{i,\sigma} + t^f_r \hat{f}_{i+r,\sigma}^\dagger \hat{f}_{i,\sigma}) + (V^{d,f}_r \hat{f}_{i+r,\sigma}^\dagger \hat{d}_{i,\sigma} + V^{f,d}_r \hat{d}_{i+r,\sigma}^\dagger \hat{f}_{i,\sigma}) + H.c.] + (V_0 \hat{n}_i^f \hat{f}_{i,\sigma} + H.c.) + E_f \hat{n}_i^f \right\}, \tag{2}
\]
where $t^b_r$ characterizes the hopping of $b$ electrons between sites $i$ and $i + r$, $V^{b,b'}_r$ is the hybridization of $b$ and $b'$ electrons at sites $i$ and $i + r$, $V_0$ is the on-site hybridization, and $E_f$ is the local on-site $f$-electron energy. The separation between a site $i$ and its neighbors in the unit cell is denoted by $r$, with $r \neq 0$. While the amplitudes $t^b_r$ are real, $V_0, V^{b,b'}_r$ can, in principle, be complex (whether $V^{b,b'}_r$ is real, imaginary or complex, depends on the linear combination of the corresponding electronic orbitals and hence on the lattice symmetry\cite{9,18,21,22,23}) and obey the relations

$$
\epsilon^b_k = E_f \delta_{b,f} + \sum_r (t^b_r e^{-i k r} + t^{b*}_r e^{+i k r}), \quad V_k = V_0 + \sum_r (V^{d,f}_r e^{-i k r} + V^{f,d}_r e^{+i k r}).
$$

(3)

In particular, for $t^f_r = 0$, the $f$-electrons are localized, and the model reduces to the conventional PAM.

**B. Transformation of the Hamiltonian.**

1. Representation of sites in a unit cell

The separation from a site $i$ in (2) is indicated by the vector $r$ which corresponds to neighboring sites located in different coordination spheres. In our investigation $r$ may extend over a unit cell $I$ of a general Bravais lattice in $D = 3$. This implies 26 different inter-site hopping and non-local hybridization amplitudes. To avoid multiple counting of contributions by the H.c. term in (2) the vector $r$ must be properly defined. To this end the sites within $I_i$, the unit cell defined at site $i$, are denoted by $r_{I_i} = i + r_{\alpha\beta\gamma}$, with $r_{\alpha\beta\gamma} = \alpha x_1 + \beta x_2 + \gamma x_3$; $\alpha, \beta, \gamma = 0, 1$. As shown in Fig. 1 the eight sites $r_{I_i}$ can be numbered by the indices $n(\alpha, \beta, \gamma) = 1 + \alpha + 3\beta + 4\gamma - 2\alpha\beta$ without reference to $I_i$. Then $r = r_{\alpha'\beta'\gamma'} - r_{\alpha\beta\gamma}$, with $n(\alpha', \beta', \gamma') > n(\alpha, \beta, \gamma)$, connects any two sites within a unit cell. It corresponds to half of the 26 possibilities, i.e., to the 13 possibilities $x_1, x_2, x_3, x_2 \pm x_1, x_3 \pm x_1, x_3 \pm x_2, x_3 \pm x_2 \pm x_1$. The remaining (negative) values of $r$ are taken into account in (2) by the H.c. contributions.

2. Transformation of $\hat{H}$ into positive semi-definite form

To construct exact ground states the Hamiltonian $\hat{H}$ needs to be rewritten in terms of positive semi-definite operators. This is made possible\cite{24} by the construction of two new operators – one for the transformation of $\hat{H}_0$ and one for $\hat{H}_U$. 
The first of these operators is the "unit cell operator" $\hat{A}^\dagger_{I_1,\sigma}$ which represents a superposition of fermionic operators creating $d$ or $f$ electrons with spin $\sigma$ inside every unit cell $I_1$ as

$$
\hat{A}^\dagger_{I_1,\sigma} = \sum_{n(\alpha, \beta, \gamma)=1}^{8} [a^*_n d^\dagger_{I_{1}+r_{n,\beta,\gamma,\sigma}} + a^*_n f^\dagger_{I_{1}+r_{n,\beta,\gamma,\sigma}}] 
= (a^*_1 d^\dagger_{1,\sigma} + a^*_2 d^\dagger_{1+x_1,\sigma} + a^*_3 d^\dagger_{1+x_1+x_2,\sigma} + a^*_4 d^\dagger_{1+x_2,\sigma} + \ldots + a^*_8 d^\dagger_{1+x_2+x_3,\sigma})
+ (a^*_1 f^\dagger_{1,\sigma} + a^*_2 f^\dagger_{1+x_1,\sigma} + a^*_3 f^\dagger_{1+x_1+x_2,\sigma} + a^*_4 f^\dagger_{1+x_2,\sigma} + \ldots + a^*_8 f^\dagger_{1+x_2+x_3,\sigma}).
$$

(4)

Because of the translational symmetry of the lattice, the numerical prefactors $a^*_n, n = n(\alpha, \beta, \gamma)$ are the same in every unit cell. The composite operators $\hat{A}^\dagger_{I_1,\sigma}$ do not obey canonical anticommutation rules, since $\{\hat{A}_{I_1,\sigma}, \hat{A}^\dagger_{I',\sigma'}\} \neq 0$ for all $I \neq I'$. This is because $\hat{A}^\dagger_{I_1,\sigma}$ creates electrons also at the boundaries of the unit cell $I_1$ with neighboring unit cells. It should be stressed that for this reason $\hat{A}^\dagger_{I_1,\sigma}$ has a genuine dependence on the lattice structure and thereby on the spatial dimension. Furthermore the relations $\{\hat{A}^\dagger_{I_1,\sigma}, \hat{A}^\dagger_{I',\sigma'}\} = \{\hat{A}_{I_1,\sigma}, \hat{A}_{I',\sigma'}\} = 0$ and $\{\hat{A}_{I_1,\sigma}, \hat{A}^\dagger_{I_1,\sigma}\} = K_d + K_f, K_b = \sum_{n=1}^{8} |a_n|^2$ imply

$$
(\hat{A}^\dagger_{I_1,\sigma})^2 = 0, \quad (5.a)
-\hat{A}^\dagger_{I,\sigma} \hat{A}_{I,\sigma} = \hat{A}_{I,\sigma} \hat{A}^\dagger_{I,\sigma} - (K_d + K_f).
$$

(5.b)

The second operator, $\hat{P}$, originates from the relation $\sum_i \hat{n}^f_{i,\uparrow} \hat{n}^f_{i,\downarrow} = \hat{P} + \sum_i \hat{n}^f_{i,\uparrow} - N_A$, where

$$
\hat{P} = \sum_i \hat{P}_i, \quad \hat{P}_i = \hat{n}^f_{i,\uparrow} \hat{n}^f_{i,\downarrow} - (\hat{n}^f_{i,\uparrow} + \hat{n}^f_{i,\downarrow}) + 1, \quad (6)
$$

and $N_A$ is the number of lattice sites. The local operators $\hat{P}_i$ are positive semi-definite and assume their lowest eigenvalue (=0) whenever there is at least one $f$ electron on site $i$. By contrast, the interaction operator $\hat{H}_U$ itself, which is also positive semi-definite for $U > 0$, assumes the eigenvalue 0 only if the double occupancy is exactly zero. For this reason $\hat{P}$ is more useful for our investigation than $\hat{H}_U$.

Taking into account periodic boundary conditions and allowing $r$ to take only the values discussed above, (1,2) may be written as

$$
\hat{H} = \hat{P}_A + U \hat{P} + E_g, \quad (7)
$$
where \( \hat{P}_A = \sum_{\alpha} \hat{A}_{i_{\alpha}} \hat{A}_{i_{\alpha}}^\dagger \), \( E_g = K_d N + U N_A - 2 N_A (2 K_d - E_f) \), and \( N \) is the total number of particles which is assumed to be fixed.

For \( \Omega \) to reproduce (1.1a) the prefactors \( a^*_{n,b} \) in \( \hat{A}_{i_{\alpha}}^\dagger \) must be expressed in terms of the microscopic parameters \( t^*_r, t^f_r, V_r, V^*_r, V_0, V^*_0, E_f, U \), for all \( r \in I_i \), taking into account periodic boundary conditions. This leads to 55 coupled, non-linear matching conditions which can be written in compact notation as

\[
\sum_{\beta_1, \beta_2, \beta_3 = -1}^1 (\prod_{i=1}^{3} D_{\beta_i, \alpha_i}) a^*_{n+b} a_{n-b} = T^{b,b'}_{r,\nu}.
\]

These matching conditions have the explicit form

\[
\begin{align*}
J^{b,b'}_{x_1} &= a^*_1 a_{2,b'} + a^*_2 a_{3,b'} + a^*_3 a_{4,b'} + a^*_4 a_{5,b'} + a^*_5 a_{6,b'} + a^*_6 a_{7,b'}, \\
J^{b,b'}_{x_2} &= a^*_1 a_{4,b'} + a^*_2 a_{5,b'} + a^*_3 a_{6,b'} + a^*_4 a_{7,b'} + a^*_5 a_{8,b'}, \\
J^{b,b'}_{x_3} &= a^*_1 a_{5,b'} + a^*_2 a_{6,b'} + a^*_3 a_{7,b'} + a^*_4 a_{8,b'}, \\
J^{b,b'}_{x_{23}} &= a^*_1 a_{7,b'} + a^*_2 a_{8,b'},
\end{align*}
\]

\[
J^{b,b'}_{x_{32}} = a^*_2 a_{4,b'} + a^*_3 a_{5,b'},
\]

\[
J^{b,b'}_{x_{32}+x_1} = a^*_1 a_{7,b'},
\]

\[
J^{b,b'}_{x_{32}-x_1} = a^*_3 a_{5,b'},
\]

\[
V_0 = -\sum_{n=1}^{8} a^*_n a_{n,f}, \quad U + E_f = K_d - K_f,
\]

where \( J^{b,b'}_r = -[\delta_{b,b'} t^b_r + (1 - \delta_{b,b'}) V^{b,b'}_r] \), \( b, b' = d, f \).

Details of this transformation are presented in Appendix A.

**C. Construction of exact ground states**

Apart from the constant term \( E_g \) in (7), \( \hat{H} \) is a positive semi-definite operator. A state \( |\Psi_g \rangle \) which fulfills the conditions

\[
\begin{align*}
\hat{P}|\Psi_g \rangle &= 0, \quad (9.a) \\
\hat{A}_{i_{\alpha}}^\dagger |\Psi_g \rangle &= 0 \quad (9.b)
\end{align*}
\]

for all \( i \), and which contains all linearly independent states with properties \( (9.a, 9.b) \), will then be the exact ground state of \( \hat{H} \) with energy \( E_g \). Since the kernel of an arbitrary operator \( \hat{O}, ker(\hat{O}) \), is defined by the linearly independent states \( |\phi \rangle \) satisfying \( \hat{O}|\phi \rangle = 0 \), the relations \( (9.a) \) and \( (9.b) \) define the kernel of the operators \( \hat{P} \) and \( \hat{P}_A \), respectively. Consequently, \( |\Psi_g \rangle \)
spans the common part of $\ker(\hat{P})$ and $\ker(\hat{P}_A)$ denoted by the Hilbert space

$$\mathcal{H}_g = \ker(\hat{P}_A) \cap \ker(\hat{P}).$$

Using this definition it is ensured that $|\Psi_g\rangle$ is the complete ground state, and that supplementary degeneracies of $E_g$ do not occur.

Using (9) and (9.a) it follows that $\ker(\hat{P})$ is defined by states $\hat{F}^\dagger|0\rangle = \prod_{i=1}^{N_A} \hat{F}_{i_1}^\dagger|0\rangle$, where $\hat{F}_{i_1}^\dagger = (\mu_{i_1,i} \hat{f}_{i_1,i}^\dagger + \mu_{i_1,i} \hat{f}_{i_1,i}^\dagger)$ and $\mu_{i_1,i}$ are arbitrary coefficients. Obviously $\hat{F}^\dagger$ creates one electron on every site $i$. Furthermore, (5.a) and (9.b) imply that $\ker(\hat{P}_A)$ is defined by states $\hat{G}^\dagger|0\rangle$, where $\hat{G}^\dagger = \prod_{i=1}^{N_A} (\hat{A}_{i_1,i}^\dagger \hat{A}_{i_1,i}^\dagger)$ creates at most two $(d \text{ or } f)$ electrons on $i$. Since $\hat{G}^\dagger$ also creates contributions without $f$ electrons, (10) implies the (unnormalized) ground state

$$|\Psi_g\rangle = \hat{G}^\dagger \hat{F}^\dagger|0\rangle = \prod_{i=1}^{N_A} (\hat{A}_{i_1,i}^\dagger \hat{A}_{i_1,i}^\dagger |0\rangle)$$

at $N = 3N_A$, e.g., $3/4$ filling. Clearly, $|\Psi_g\rangle$ has the desired property $\hat{H}|\Psi_g\rangle = E_g|\Psi_g\rangle$ and spans $\mathcal{H}_g$ at $3/4$ filling. Thus it is the exact ground state of $\hat{H}$ with energy $E_g$.

Since the operator $\hat{F}^\dagger$ was introduced into $|\Psi_g\rangle$ to take into account the operator $\hat{P}$ in (7), i.e., the Hubbard interaction $U$, $|\Psi_g\rangle$ can only be a ground state for $U > 0$.

Eq. (11) implies that (i) the linearly independent basis vectors of $\mathcal{H}_g$ have the form $|\Psi_g\{\sigma_1\}\rangle = \hat{G}^\dagger \hat{F}_{\{\sigma_1\}}^\dagger|0\rangle$, where $\hat{F}_{\{\sigma_1\}}^\dagger = \prod_{i=1}^{N_A} \hat{f}_{i_1,\sigma_1}^\dagger$, and (ii) $\hat{G}^\dagger$ does not contribute to the total spin of the ground state. The overall degeneracy and total spin $S \in [0, N_A/2]$ of $|\Psi_g\rangle$ are then determined only by the (arbitrary) set of coefficients $\mu_{i_1,i}$ (see also Sect. III.A.2., Sect.IV.E., and footnote [25]). Consequently, the degeneracy of $E_g$ is determined by the (high) spin degeneracy of $|\Psi_g\rangle$. Since in $|\Psi_g\rangle$ all possible values $S$ and orientations $\mathbf{S}$ occur the ground state is globally non-magnetic.

Exact ground states can also be constructed away from $3/4$ filling. For example, the operator $\hat{V}_M = \prod_{j=1}^{M} [\sum_{i=1}^{N_A} \sum_{b=d,f} a_{b,i,j,\sigma} \hat{b}_{i,j,\sigma}^\dagger] |0\rangle$ with numerical coefficients $a_{b,i,j,\sigma}$ creates $M < N_A$ additional particles into the system such that

$$|\Psi_g\rangle = \prod_{i=1}^{N_A} (\hat{A}_{i_1,i}^\dagger \hat{A}_{i_1,i}^\dagger \hat{F}_{i_1}^\dagger |0\rangle \hat{V}_M^\dagger$$

(12)
is a ground state for $U > 0$ and $N > 3N_A$. 

7
III. EXACT LOCALIZED GROUND STATE

The physical properties of $|\Psi_g\rangle$ depend on the values of the coefficients $a_{n,b}$ in (1) which are solutions of (8) for given microscopic parameters. We now identify different solutions for nonlocal hybridization amplitudes with $V_r^{df} = V_r^{fd} = V_r$ and discuss their physical properties. We start with a localized ground state at $3/4$ filling.

A. Derivation of the localized ground state

From (1) it follows that if $a_{n,d}^*$ and $a_{n,f}^*$ are proportional, i.e., $a_{n,d}^* = pa_{n,f}^*$ for all $n$, the operators $\hat{A}_{i,\sigma}^\dagger$ take the form

$$\hat{A}_{i,\sigma}^\dagger = \sum_{n(\alpha,\beta,\gamma)=1}^8 a_{n(\alpha,\beta,\gamma),f}^* E_{i+r_{\alpha,\beta,\gamma,\sigma}}^\dagger,$$

(13)

where $E_{i+r_{\alpha,\beta,\gamma,\sigma}}^\dagger = (p\hat{d}_{r_{\alpha,\beta,\gamma,\sigma}}^\dagger + \hat{f}_{r_{\alpha,\beta,\gamma,\sigma}}^\dagger)$. The ground state $|\Psi_g\rangle$, (11), then transforms into $|\Psi_{loc}\rangle = \Pi_{i=1}^{N_\Lambda}(\hat{E}_{i,\uparrow}^\dagger \hat{E}_{i,\downarrow}^\dagger \hat{F}_1^\dagger)|0\rangle$. Evaluating the product $\hat{E}_{i,\uparrow}^\dagger \hat{F}_{i,\downarrow}^\dagger$, one finds

$$|\Psi_{loc}\rangle = \prod_{\sigma}^{N_\Lambda} \mu_{i,\sigma} (p\hat{d}_{i,\sigma}^\dagger \hat{f}_{i,\sigma}^\dagger + \hat{f}_{i,\sigma}^\dagger \hat{d}_{i,\sigma}^\dagger)|0\rangle.$$

(14)

Since $\langle \Psi_{loc}| \Psi_{loc}\rangle = (1 + |p|^2)^{N_\Lambda} \prod_{i=1}^{N_\Lambda} (|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2) \neq 0$ the ground state is well-defined.

1. The insulating nature of the ground state

The state $|\Psi_{loc}\rangle$ has exactly three particles on each site, corresponding to a uniform electron distribution in the system. Indeed, for $\hat{n}_i = \sum_{b=d,f} \sum_{\sigma} \hat{n}_{i,\sigma}^b$ one finds $\hat{n}_i|\Psi_{loc}\rangle = 3|\Psi_{loc}\rangle$. Denoting ground state expectation values in terms of $|\Psi_{loc}\rangle$ by $\langle ... \rangle$, one obtains

$$\langle \hat{d}_{i,\sigma}^\dagger \hat{d}_{j,\sigma'} \rangle = 0, \quad \langle \hat{d}_{i,\sigma}^\dagger \hat{f}_{j,\sigma'} \rangle = 0, \quad \langle \hat{f}_{i,\sigma}^\dagger \hat{d}_{j,\sigma'} \rangle = 0, \quad \langle \hat{f}_{i,\sigma}^\dagger \hat{f}_{j,\sigma'} \rangle = 0,$$

(15)

for all $\sigma, \sigma'$ and all $i \neq j$. Hence hopping or non-local hybridization does not occur.

By separating the Hamiltonian $\hat{H}$ into an itinerant part $\hat{H}_{\text{itin}} = \sum_{\mathbf{r}} \hat{H}_{\text{itin}}(\mathbf{r})$ and a complementary localized part $\hat{H}_{\text{loc}} = \hat{H} - \hat{H}_{\text{itin}}$ (see Appendix B), and using (13), one finds $\langle \hat{H}_{\text{itin}}(\mathbf{r}) \rangle = 0$ for all $\mathbf{r}$, and $\langle \hat{H}_{\text{loc}} \rangle = E_g$. This clearly demonstrates the localized nature of the ground state. Furthermore, from (13), the sum rule for the charge conductivity is obtained as $\int_0^\infty d\omega \text{Re} \sigma_{\tau,\tau}(\omega) = 0$. Since $\text{Re} \sigma_{\tau,\tau}(\omega)$ is non-negative this relation implies
$Re\sigma_{\tau,\tau}(\omega) = 0$. In particular, $Re\sigma_{\tau,\tau}(0) = 0$, the DC-conductivity, is also zero. The ground state \cite{14} is therefore insulating\textsuperscript{27,28}. It should be noted that the nature of this state is quite nontrivial, since the localization of the electrons is due to a subtle quantum mechanical interference between states with two $d$ and one $f$ electron ($d^{\dagger}_i\sigma \sigma^{\dagger}_i f^{\dagger}_i\sigma$) and two $f$ and one $d$ electron ($f^{\dagger}_i\sigma \sigma^{\dagger}_i d^{\dagger}_i\sigma$) on every site $i$.

A state with $Re\sigma_{\tau,\tau}(\omega) = 0$ for all $\omega$ appears to be rather unphysical since it implies that not only the DC-conductivity but even the dynamic conductivity vanishes for all excitation energies. It should be stressed, however, that the relation $Re\sigma_{\tau,\tau}(\omega) = 0$ was derived in the framework of the Kubo formula for the charge conductivity, i.e., within linear response theory. Consequently, this result is not valid at high excitation energies $\omega$.

2. Global magnetic properties

The expectation value of the spin\textsuperscript{29} in terms of the ground state \cite{14} in Cartesian coordinates is found as

$$\langle \hat{S} \rangle = x \sum_{i=1}^{N_A} \frac{\mu_i \mu^*_{i,\uparrow} + \mu_{i,\downarrow} \mu^*_{i,\uparrow}}{2(|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2)} + y \sum_{i=1}^{N_A} \frac{(-i)(\mu_{i,\uparrow} \mu^*_{i,\downarrow} - \mu_{i,\downarrow} \mu^*_{i,\uparrow})}{2(|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2)} + z \sum_{i=1}^{N_A} \frac{|\mu_{i,\uparrow}|^2 - |\mu_{i,\downarrow}|^2}{2(|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2)},$$

where $|x| = |y| = |z| = 1$. The total spin is seen to depend on the arbitrary coefficients \{\mu_{i,\sigma}\}. Here the site dependence of the $\mu_{i,\sigma}$ coefficients should be stressed. Namely, by choosing $\mu_{i,\sigma} = \mu_{\sigma}$ one obtains

$$\langle \hat{S}^2 \rangle = \frac{N_A}{2} \left( \frac{N_A}{2} + 1 \right), \quad \langle \hat{S}^z \rangle = \frac{N_A}{2} \frac{(|\mu_{\uparrow}|^2 - |\mu_{\downarrow}|^2)}{(|\mu_{\uparrow}|^2 + |\mu_{\downarrow}|^2)},$$

which represents a ferromagnetic state with maximal total spin $S/N_A = 1/2$, leading to $\sqrt{\langle \hat{S}^2 \rangle}/N_A = 1/2$ in the thermodynamic limit; $\mu_{\sigma}$ is seen to influence only the orientation of $\mathbf{S}$.

The minimal total spin can be found by considering two distinct subsystems of arbitrary shape, both containing the same number of lattice sites $N_A/2$. Taking $\mu_{i,\sigma} = \mu_{\sigma}, \mu_{i,-\sigma} = 0$ in each subsystem one finds

$$\sqrt{\langle \hat{S}^2 \rangle}/N_A = \frac{1}{\sqrt{2N_A}}, \quad \langle \hat{S}^x \rangle = \langle \hat{S}^y \rangle = \langle \hat{S}^z \rangle = 0,$$

which implies zero total spin (i.e., a global singlet state) in the thermodynamic limit. Depending on the choice of the parameters \{\mu_{i,\sigma}\} all values of $S$ between these two extreme values for $S$, and all orientations of $\mathbf{S}$, can be constructed (see Sec.II.C).
3. Local magnetic properties

Analyzing the local magnetic properties of the ground state one observes that the expectation value of the double occupancy per site for both $b = d, f$ electrons is smaller than unity since $\langle \hat{n}_{i,b}^b \hat{n}_{i,d}^d \rangle = (\delta_{b,f} + |p|^2 \delta_{b,d})/(1 + |p|^2)$. Consequently, each site carries a local moment. Indeed, irrespective of the values of $\mu_{i,\sigma}$ and $p$ one has $\langle \hat{S}_{i}^{\sigma} \rangle = 3/4$ on each site $i$; this is the result of a quantum mechanical superposition of the corresponding contributions of $d$ and $f$ electrons. The $f$ and $d$ moments do not compensate each other locally since

$$\langle \hat{S}_{i,f} + \hat{S}_{i,d} \rangle = xRe(\mu_{i,\mu_{i,\uparrow}}) + yIm(\mu_{i,\mu_{i,\uparrow}}) + z \frac{|\mu_{i,\uparrow}|^2 - |\mu_{i,\downarrow}|^2}{2},$$

where $\langle \hat{S}_{i,f} \rangle = |p|^2 \langle \hat{S}_{i,f} \rangle$ holds. Furthermore, taking into account fixed (but arbitrary) $\mu_{i,\sigma}$ the spin-spin correlation function for $\sigma = \{ \uparrow, \downarrow \}$ is found as

$$\langle \hat{S}_{i}^{\uparrow} \hat{S}_{j}^{\downarrow} \rangle = \frac{1}{4} \frac{|\mu_{i,\uparrow}|^2 - |\mu_{i,\downarrow}|^2}{|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2} \frac{|\mu_{j,\uparrow}|^2 - |\mu_{j,\downarrow}|^2}{|\mu_{j,\uparrow}|^2 + |\mu_{j,\downarrow}|^2}. \tag{19}$$

An average over all possible values of $\mu_{i,\sigma}, \mu_{j,\sigma}$ therefore implies $\langle \hat{S}_{i} \hat{S}_{j} \rangle = 0$. Therefore, in spite of the existence of local moments the system is globally non-magnetic; this is a consequence of the large spin degeneracy of the ground state.

B. Solutions of the matching conditions

The matching conditions for the nonlocal hybridization amplitudes along the space diagonals of the unit cell read

$$-V_{x_3 + x_2 + x_1} = a_{1,d}^* a_{7,f} = a_{1,f}^* a_{7,d}, \quad -V_{x_3 + x_2 - x_1} = a_{2,d}^* a_{8,f} = a_{2,f}^* a_{8,d},$$

$$-V_{x_3 - x_2 + x_1} = a_{3,d}^* a_{6,f} = a_{4,f}^* a_{6,d}, \quad -V_{x_3 - x_2 - x_1} = a_{3,d}^* a_{5,f} = a_{3,f}^* a_{5,d}. \tag{21}$$

They hold for all $\{ x_{\tau} \}, \tau = 1, 2, 3$ and hence imply $a_{n,d}^* / a_{n,f}^* = a_{n',d} / a_{n',f} = p = p^*$. Since for real $p$, leads to the relations

$$t_{r}^f = \frac{t_{r}^d}{p^2}, \quad V_r = \frac{t_{r}^d}{p}, \quad \frac{U + E_f}{V_0} = \frac{1 - p^2}{p}. \tag{22}$$

Real $p$ are seen to imply real hybridization amplitudes. In addition to (22), (8) yields the following system of 14 coupled nonlinear equations

$$-t_{x_1}^d = a_{1,d}^* a_{2,d} + a_{8,d}^* a_{7,d} + a_{4,d}^* a_{3,d} + a_{5,d}^* a_{6,d}.$$
The relative sizes of the hopping and hybridization amplitudes are physically very reasonable, analyzed below.

\[ -t^d_{x_2} = a^*_1 t^d_{4} a^d_4 + a^*_6 t^d_{7} a^d_7 + a^*_2 t^d_{3} a^d_3 + a^*_5 t^d_{8} a^d_8, \]
\[ -t^d_{x_3} = a^*_1 t^d_{5} a^d_5 + a^*_3 t^d_{7} a^d_7 + a^*_2 t^d_{6} a^d_6 + a^*_4 t^d_{8} a^d_8, \]
\[ -t^d_{x_2+x_1} = a^*_1 t^d_{3} a^d_3 + a^*_5 t^d_{7} a^d_7, \]
\[ -t^d_{x_3+x_1} = a^*_1 t^d_{6} a^d_6 + a^*_4 t^d_{7} a^d_7, \]
\[ -t^d_{x_3+x_2} = a^*_1 t^d_{8} a^d_8 + a^*_2 t^d_{7} a^d_7, \]
\[ -t^d_{x_3-x_2+x_1} = a^*_3 t^d_{5} a^d_5, \]
\[ pV_0 = -\sum_{n=1}^8 |a_{n,d}|^2. \] (23)

They determine the unknown complex coefficients \( a_{n,d} \) (i.e., 16 unknown real values) from the input parameters \( t^d_8 \). A study of the possible solutions shows that for \(|p| > 1\) the relative sizes of the hopping and hybridization amplitudes are physically very reasonable, e.g., \(|t^f_{x_1}| < |t^d_{x_2}|, |t^d_{x_1+x_2}| < |t^d_{x_3}|, |t^f_{x_1}| < |t^f_{x_2}|\). That is, they decrease with distance, and the magnitude of the amplitudes of the \( d \) electrons is larger than those of the almost localized \( f \) electrons.

Based on (24), the corresponding ground state energy becomes \( E_g/N_A = -U + (1 - 2/p^2) \sum_{n=1}^8 |a_{n,d}|^2 \). Depending on the solution, \( E_g \) has a nontrivial structure which will be analyzed below.

1. **Solution for a cubic lattice**

For a simple cubic lattice one has \( t^d_{x_1} = t^d_{x_2} = t^d_{x_3} = t^d_{x_1} = t^d_{x_3} = t^d_{x_5} = t^d_{x_3} = t^d_{x_2} = t^d_3 \). Then (23) has a solution

\[ a_{1,d} = a_1, \quad a_{2,d} = a_{4,d} = a_{5,d} = ua_1, \quad a_{3,d} = a_{6,d} = a_{8,d} = u^2 a_1, \quad a_{7,d} = u^3 a_1, \] (24)

where \( a_1 \) is an arbitrary, real quantity which is fixed by the energy unit. Furthermore, \( u \) is real and is determined by the parameters entering in \( \tilde{H} \) through (23,24). Due to the almost localized nature of the \( f \) electrons their nearest-neighbor hopping amplitude can be expected to be much smaller than that of the \( d \) electrons. Indeed, for \( z \equiv |t^f_1/t^d_1| < 1/2 \) the ground state energy is given by

\[ \frac{E_g}{UN_A} = -1 + (1 - 2 |t^f_1| |t^d_1|)(1 + \frac{(1 - \sqrt{1 - 4y^2})^2}{4y^2})^3, \] (25)
where \( u = \frac{1 - \sqrt{1 - 4y^2}}{2y} \), and \( y = |t_2^d/t_1^d| \in (0, 1/2) \) holds. We see that \( |\Psi_{\text{loc}}\rangle \) ceases to be the ground state for \( y = |t_2^d/t_1^d| > 1/2 = y_c \). This corresponds to rather strong next-nearest neighbor hopping of \( d \) electrons. Apparently, at \( y_c = 1/2 \) a different — most probably itinerant — phase becomes stable. At \( y_c \) the ground state energy \( E_g(y) \) has a finite value, but its derivative diverges due to \( \partial u/\partial y = +\infty \) (see Fig.2). Since the size of the hopping element may be tuned by pressure, the infinite slope of \( E_g \) at \( y = y_c \) is expected to correspond to an anomaly in the volume, or the compressibility, at a critical pressure \( P_c \). Such a feature is indeed observed in some heavy-fermion materials.

2. Solutions for non-cubic lattices

Similar results may be deduced for other lattice structures. In the most general case, i.e., when all hopping amplitudes \( t_i^d \) are different, the ground state energy for the localized solution becomes

\[
E_g/N_{\Lambda} = -U + (1 - 2|t_1^f/|t_1^d|) \sum_{n=1}^{8} |a_{n,d}|^2.
\]

When at least one of the terms \( |a_{n,d}|^2 \) (see (C2) in Appendix C) is mathematically no longer defined the localized solution becomes unstable. Except for accidental cancellations in the ground state energy an infinite slope of \( E_g \) as a function of the hopping amplitudes is also found in this more general case (see Appendix C).

IV. EXACT ITINERANT GROUND STATES

The localized ground state discussed above has exactly three electrons per site. In general, however, the inter-site hopping and hybridization will lead to a variable number of electrons on each site. In that case the ground state \( |\Psi_g\rangle \), (11), becomes conducting. We will now describe solutions of this kind.

A. Solution for \( a_{n,b} \neq 0 \text{ for all } n, b \).

To solve the matching conditions (S) for the case where \( a_{n,b} \neq 0 \text{ for all } n, b \), we define

\[
p_n = \frac{a_{n,d}}{a_{n,f}}, n = 1, 2, 3, 4, \tag{26.a}
\]

\[
p_{n'} = \frac{a_{n',d}}{a_{n',f}}, n' = 5, 6, 7, 8, \tag{26.b}
\]
and consider again $V_r^{d,f} = V_r^{f,d} = V_r$. Eq. (26.5) is seen to contain coefficients $a_{n,b}$ instead of $a_{n,b}^*$ since (21) holds as well. An itinerant solution is obtained by choosing $p_n = p = -p^*$, i.e., imaginary $p$. For this choice (8) leads to

$$t_{r_1}^f = \frac{t_{r_1}^d}{|p|^2}, \quad t_{r_2}^f = -\frac{t_{r_2}^d}{|p|^2}, \quad V_{r_2} = pt_{r_2}^f, \quad V_{r_1} = 0, \quad (27)$$

where $r_1 = x_1, x_2, x_2 \pm x_1, r_2 = x_3, x_3 \pm x_2, x_3 \pm x_1, x_3 \pm x_2 \pm x_1$, and $V_{r_1} = 0$ follows from $V_{r_1} = -V_{r_2}$. As discussed earlier, imaginary $p$ imply imaginary $V_r$. The local parameters $U$ and $V_0$ become

$$U + E_f = \frac{|p|^2 - 1}{|p|^2} \sum_{n=1}^{8} |a_{n,d}|^2, \quad p^*V_0 = \sum_{n=5}^{8} |a_{n,d}|^2 - \sum_{n=1}^{4} |a_{n,d}|^2. \quad (28)$$

The remaining relations following from (8) are

$$-t_{x_1}^d = a_{1,d}^*a_{2,d} + a_{8,d}^*a_{7,d} + a_{4,d}^*a_{3,d} + a_{5,d}^*a_{6,d},
-t_{x_2}^d = a_{1,d}^*a_{4,d} + a_{6,d}^*a_{7,d} + a_{2,d}^*a_{3,d} + a_{5,d}^*a_{8,d},
-t_{x_3}^d = a_{1,d}^*a_{5,d} + a_{3,d}^*a_{7,d} + a_{2,d}^*a_{6,d} + a_{4,d}^*a_{8,d},
-t_{x_2 + x_1}^d = a_{1,d}^*a_{3,d} + a_{5,d}^*a_{7,d}, \quad -t_{x_2 - x_1}^d = a_{2,d}^*a_{4,d} + a_{6,d}^*a_{8,d},
-t_{x_3 + x_1}^d = a_{1,d}^*a_{6,d} + a_{4,d}^*a_{7,d}, \quad -t_{x_3 - x_1}^d = a_{2,d}^*a_{5,d} + a_{3,d}^*a_{8,d},
-t_{x_3 + x_2}^d = a_{1,d}^*a_{8,d} + a_{2,d}^*a_{7,d}, \quad -t_{x_3 - x_2}^d = a_{4,d}^*a_{5,d} + a_{3,d}^*a_{6,d},
-t_{x_3 + x_2 + x_1}^d = a_{1,d}^*a_{6,d}, \quad -t_{x_3 + x_2 - x_1}^d = a_{2,d}^*a_{8,d},
-t_{x_3 - x_2 + x_1}^d = a_{4,d}^*a_{6,d}, \quad -t_{x_3 - x_2 - x_1}^d = a_{3,d}^*a_{5,d}. \quad (29)$$

Furthermore, $V_{r_1} = 0$ implies

$$a_{1,d}^*a_{2,d} + a_{4,d}^*a_{3,d} = a_{5,d}^*a_{6,d} + a_{8,d}^*a_{7,d}, \quad a_{1,d}^*a_{3,d} = a_{5,d}^*a_{7,d},$$

$$a_{1,d}^*a_{4,d} + a_{2,d}^*a_{3,d} = a_{6,d}^*a_{7,d} + a_{5,d}^*a_{8,d}, \quad a_{2,d}^*a_{4,d} = a_{6,d}^*a_{8,d}. \quad (30)$$

From (29, 30) it follows that

$$a_{1,d}^* = a_1, \quad a_{2,d}^* = ua_1^*, \quad a_{3,d}^* = u^2a_1^*, \quad a_{4,d}^* = ua_1^*,$$

$$a_{5,d}^* = ua_1^*, \quad a_{6,d}^* = u^2a_1^*, \quad a_{7,d} = ua_1, \quad a_{8,d} = a_1. \quad (31)$$

where $u$ is real, $|u| \neq 1$, $V_0 = 0$, and $\sum_{n=1}^{8} |a_{n,d}|^2 = 2|a_1|^2(1 + u^2)^2$. These relations can only be fulfilled for anisotropic hopping and hybridization amplitudes, e.g., for vanishing hybridization in the basal $(x,y)$ plane. Namely, (29, 31) yield $|u| = \sqrt{|t_{x_3 - x_2}^d/t_{x_3 + x_2}^d|}$ and $|t_{x_1}^b| = |t_{x_2}^b|$. The anisotropy in the hopping amplitudes is seen to start at the level of next-nearest neighbors. The stability region of this phase is presented in Fig.3.
B. Exact itinerant ground state of the conventional PAM.

The solutions obtained so far, namely (21-25), and (27-31), require the $f$ electrons to be itinerant, i.e., $t_f^d \neq 0$. We will now show that exact itinerant ground states can even be constructed for the conventional PAM, i.e., for $t_f^d = 0$. This requires nonzero $d$-electron hopping up to next-nearest neighbors together with local and nearest-neighbor hybridizations.

Such a solution can be constructed, for example, for nonzero coefficients $a_{1,f}, a_{1,d}, a_{2,d}, a_{4,d}, a_{5,d}$, with the remaining coefficients $a_{n,b} = 0$. This is realized in a tilted unit cell (see Fig.4) where the distances between lattice sites with indices $(n = 1, n = 3), (n = 1, n = 6), (n = 1, n = 8)$ and corresponding hopping elements ($t^d_{x_2 + x_1}, t^d_{x_3 + x_1}, t^d_{x_3 + x_2}$) are considerably larger than the distances between lattice sites with indices $(n = 2, n = 4), (n = 2, n = 5), (n = 4, n = 5)$ and hopping elements ($t^d_{x_2 - x_1}, t^d_{x_3 - x_1}, t^d_{x_3 - x_2}$). For this reason the former hopping elements are neglected (i.e., put to zero). In this case (8) reduces to the following eleven equations

\[
\begin{align*}
    t^d_{x_1} &= -a^*_{1,d} a^*_{2,d}, \quad t^d_{x_2} = -a^*_{1,d} a^*_{4,d}, \quad t^d_{x_3} = -a^*_{1,d} a^*_{5,d}, \\
    t^d_{x_2 - x_1} &= -a^*_{2,d} a^*_{4,d}, \quad t^d_{x_3 - x_1} = -a^*_{2,d} a^*_{5,d}, \quad t^d_{x_3 - x_2} = -a^*_{4,d} a^*_{5,d}, \\
    V^f_{x_1} &= -a^*_{1,f} a^*_{2,d}, \quad V^f_{x_2} = -a^*_{1,f} a^*_{4,d}, \quad V^f_{x_3} = -a^*_{1,f} a^*_{5,d}, \\
    V_0 &= -a^*_{1,d} a^*_{1,f}, \quad U + E_f = K_d - |a_{1,f}|^2, 
\end{align*}
\]

where $K_d = |a_{1,d}|^2 + |a_{2,d}|^2 + |a_{4,d}|^2 + |a_{5,d}|^2$, and all other amplitudes are identically zero.

Considering only the simplest case, i.e., $t_1^d = t^d_{x_1}, V_1 = V^f_{x_1}, \tau = 1, 2, 3$, and $t_2^d = t^d_{x_2 - x_1}$, $\tau > \tau'$, with real hopping amplitudes, the corresponding stability region corresponds to the surface in parameter space (see Fig.5) described by

\[
\frac{U + E_f}{|t_1^d|} = x + \frac{1}{x} (1 - y^2),
\]

where $x = |t_2^d|/|t_1^d|$ and $y = |V_1|/|t_1^d|$. Further properties of the solution are discussed in footnotes. The fact that $a_{n,d}^* = p a_{n,f}^*$ with $p = p^*$ does not hold for all $n = 1, 2, \ldots, 8$, implies a variable number of electrons at each site, i.e., an itinerant ground state.

C. Diagonalization of the Hamiltonian

To describe properties of the itinerant state, a $k$-representation is more suitable. This can be introduced without restriction on the $a_{n,b}$ coefficients. Therefore the two conducting
solutions presented in Sections IV.A. and IV.B. can be treated simultaneously.

Denoting the Fourier transforms of $\hat{A}_{i,\sigma}^\dagger$ by $\hat{A}_{k\sigma}^\dagger = \sum_{b=d,f} a_{k,b}^* \hat{b}_{k\sigma}^*$, with

\[
 a_{k,b}^* = a_{1,b}^* + a_{2,b}^* e^{i k x_1} + a_{3,b}^* e^{i k (x_1 + x_2)} + a_{4,b}^* e^{i k x_2} + a_{5,b}^* e^{i k x_3} + a_{6,b}^* e^{i k (x_1 + x_3)} + a_{7,b}^* e^{i k (x_1 + x_2 + x_3)} + a_{8,b}^* e^{i k (x_2 + x_3)},
\]

one may define new canonical Fermi operators describing composite fermions $\hat{C}_{\delta,k\sigma}$, $\delta = 1, 2$, \{\(\hat{C}_{\delta,k\sigma}, \hat{C}_{\delta',k'\sigma'}\)\} = 0. Here\(^{32,33}\)

\[
\hat{C}_{1,k\sigma} = \sqrt{R_k} \hat{A}_{k\sigma} = \sqrt{R_k} (a_{k,d} \hat{d}_{k\sigma} + a_{k,f} \hat{f}_{k\sigma}), \quad \hat{C}_{2,k\sigma} = \sqrt{R_k} (a_{k,d}^* \hat{d}_{k\sigma} - a_{k,d}^* \hat{f}_{k\sigma}),
\]

where $R_k^{-1} = \sum_{b=d,f} |a_{k,b}|^2$. Then the Hamiltonian becomes\(^{34}\)

\[
\hat{H} = \hat{H}_g + U \hat{P} - UN_{\Lambda}, \quad \hat{H}_g = \sum_{k,\sigma} [(K_d - R_k^{-1})\hat{C}_{1,k\sigma}^\dagger \hat{C}_{1,k\sigma} + K_d \hat{C}_{2,k\sigma}^\dagger \hat{C}_{2,k\sigma}].
\]

In the ground state where $\hat{P}|\Psi_g\rangle = 0$ the Hamiltonian $\hat{H}$ reduces to $\hat{H}_g$. Hence the composite fermion operators introduced above indeed diagonalize $\hat{H}$. There are two bands, the lower one having a dispersion $\xi_{1,k} = K_d - R_k^{-1}$, while the upper one is dispersionless, i.e., flat, since $\xi_{2,k} = K_d =$const. The lower (upper) diagonalized band contains fermions created by $\hat{C}_{1,k\sigma}$ ($\hat{C}_{2,k\sigma}$), respectively. Since the total band filling is $3/4$ the lower band is completely filled, while the upper band is half filled. Thus the Fermi energy is given by $E_F = K_d$. Band structures containing a partially filled flat band around $E_F$ have indeed been observed experimentally\(^{35,36,37}\).

D. Conductivity of the itinerant state

The ground state expectation value of $\hat{H}_{\it{itin}}$, the itinerant part of $\hat{H}$, is obtained as

\[
\langle \hat{H}_{\it{itin}} \rangle = - \sum_k K_d |a_{k,d}|^2 + K_f |a_{k,f}|^2 \left/ \left( |a_{k,d}|^2 + |a_{k,f}|^2 \right) \right. < 0.
\]

This is in contrast to the localized case where $\langle \hat{H}_{\it{itin}} \rangle = 0$\(^{38}\).

Since $\langle \hat{H}_{\it{itin}}(r) \rangle \neq 0$ the charge sum rule\(^{39}\) implies $\int_0^\infty d\omega \text{Re} \sigma_{\tau,\tau}(\omega) \neq 0$, i.e., the (dynamic) conductivity is in general non-zero. However, the sum rule does not allow us to draw conclusions about the DC-conductivity $\sigma(0)$. This becomes possible if we calculate the chemical potential of the system as a function of the particle number. To this end we observe
that in the case of a variable number of particles per site the itinerant ground state is defined at and above $3/4$ filling, such that $|\Psi_g\rangle$ in (11) can be generalized to fillings beyond $3/4$ via (12). Using (11) this allows one to calculate the energy $E_g$ for different particle numbers. In particular, one finds $\mu^+ = E_g(N+2) - E_g(N+1) = K_d$, $\mu^- = E_g(N+1) - E_g(N) = K_d$, i.e., $\mu^+ - \mu^- = 0$. Therefore, the described itinerant solutions are indeed conducting.

E. Magnetic properties.

Using $k$-space notation the unnormalized ground state, (11), can be written as

$$|\Psi_g\rangle = \prod_{k}^{N_{\Lambda}} \hat{A}^+_k \hat{A}^+_k \prod_{i}^{N_{\Lambda}} \sum_{k} e^{ik} (\mu_{i,k}^+ \hat{f}^+_k + \mu_{i,k}^- \hat{f}^+_k) |0\rangle,$$

where the sum and product over $k$ extend over the first Brillouin zone, and the set $\{\mu_{i,\sigma}\}$ is arbitrary. Using (38) we will now calculate ground state expectation values of the spin for different sets of $\{\mu_{i,\sigma}\}$.\n
1. Maximum total spin

As in the localized case $\mu_{i,\sigma} = \mu_{\sigma}$ corresponds to maximum total spin. Defining $\hat{F}^+_k = (\mu_{i,k}^+ \hat{f}^+_k + \mu_{i,k}^- \hat{f}^+_k)$ and employing $(\hat{F}^+_k)^2 = 0$ the product over sites $i$ in (38) may be written as

$$\prod_{i}^{N_{\Lambda}} \sum_{k} e^{ik} \hat{F}^+_k = Z \prod_{k}^{N_{\Lambda}} \hat{F}^+_k,$$

where $Z$ is defined in footnote (40). Then the normalized ground state becomes

$$|\Psi_g\rangle = \prod_{k}^{N_{\Lambda}} \frac{a^*_{k,d} \hat{a}^+_k \hat{f}^+_k + a^*_{k,f} \hat{f}^+_k \hat{f}^+_k \hat{f}^+_k}{\sqrt{(|\mu|^2 + |\mu|^2)(|a_{k,d}|^2 + |a_{k,f}|^2)}} |0\rangle.$$

The spin expectation value then follows as

$$\frac{2\langle \hat{S} \rangle}{N_{\Lambda}} = x \frac{\mu^+ \mu^- + \mu^+ \mu^-}{|\mu|^2 + |\mu|^2} + y \frac{i(\mu^+ \mu^- - \mu^+ \mu^-)}{|\mu|^2 + |\mu|^2} + z \frac{|\mu^2| - |\mu|^2}{|\mu|^2 + |\mu|^2},$$

resulting in $|\langle \hat{S} \rangle|/N_{\Lambda} = 1/4$, and $\langle \hat{S}^2 \rangle = (N_{\Lambda}/2)(N_{\Lambda}/2+1)$. Thus we recover (17), the results for the localized solution. The maximum total spin is again given by $\sqrt{\langle \hat{S}^2 \rangle}/N_{\Lambda} = 1/2$ in the thermodynamic limit.
2. Minimum total spin

To determine the minimum spin value we proceed as in the localized case, i.e., divide the system in two sublattices $D_\uparrow$ and $D_\downarrow$ containing both $N_\Lambda/2$ lattice sites, such that for all $i_n \in D_\uparrow$ and $j_n \in D_\downarrow$ we have $j_n = i_n + \mathbf{R}$, where $\mathbf{R}$ is a fixed Bravais vector. Choosing $\mu_{i,\sigma} = \mu_\sigma$, $\mu_{i,-\sigma} = 0$ for $D_\sigma$ in (38) the unnormalized ground state becomes

$$|\Psi_g\rangle = \prod_{n=1}^{N_\Lambda} \hat{A}_{\uparrow,n} \hat{A}_{\uparrow,n} \prod_{i \in D_\uparrow} \left( \sum_{k} e^{ik_i \hat{f}_{\uparrow,k}} \right) \prod_{j \in D_\downarrow} \left( \sum_{k} e^{ik_j \hat{f}_{\downarrow,k}} \right) |0\rangle,$$  

(D1)

Details of the calculation of ground state expectation values in terms of (41) are presented in Appendix D. Based on (D3) one finds $\langle \hat{S} \rangle = 0$, and using (D4), $\sqrt{\langle \hat{S}^2 \rangle/N_\Lambda} < \sqrt{3}/(2\sqrt{N_\Lambda})$. As a consequence, this itinerant ground state has zero total spin in the thermodynamic limit.

Between the two limiting cases of the total spin discussed above all values of $S$ may exist, depending on the choice of the set ${\{\mu_{i,\sigma}\}}$. The statement regarding the degeneracy of the ground state presented below (18) holds in the itinerant case as well.

F. Momentum distribution function

To calculate ground state expectation values of $\mathbf{k}$-dependent operators involving $\hat{C}_{\delta,\mathbf{k}\sigma}$ operators, (35), we need to express $|\Psi_g\rangle$, (38), in terms of $\hat{C}_{\delta,\mathbf{k}\sigma}$, too. For the unnormalized ground state one finds

$$|\Psi_g\rangle = \prod_{n=1}^{N_\Lambda} \hat{C}_{\uparrow,n} \hat{C}_{\uparrow,n} \prod_{i \in D_\uparrow} \left( \sum_{k} X_k e^{ik_i \hat{f}_{\uparrow,k}} \right) \prod_{j \in D_\downarrow} \left( \sum_{k} X_k e^{ik_j \hat{f}_{\downarrow,k}} \right) |0\rangle,$$  

(42)

where $\{\mu_{i,\sigma}\}$ is arbitrary, and $X_k = -a_{k,d}\sqrt{R_k}$; in the following we consider $X_k \neq 0$ for all $\mathbf{k}$. From (42) it follows that

$$\hat{C}_{\delta,\mathbf{k}\sigma} \hat{C}_{\delta',\mathbf{k}\sigma'} |\Psi_g\rangle = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma',\sigma} |\Psi_g\rangle, \quad \hat{C}_{\delta,\mathbf{k}\sigma} \hat{C}_{\delta',\mathbf{k}'\sigma'} |\Psi_g\rangle = 0.$$  

(43)

Details of the calculation of ground state expectation values of $\hat{C}_{\delta,\mathbf{k}\sigma} \hat{C}_{\delta,\mathbf{k}\sigma}$ operators are presented in Appendix E. Using (13, 18), one finds in particular

$$\langle \hat{C}_{\delta,\mathbf{k}\sigma} \hat{C}_{\delta,\mathbf{k}\sigma} \rangle = \delta_{1,\delta} + \frac{1}{2} \delta_{2,\delta}$$  

(44)

for all $\mathbf{k}$. This expresses the fact that the lower band ($\delta = 1$) is completely filled, while the upper band ($\delta = 2$) is flat and half filled.
Employing (44) the momentum distribution of $b = d, f$ electrons is then obtained as

$$n_k^b = \langle \hat{n}_k^b \hat{n}_k^b \rangle = \frac{1}{2} + \frac{1}{2} R_k |a_{k,b}|^2, \quad (45)$$

which implies $n_k = \sum_{b=d,f} n_k^b = 3/2$. Since the coefficients $R_k |a_{k,b}|^2 = |a_{k,b}|^2/(|a_{k,d}|^2 + |a_{k,f}|^2)$ are regular functions of $k$, this is also the case for $n_k^b$ and $n_k^\sigma$ (see Fig.6)\textsuperscript{33}. Consequently, the momentum distributions of the electrons in the interacting ground state have no discontinuities. Since the ground state is nonmagnetic and metallic, the system is therefore a non-Fermi liquid. This is a consequence of the macroscopic degeneracy of the electrons in the upper band. Due to the flatness of the upper half-filled band all $k$ states are equivalent. Hence, even if a Fermi energy $E_F = K_d$ exists the Fermi surface, and the Fermi momentum are not defined. Consequently, Luttinger’s theorem\textsuperscript{44} does not apply. Non-Fermi liquid properties connected to a flat band have also been observed in other investigations\textsuperscript{45,46,47}.

G. Correlation functions

To characterize the itinerant ground states further we now calculate correlation functions of the interacting systems in $D = 3$. This is made possible by the explicit form of the exact ground states.

1. Density-density correlation function

Using (43) the density-density correlation function

$$\rho_{n,n}(r) = \frac{1}{N_A} \sum_{i}(\langle \hat{n}_i \hat{n}_{i+r} \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_{i+r} \rangle), \quad (46)$$

where $\hat{n}_i = \sum_\sigma \sum_{b=d,f} \hat{n}_i^b_\sigma$, may be written as

$$\rho_{n,n}(r) = \frac{1}{N_A^2} \sum_{\sigma,\sigma'} \sum_{k_1,k_2,k_3} e^{i(k_1-k_2)r} \sqrt{R_{k_1} R_{k_2} R_{k_3} R_{k_4} \delta_{\sigma,\sigma'}} [(a_{k_1,d}^* a_{k_1,d} + a_{k_1,f}^* a_{k_1,f}) \times (a_{k_3,d}^* a_{k_2,d} + a_{k_1,f}^* a_{k_2,f}) (\langle \hat{C}^\dagger_{2,k_3\sigma} \hat{C}^\dagger_{2,k_4\sigma} \hat{C}_{2,k_1\sigma} \hat{C}_{2,k_2\sigma} \rangle - (\langle \hat{C}^\dagger_{2,k_3\sigma'} \hat{C}^\dagger_{2,k_4\sigma'} \hat{C}_{2,k_1\sigma'} \hat{C}_{2,k_2\sigma'} \rangle \langle \hat{C}^\dagger_{2,k_1\sigma} \hat{C}^\dagger_{2,k_2\sigma} \rangle) \rangle + \langle \hat{C}^\dagger_{1,k_3\sigma} \hat{C}^\dagger_{2,k_4\sigma} \hat{C}_{2,k_1\sigma} \hat{C}_{2,k_2\sigma} \rangle], \quad (47)$$

where $k_4 = k_3 + k_1 - k_2$. Employing (45,46,47) in the first term and (43,46) in the second term of (47) one finds

$$\sum_{\sigma,\sigma'} (\langle \hat{C}^\dagger_{2,k_3\sigma} \hat{C}^\dagger_{2,k_4\sigma} \hat{C}_{2,k_1\sigma} \hat{C}_{2,k_2\sigma} \rangle - (\langle \hat{C}^\dagger_{2,k_3\sigma'} \hat{C}^\dagger_{2,k_4\sigma'} \hat{C}_{2,k_1\sigma'} \hat{C}_{2,k_2\sigma'} \rangle \langle \hat{C}^\dagger_{2,k_1\sigma} \hat{C}^\dagger_{2,k_2\sigma} \rangle) = \delta_{k_1,k_4} \delta_{k_2,k_3} -$$
\[
\frac{1}{N_\Lambda} \sum_{k_1 \neq k_2} \sum_{k_3 \neq k_4} \sum_{k_1 + k_3 = k_2 - k_4} \delta_{k_4,k_3} \delta_{k_1,k_2}, \quad \sum_{\sigma,\sigma'} \langle \hat{C}_{1,\sigma}^\dagger \hat{C}_{2,\sigma'} \hat{C}_{2,\sigma}^\dagger \hat{C}_{1,\sigma'} \rangle = \delta_{k_4,k_1} \delta_{k_3,k_2}.
\]

Then the density-density correlation function becomes
\[
\rho_{n,n}(r) = \delta_{r,0} - \frac{1}{N_\Lambda^3} \sum_{k_1,k_2,k_3,k_4} e^{i(k_1 - k_2)r} a_{k_1,k_2,k_3,k_4}^* \times \left( \frac{(a_{k_3,d}^* a_{k_4,d} + a_{k_3,f}^* a_{k_4,f})(a_{k_1,d}^* a_{k_2,d} + a_{k_1,f}^* a_{k_2,f})}{(|a_{k_2,d}|^2 + |a_{k_2,f}|^2)(|a_{k_1,d}|^2 + |a_{k_1,f}|^2)} \right) \delta_{k_4,k_3 + k_1 - k_2}.
\]

In the thermodynamic limit the contributions from \( k_4 = k_2 \) and \( k_3 = k_1 \) in the second term have zero measure. Hence all \( k \) sums can be calculated without restriction. \( \rho_{n,n}(r) \) is seen to vanish for all \( r \) whenever the \( k \)-dependence of the \( a_{k,b} \) coefficients is negligible (for example in the case \(|t_1^d/t_2^d| >> 1\) for the solution from Sec.IV.B). It also vanishes in the limit \( |r| \to \infty \), where the \( k \to 0 \) limit of the coefficients \( a_{k,b} \) gives the dominant contribution to (48); this behavior is indeed seen in Fig.7.

2. Spin-spin correlation function

Similarly, the spin-spin correlation function
\[
\rho_{s,s}(r) = \frac{1}{N_\Lambda} \sum_i \left( \langle \hat{S}_i^z \hat{S}_{i+r}^z \rangle - \langle \hat{S}_i^z \rangle \langle \hat{S}_{i+r}^z \rangle \right)
\]

is given by
\[
\rho_{s_z,s_z}(r) = \frac{1}{N_\Lambda} \sum_i \left( \langle \hat{S}_i^z \hat{S}_{i+r}^z \rangle - \langle \hat{S}_i^z \rangle \langle \hat{S}_{i+r}^z \rangle \right)
\]
\[(a_{k_1,d}^* a_{k_2,d} + a_{k_1,f}^* a_{k_2,f}) (\langle \hat{C}^\dagger_{2,k_3} \hat{C}_{2,k_4} \hat{C}_{2,k_5} \rangle - \langle \hat{C}^\dagger_{2,k_3} \hat{C}_{2,k_4} \hat{C}_{2,k_5} \rangle) + (a_{k_3,d}^* a_{k_4,f} - a_{k_3,f}^* a_{k_4,d}) (a_{k_1,f}^* a_{k_2,d} - a_{k_1,d}^* a_{k_2,f}) (\langle \hat{C}^\dagger_{1,k_3} \hat{C}_{2,k_4} \hat{C}_{2,k_5} \rangle - \langle \hat{C}^\dagger_{1,k_3} \hat{C}_{2,k_4} \hat{C}_{2,k_5} \rangle) \delta_{k_4,k_1-k_2+k_3}.\]

Thus one finds \(\rho_{S_z,S_z}(r) = \delta_{r,0}/4\) and \(\rho_{S_\perp,S_\perp}(r) = \delta_{r,0}/2\) in the thermodynamic limit. Consequently, the spins are uncorrelated at distances \(|r| \neq 0\). This is a result of the macroscopic spin degeneracy of the ground state.

V. ALTERNATIVE TRANSFORMATIONS OF THE HAMILTONIAN

A. Generalized cell operators

The transformation of the PAM Hamiltonian into positive semi-definite form in terms of composite operators (the unit cell operators \(\hat{A}_{i,\sigma}\) in Sect. II.B.2) is relatively independent of the form of \(\hat{A}\). Instead of defining linear combinations of fermionic operators inside a *unit cell* of the Bravais lattice one may also define this superposition on an *arbitrary* substructure of the underlying lattice, e.g., a cell larger than a unit cell (for example, see Fig. 8). This leads to more general cell operators which may then be employed to transform the Hamiltonian into a form similar to (7). The corresponding matching conditions are similar to (8) but are now fulfilled in a different region of parameter space. In this way it is possible to construct and investigate various regions of parameter space.

Below we present a different transformation of the PAM Hamiltonian based on cell operators with octahedral shape, as shown in Fig. 8. Thereby it is possible to make direct contact with the conventional PAM. This clearly shows that a transformation of the PAM Hamiltonian into positive semi-definite form is *not* linked to finite \(f\)-electron hopping amplitudes in the PAM as one might have suspected from the steps performed in Sect. II.B. It also shows that the conventional PAM and the generalized version with extended hopping and hybridization amplitudes can have ground states with quite similar properties. This emphasizes the fact that the physical properties of an interacting electronic system need not depend on the precise form of the non-interacting bands.

We consider an octahedral cell \(B_i\) at each lattice site \(i\). The seven sites within \(B_i\) are denoted by \(r_{B_i} = i + r_{\alpha_1,\alpha_2,\alpha_3}\), where \(r_{\alpha_1,\alpha_2,\alpha_3} = \alpha_1 (1 - |\alpha_2|)(1 - |\alpha_3|)x_1 + \alpha_2 (1 - |\alpha_1|)(1 - |\alpha_3|)x_2 + \alpha_3 (1 - |\alpha_1|)(1 - |\alpha_2|)x_3, \alpha_\tau = -1,0,1\). Here \(x_\tau\) are the primitive vectors of the
unit cell of the lattice. As seen from Fig.8., the seven sites \( \mathbf{r}_{B_i} \) can be numbered by the indices \( n_{a_1,a_2,a_3} = (1 - |\alpha_2|)(1 - |\alpha_3|)(\alpha_1|\alpha_1| + 2) + (1 - |\alpha_1|)(1 - |\alpha_3|)(|\alpha_2|\alpha_2| + |\alpha_2| + 2) + (1 - |\alpha_1|)(1 - |\alpha_2|)(\alpha_3|\alpha_3| + 4|\alpha_3| + 2) \) without reference to \( B_i \). The separation vector \( \mathbf{r} \) between a site \( i \) and its neighbors in the cell \( B_i \) can take 11 distinct values \( (\mathbf{x}_\tau, \mathbf{x}_\tau \pm \mathbf{x}_{\tau'}, 2\mathbf{x}_\tau, \tau, \tau' = 1, 2, 3, \tau > \tau') \) over which the summation in (28) must be performed. Instead of (28) the cell operator is now defined as

\[
\hat{B}^\dagger_{B_i,\sigma} = a_{n,f}^* f_{i,\sigma}^\dagger + \sum_{n_{a_1,a_2,a_3}=1}^{7} a_{n,d}^* d_{i+r_{a_1,a_2,a_3},\sigma}^\dagger \tag{53}
\]

where \( n = n_{a_1,a_2,a_3} \), and the seven vectors \( \mathbf{r}_{a_1,a_2,a_3} \equiv \mathbf{r}_{n_{a_1,a_2,a_3}} \equiv \mathbf{r}_n \) in the sum are, in the increasing order of the index \( n, -\mathbf{x}_1, -\mathbf{x}_2, -\mathbf{x}_1, \mathbf{x}_2, -\mathbf{x}_3, 0, \mathbf{x}_3 \), (see Fig.8.). We note that \( a_{n,f} \neq 0 \) only on the central site (e.g., \( n = 6 \)) of the cell \( B_i \). Consequently the product \( \hat{B}^\dagger_{B_i,\sigma} \hat{B}_{B_i,\sigma} \) does not introduce \( f \)-electron hopping terms into the Hamiltonian, implying that the decomposition discussed here directly applies to the conventional PAM. In addition, the Hamiltonian contains only on-site and nearest-neighbor hybridization amplitudes, and \( d \)-electron hopping occurs between nearest and next-nearest neighbor sites.

Instead of (28) the transformed Hamiltonian then becomes

\[
\hat{H} = \sum_{i,\sigma} \hat{B}^\dagger_{B_i,\sigma} \hat{B}_{B_i,\sigma} + U \hat{P} + E_{g,b}, \tag{54}
\]

where \( E_{g,b} = K\hat{N} - UN_A - 2N_A(|a_{6,f}|^2 + K) \), \( K = \sum_{n=1}^{7} |a_{n,d}|^2 \). Furthermore, the matching conditions from (28) transform into the following non-linear system of 19 coupled complex algebraic equations

\[
\begin{align*}
-t^d_{x_1} &= a_{6,d}^* a_{3,d} + a_{1,d}^* a_{6,d}, \\
-t^d_{x_2} &= a_{6,d}^* a_{4,d} + a_{2,d}^* a_{6,d}, \\
-t^d_{x_3} &= a_{6,d}^* a_{7,d} + a_{5,d}^* a_{6,d}; \\
-t^d_{x_2-x_1} &= a_{2,d}^* a_{3,d} + a_{1,d}^* a_{4,d}, \\
-t^d_{x_3-x_1} &= a_{3,d}^* a_{4,d} + a_{2,d}^* a_{1,d}, \\
-t^d_{x_3+x_1} &= a_{5,d}^* a_{3,d} + a_{1,d}^* a_{7,d}; \\
-t^d_{x_3-x_2} &= a_{4,d}^* a_{7,d} + a_{5,d}^* a_{2,d}, \\
-t^d_{x_3+x_2} &= a_{5,d}^* a_{7,d} + a_{5,d}^* a_{1,d}; \\
-t^d_{2x_1} &= a_{1,d}^* a_{6,f} + a_{6,f}^* a_{3,d}, \\
-t^d_{2x_2} &= a_{2,d}^* a_{4,d}, \\
-t^d_{2x_3} &= a_{5,d}^* a_{7,d}, \\
-V_{x_1} &= a_{1,d}^* a_{6,f} + a_{6,f}^* a_{3,d}, \\
-V_{x_2} &= a_{2,d}^* a_{6,f} + a_{6,f}^* a_{4,d}, \\
-V_{x_3} &= a_{5,d}^* a_{6,f} + a_{6,f}^* a_{7,d}, \tag{55}
\end{align*}
\]

where \( V_{r}^{f,d} = V_{r}^{d,f} = V_{r} \), \( E_f = K - U - |a_{6,f}|^2 \), and \( a_{n,f} = 0 \) for \( n \neq 6 \). The ground state wave function valid for \( N \geq 3N_A \) now has the form

\[
|\Psi_{g,b}\rangle = \prod_{i=1}^{N_A} \hat{B}^\dagger_{B_{i,\uparrow}} \hat{B}^\dagger_{B_{i,\downarrow}} \hat{F}_{i}^\dagger |\bar{V}_{M}\rangle |0\rangle, \tag{56}
\]
where, for $N = 3N$, $\hat{V}_M^+ = 1$ holds. Since $a_{n,d}/a_{n,f}$ cannot be constant for all $n = 1, 2, \ldots, 7$ (see Sec. III), $|\Psi_{g,b}\rangle$ describes an itinerant ground state with properties similar to those presented in Sec. IV. An isotropic solution is obtained for
d
$$a_{1,d} = \sqrt{\frac{|t_d^2|}{2}} e^{i\phi}, \quad a_{6,d} = \frac{|V_0|}{V_1} \sqrt{\frac{|t_d^2|}{2}} e^{i(\phi - \phi_{V_0})}, \quad a_{6,f} = -V_1 \sqrt{\frac{2}{|t_d^2|}} e^{i\phi}. \quad (57)$$

where $\phi$ is an arbitrary phase and $\phi_{V_0}$ is the phase of the hybridization amplitude $V_0$. Introducing the notation $t = |t_d^2/t_1^d|$, $v = |V_1/t_1^d|$, this solution emerges in the parameter region with

$$\frac{U + E_f}{|t_1^d|} = 3t - \frac{2v^2}{t} + \frac{1}{2t \cos^2 \phi_{V_0}}. \quad (58)$$

Since $V_0$ and thereby $Im(V_0)$ is in principle arbitrary, (58) defines an entire region in the parameter space where the solution exists (see Fig.9.). For $Im(V_0) \neq 0$, or real $V_0$ at $|t_1^d/t_d^2| > 6$, the properties presented in Sec.IV. remain valid.

The results presented in this Section show that an itinerant non-Fermi liquid phase emerges also for real hybridization — even in the conventional PAM.

### B. Alternative decomposition using unit cell operators

To emphasize the flexibility of our method for constructing exact ground states of the PAM we will now show that even if unit cell operators $\hat{A}_{l_i,\sigma}$ are used, alternative decompositions are possible which lead to qualitatively different ground states in other regions of the parameter space. For example, instead of (7) the Hamiltonian $\hat{H}$ defined by (1a,1c,2) can also be cast into the form

$$\hat{H} = \sum_{l_i,\sigma} \hat{A}_{l_i,\sigma}^+ \hat{A}_{l_i,\sigma} + U \sum_i \hat{n}_{l_i^\uparrow} \hat{n}_{l_i^\downarrow} + E'_{g}. \quad (59)$$

For periodic boundary conditions the matching conditions can then be obtained from (8) by (i) replacing $J_{r}^{b,b'}$ by $\bar{J}_{r}^{b,b'} = -J_{r}^{b,b'}$, and (ii) replacing the last two equations (for $V_0$ and $U + E_f$) by $V_0 = \sum_{n=1}^8 a_{n,d,a_{n,f}}$ and $E_f = K_d - K_f$, with $E'_{g}/N = K_d$.

Using the new solutions of the matching conditions for arbitrary $U > 0$ we will now identify new ground states of (59) at and below quarter filling.
1. Insulating ground state at quarter filling

There exist solutions of the form \( q_{n,d}/q_{n,f} = p \) for all \( n \), with the additional constraint \( p = p^* \). In this case, the unit cell operator \( \hat{A}_{i,\sigma} \) contains only contributions of the form \( \hat{f}_{i,\sigma} + p\hat{d}_{i,\sigma} \) for all \( i \) and \( \sigma \). Introducing \( \hat{I}_i^\dagger(\mu_i) = [\hat{f}_{i,\uparrow} - (1/p)\hat{d}_{i,\uparrow}] + \mu_i[\hat{f}_{i,\downarrow} - (1/p)\hat{d}_{i,\downarrow}] \), where \( \mu_i \) is an arbitrary site dependent constant, one observes that

\[
\{ \hat{f}_{j,\sigma} + p\hat{d}_{j,\sigma}, \hat{I}_i^\dagger(\mu_i) \} = 0, \quad \forall j, j', \mu_j', \sigma.
\]

(60)

Since the operator \( \hat{I}_i^\dagger(\mu_i) \) acts only on site \( i \), the operator \( \hat{I}^\dagger = \prod_i^{N_A} \hat{I}_i^\dagger(\mu_i) \) does not introduce \( f \)-electron double occupancies. Consequently, \( \sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} \hat{I}^\dagger |0\rangle = 0 \), \( U \sum_i n_{i,\uparrow} n_{i,\downarrow} \hat{f}_i^\dagger |0\rangle = 0 \), and the ground state becomes

\[
|\Psi_\theta\rangle = \prod_{i=1}^{N_A} [(\hat{f}_{i,\uparrow} - \frac{1}{p}\hat{d}_{i,\uparrow}) + \mu_i(\hat{f}_{i,\downarrow} - \frac{1}{p}\hat{d}_{i,\downarrow})] |0\rangle.
\]

(61)

The ground state (61) has exactly one electron per site, and is degenerate, localized and globally non-magnetic. One can directly show that \( \text{Re} \sigma_{\tau,\tau}(0) = 0 \) (see Sec.III.A.1.), i.e., the state is indeed insulating.

2. Conducting ferromagnetic ground state at quarter filling

If \( q_{n,d}/q_{n,f} \) depends on \( n \), \( \hat{A}_{i,\sigma} \) does not anticommute with \( \hat{I}_i^\dagger(\mu_i) \); hence \( \sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} \hat{I}^\dagger |0\rangle = 0 \) does not hold. In this case one may introduce a complementary unit cell operator\(^{32}\)

\[
\hat{Q}_{i,\sigma}^\dagger = \sum_{n(\alpha,\beta,\gamma)=1}^8 [q_{n,d}^* \hat{d}_{i+\alpha,\beta,\gamma,\sigma} + q_{n,f}^* \hat{f}_{i+\alpha,\beta,\gamma,\sigma}]
\]

\[
= (q_{1,d}^* \hat{d}_{i+1,\sigma} + q_{2,d}^* \hat{d}_{i+1+x_1,\sigma} + q_{3,d}^* \hat{d}_{i+1+x_2,\sigma} + q_{4,d}^* \hat{d}_{i+1+x_3,\sigma} + \ldots + q_{8,d}^* \hat{d}_{i+1+x_3,\sigma})
\]

\[
+ (q_{1,f}^* \hat{f}_{i+1,\sigma} + q_{2,f}^* \hat{f}_{i+1+x_1,\sigma} + q_{3,f}^* \hat{f}_{i+1+x_2,\sigma} + q_{4,f}^* \hat{f}_{i+1+x_3,\sigma} + \ldots + q_{8,f}^* \hat{f}_{i+1+x_3,\sigma}),
\]

(62)

with the property \( \{ \hat{A}_{i,\sigma}, \hat{Q}_{j,\sigma'}^\dagger \} = 0 \) for all \( i, j \) and \( \sigma, \sigma' \). The numerical coefficients are given by the relations

\[
q_{1,d}^* = wa_{7,f}, \quad q_{2,d}^* = wa_{8,f}, \quad q_{3,d}^* = wa_{5,f}, \quad q_{4,d}^* = wa_{6,f},
\]

\[
q_{5,d}^* = wa_{3,f}, \quad q_{6,d}^* = wa_{4,f}, \quad q_{7,d}^* = wa_{1,f}, \quad q_{8,d}^* = wa_{2,f},
\]

\[
q_{1,f}^* = -wa_{7,d}, \quad q_{2,f}^* = -wa_{8,d}, \quad q_{3,f}^* = -wa_{5,d}, \quad q_{4,f}^* = -wa_{6,d},
\]

\[
q_{5,f}^* = -wa_{3,d}, \quad q_{6,f}^* = -wa_{4,d}, \quad q_{7,f}^* = -wa_{1,d}, \quad q_{8,f}^* = -wa_{2,d},
\]

(63)
where \( w \) is an arbitrary non-zero constant. Introducing \( \hat{Q}_1^{\dagger}, \sigma_1, \sigma_2, \ldots, \sigma_{N_L} \) one has \( \sum_{i,\sigma} \hat{A}_{1,i,\sigma} \hat{A}_{1,i,\sigma} \hat{Q}_1^{\dagger} \sigma_1, \sigma_2, \ldots, \sigma_{N_L} |0\rangle = 0 \) for arbitrary \( \sigma \). If the sites \( i, i' \) are adjacent the operator \( \hat{Q}_{1,i,\sigma} \hat{Q}_{1,i',\sigma} \) introduces two electrons on the common sites of \( I_i \) and \( I_{i'} \). The state \( \hat{Q}_{1,i,\sigma} \sigma_1, \sigma_2, \ldots, \sigma_{N_L} |0\rangle \) then provides the minimum possible eigenvalue (e.g., zero) in the presence of the Hubbard term only when \( \sigma = \sigma \) for all \( i \). Consequently, the ground state becomes

\[
|\Psi_g\rangle = \prod_{i=1}^{N_L} \hat{Q}_{1,i}^{\dagger} |0\rangle ; \sigma = \uparrow, \downarrow .
\]  

This corresponds to a fully saturated, non-degenerate ferromagnetic phase, which is metallic since in (64) double occupancies (e.g., \( \hat{d}_i^{\dagger} \hat{f}_i^{\dagger} \)), empty sites, and single occupancies are simultaneously present.\(^{54}\)

Ferromagnetism in the PAM at and around quarter filling has been investigated rather extensively in the past already. Following variational results for Kondo lattices by Fazekas and Müller-Hartmann\(^{55}\) ferromagnetic phases in the PAM itself were found by Dorin and Schlottmann\(^{56}\) in the limit \( U \to \infty \), and at finite \( U \) by Möller and Wölfle\(^{57}\) within a slave-boson approach. Subsequently, ferromagnetic solutions of the PAM at and near quarter filling were obtained within various other approximation schemes.\(^{58,59,60,61,62,63,64,65,66}\) Exact results were derived in \( D = 1 \) for \( U = \infty \) by Yanagisawa\(^{67}\).

In the exact solution discussed here ferromagnetism emerges when the lower diagonalized band of (2) becomes non-dispersive (flat). We note that this can happen even if the bare bands of the Hamiltonian are dispersive.

3. Ground states below quarter filling

Exact ground states of the PAM can even be constructed for \( N < N_L \), i.e., below quarter filling. For the two cases discussed in Sec.V.B.1-2. they have the same form as (64) and (61). However, the upper limit of the products has to be replaced by \( N \), and the additional geometrical degeneracy of the electrons needs to be taken into account.

For \( n \)-dependent \( q_{n,d}/q_{n,f} \), the ground state becomes

\[
|\Psi_g\rangle = \sum_{\mathcal{D}_N} \sum_{\{\mathcal{D}_{N,m}\}} \sum_{\{\sigma_m\}} \alpha_{\mathcal{D}_N,\{\mathcal{D}_{N,m}\},\{\sigma_m\}} \prod_{m \in \mathcal{D}_{N,m}} (\prod_{i \in \mathcal{D}_{N,m}} \hat{Q}_{1,i,\sigma_m}) |0\rangle
\]  

where \( \mathcal{D}_N \) denotes an arbitrary domain (a subset of lattice points) of the full lattice containing \( N < N_L \) lattice sites. A given domain \( \mathcal{D}_N \) consists of disjoint subdomains (clusters)
denoted by $D_{N,m}$ where $m$ enumerates the clusters in $D_N$; the maximum of $m$ is denoted by $N_m$. Clearly one has $D_N = D_{N,1} \cup D_{N,2} \cup \ldots \cup D_{N,N_m}$, and $D_{N,m_1} \cap D_{N,m_2} = 0$ for $m_1 \neq m_2$. Furthermore, $\sigma_m = \pm 1/2$ represents a fixed, but arbitrary, spin-index in the sub-domain $D_{N,m}$, and $\alpha_{D_N,\{D_{N,m}\},\{\sigma_m\}}$ are arbitrary coefficients. From a physical point of view (65) contains disjoint, fully saturated ferromagnetic, conducting clusters of arbitrary shape and size, whose spin orientation is arbitrary.

For $q_{n,d}/q_{n,f} = p = p^*$ the ground state becomes

$$|\Psi_g\rangle = \sum_{D_N} \sum_{\{D_{N,m}\}} \alpha_{D_N,\{D_{N,m}\}} \prod_m \left( \prod_{i \in D_{N,m}} \left[ (\hat{f}^\dagger_{i\uparrow} - \frac{1}{p} \hat{d}^\dagger_{i\uparrow}) + \mu_i (\hat{f}^\dagger_{i\downarrow} - \frac{1}{p} \hat{d}^\dagger_{i\downarrow}) \right] \right) |0\rangle$$

containing again clusters of arbitrary shape and size. But now the clusters are insulating and non-magnetic, containing strictly one particle per site with arbitrary spin.

The parameter region corresponding to the ground state solutions in Sec.V.B. can be obtained from that derived from the matching conditions (8) by the replacements $t^b_r \rightarrow -t^b_r$, $V_r \rightarrow -V_r$, $U \rightarrow 0$. The results are valid for all $U > 0$.

VI. SUMMARY

We presented details of an analytic scheme which allows one to construct exact ground states for a general class of three-dimensional periodic Anderson models (PAM), including the conventional PAM, on regular Bravais lattices. First the Hamiltonian is cast into positive semi-definite form with the help of composite fermionic operators in combination with a set of coupled, non-linear matching conditions for the microscopic parameters of the Hamiltonian. Then a non-local product state of these composite operators in position space, corresponding to $3/4$ filling is constructed which yields exact grounds in various parts of parameter space.

Depending on the choice of the composite operators and the geometry of the building blocks of the lattice on which they are defined, the transformation of the Hamiltonian into positive semi-definite form can be performed in several ways. Thereby it is possible to construct exact ground states in different regions of the parameter space of the model.

For real $d, f$ hybridization amplitudes we constructed an insulating, non-magnetic ground state which is stable on several different lattice structures. Its ground state energy was shown to diverge at the boundary of the stability region, implying a divergence of its compressibility. Such an anomaly is known to occur in several heavy-fermion materials. Furthermore,
we identified an exact metallic non-Fermi liquid ground state, characterized by one dispersing band and one upper flat band, which is stable in different regions of parameter space. This state is non-magnetic and has vanishing non-local spin-spin correlations in the thermodynamic limit. Its density-density correlations are short ranged, and the momentum distributions of the electrons in the interacting ground state have no discontinuities. The stability regions of these ground states extend through a large region of the parameter space – from weak to strong on-site interactions $U$.

Exact ground states with conducting and insulating properties, respectively, were also constructed at and below quarter filling. In particular, a conducting, fully polarized ferromagnetic state was found to be the ground state at quarter filling. At lower fillings a ground state characterized by ferromagnetic clusters of arbitrary shape was identified.

Our results show that ground states of the conventional PAM and of generalizations with extended hopping and hybridization amplitudes can have quite similar properties.

The exact ground states discussed in this paper correspond to simple solutions of the coupled matching conditions for the microscopic parameters of the Hamiltonian. In view of their large number (e.g., 55 conditions in the case of the unit cell operators in Sec. II.B) and their non-linearity it almost certain that other solutions exist which then lead to yet other exact ground states of the three-dimensional PAM and its extensions. In view of the great relevance of this model for our understanding of correlated electronic systems, both on the level of models and real materials, more detailed investigations of the matching conditions derived here will be worthwhile. Finally it should be stressed that the concept behind the construction of exact ground states for the PAM in $D = 3$ presented here is quite general, and is also applicable to other electronic correlation models.

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APPENDIX A: TRANSFORMATION OF THE PERIODIC ANDERSON MODEL HAMILTONIAN

In this appendix we present details of the transformation of the PAM Hamiltonian in its original form with $d$ and $f$ operators [see (1), (2), (6)]

\[
\hat{H} = \sum_{i,\sigma} \left\{ \sum_r \left[ (t_r^d \hat{d}_{i,\sigma} \hat{a}_{i+r,\sigma} + t_r^f \hat{f}_{i,\sigma} \hat{f}_{i+r,\sigma}) + (V_r^d \hat{d}_{i,\sigma} \hat{a}_{i+r,\sigma} + V_r^f \hat{f}_{i,\sigma} \hat{a}_{i+r,\sigma}) \right] \right. \\
+ \left. (V_0 \hat{d}_{i,\sigma} \hat{f}_{i,\sigma} + H.c.) + (E_f + U) \hat{n}_{i,\sigma} \right\} + U \hat{P} - U N_A, \\
\]  

\[\text{(A1)}\]

into the form with unit cell operators, (4),

\[
\hat{H} = - \sum_{i,\sigma} \hat{A}_{i,\sigma}^+ \hat{A}_{i,\sigma} + K_d \hat{N} + U \hat{P} - U N_A, \\
\]  

\[\text{(A2)}\]

and explain how the matching conditions arise in this process.

One first calculates all terms in the sum \(- \sum_{i,\sigma} \hat{A}_{i,\sigma}^+ \hat{A}_{i,\sigma}\) from (A2). To identify the contributions generated thereby with those defined by (A1) one needs altogether 55 matching equations. This procedure will now be illustrated by four typical examples. Here we refer to Fig.10 where four neighboring unit cells $I_{i_1}, I_{i_2}, I_{j_1},$ and $I_{j_2}$ – each denoted according to the notation introduced in Sec. II.B.1 – is depicted. Since the precise shape of the unit cells is unimportance here we use orthorhombic cells for simplicity.

Nearest neighbor contributions: First we analyze a nearest neighbor amplitude, e.g., $t_{j_2,j_5}^d,$ which appears in the kinetic energy of (A1) as $t_{j_2,j_5}^d \hat{d}_{j_2,\sigma}^\dagger \hat{d}_{j_5,\sigma}.$ This term acts along the bond $(j_2,j_5)$ represented by the horizontal, thick dashed line in Fig.10. In (A2) this term originates from \(- \sum_{i,\sigma} \hat{A}_{j_1,\sigma}^+ \hat{A}_{j_1,\sigma}\), but only for sites $i = i_1,i_2,j_1,j_2$ in $I_i.$ To calculate \(- \sum_{i=i_1,i_2,j_1,j_2} \hat{A}_{j_1,\sigma}^+ \hat{A}_{j_1,\sigma}\) one must write down the unit cell operators $\hat{A}_{j_1,\sigma}^+,$ (4), corresponding to the aforementioned four unit cells. For example one finds

\[
\hat{A}_{j_1,\sigma}^+ = \sum_{b=d,f} \left[ a_{1,b}^* \hat{b}_{1,j_1,\sigma} + a_{2,b}^* \hat{b}_{2,j_1,\sigma} + a_{3,b}^* \hat{b}_{3,j_5,\sigma} + a_{4,b}^* \hat{b}_{4,j_1,\sigma} + a_{5,b}^* \hat{b}_{5,j_1,\sigma} + a_{6,b}^* \hat{b}_{6,j_2,\sigma} + a_{7,b}^* \hat{b}_{7,j_5,\sigma} + a_{8,b}^* \hat{b}_{8,j_5,\sigma}, \right] \\
\hat{A}_{j_1,\sigma} = \sum_{b=d,f} \left[ a_{1,b} \hat{b}_{1,j_1,\sigma} + a_{2,b} \hat{b}_{2,j_1,\sigma} + a_{3,b} \hat{b}_{3,j_5,\sigma} + a_{4,b} \hat{b}_{4,j_1,\sigma} + a_{5,b} \hat{b}_{5,j_1,\sigma} + a_{6,b} \hat{b}_{6,j_2,\sigma} + a_{7,b} \hat{b}_{7,j_5,\sigma} + a_{8,b} \hat{b}_{8,j_5,\sigma}. \right]
\]

Thereby one obtains contributions of the form \(-a_{6,b}^* a_{7,d} \hat{d}_{j_2,\sigma}^\dagger \hat{d}_{j_5,\sigma},\ -a_{5,b}^* a_{8,d} \hat{d}_{j_2,\sigma}^\dagger \hat{d}_{j_5,\sigma},\ -a_{2,d} a_{3,d} \hat{d}_{j_2,\sigma}^\dagger \hat{d}_{j_5,\sigma},\) and \(-a_{1,d} a_{4,d} \hat{d}_{j_2,\sigma}^\dagger \hat{d}_{j_5,\sigma}\) implying $t_{j_2,j_5}^d = -(a_{1,d} a_{4,d} + a_{2,d} a_{3,d} + a_{5,d} a_{8,d} + a_{6,d} a_{7,d}).$ Since (i) $t_{j_2,j_5}^d$ is a specific example of the general hopping amplitude $t_{i_1,i_2+x_2}^d,$ (ii) all amplitudes $t_{j_2,j_5}^d$ amplitudes have the same form (i.e., $t_{x_2}^d = t_{i_1,i_2+x_2}^d$), and (iii) this also holds for
the \( f \) electrons, i.e., \( t_{x_2}^f = t_{i,i+x_2}^f \), one finds \( -t_{x_2}^b = a_{1,b}^* a_{4,b} + a_{2,b}^* a_{3,b} + a_{5,b}^* a_{8,b} + a_{6,b}^* a_{7,b} \), where \( b = d, f \).

The same analysis applies to the hybridization amplitudes. Hence, for the terms \( V_{x_2}^{d,f} \hat{d}_{1+i,x_2} \hat{f}_{1+i,x_2} \) and \( V_{x_2}^{f,d} \hat{f}_{1+i,x_2} \hat{d}_{1+i,x_2} \) one finds \( -V_{x_2}^{b,b'} = a_{1,b}^* a_{4,b'} + a_{2,b}^* a_{3,b'} + a_{5,b}^* a_{8,b'} + a_{6,b}^* a_{7,b'} \).

Thus we have derived the matching condition \( J_{x_2}^{b,b'} = -[\delta_{b,b'} t_{x_2}^b + (1 - \delta_{b,b'}) V_{x_2}^{b,b'}] \) [the third relation in (8)].

It should be noted that the sum \( -\sum_i \hat{A}_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \) also produces the Hermitian conjugates of the terms represented by (A1). Therefore, in addition to the result for \( t_{j_2,j_3}^d \), one also finds \( t_{j_3,j_2}^d = -(a_{1,d}^* a_{1,d} + a_{3,d}^* a_{2,d} + a_{3,d}^* a_{5,d} + a_{7,d}^* a_{6,d}) \), where \( t_{j_3,j_2}^d = t_{i_1-x_2}^d = t_{-x_2}^d = t_{x_2}^d \).

Second-nearest neighbor contributions: We now consider a plaquette-diagonal next-nearest neighbor term, namely \( t_{i_2,j_3}^d \), acting on the oblique thick dashed line in Fig.10. Since the bond \((i_2,j_3)\) appears only in the unit cells \( I_i \) and \( I_{i_2} \), only the contributions from \(-\sum_i \hat{A}_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \) in (A2) with \( i = i_1, i_2 \) give rise to \( t_{i_2,j_3}^d \hat{d}_{i_2} \hat{d}_{j_3} \) in (A1). The sum \(-\sum_{i_1,i_2} \hat{A}_{i_1,\sigma} \hat{A}_{i_2,\sigma} \) leads to the expressions \(-a_{1,d} a_{7,d}^\dagger \hat{d}_{i_2} \hat{d}_{j_3} \), and \(-a_{1,d} a_{8,d} \hat{d}_{i_2} \hat{d}_{j_3} \), implying \( t_{i_2,j_3}^d = -(a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d}) \). Since (i) \( t_{i_2,j_3}^d \) is a specific example of the general hopping amplitude \( t_{i_1-x_2}^d \), and (ii) all the amplitudes \( t_{i_1-x_2}^d \) have the same form (i.e., \( t_{i_1-x_2}^d = t_{x_3+x_2}^d \)) one finds \( -t_{x_3+x_2}^d = a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d} \). These relations also hold for the \( f \) electrons. Therefore we arrive at the matching condition \( J_{x_3+x_2}^{b,b'} = a_{1,b}^* a_{8,b'} + a_{2,b}^* a_{7,b'} \) [the sixth relation in (8)].

Third-nearest neighbor contributions: The third neighbor contributions, located along the space diagonals of the unit cell, are the same in every cell. For example, studying the bond \((j_1,j_3)\) of the cell \( I_i \), the product \(-\hat{A}_{i_1,\sigma} \hat{A}_{i_1,\sigma} \) leads to the term \(-a_{1,d} a_{7,d} \hat{d}_{i_1} \hat{d}_{j_3} \). Hence one finds \( t_{i_1,j_3}^d = t_{i_1+x_2+x_2}^d = t_{x_3+x_2+x_3}^d = a_{1,d}^* a_{7,d} \) and, consequently, \( J_{x_3+x_2+x_3}^{b,b'} = a_{1,d}^* a_{7,d} \) [the tenth relation in (8)].

Single-site contributions: Since any site is common to 8 unit cells, single site contributions require the consideration of 8 neighboring unit cells. For example, the term \( V_0 \sum_{i,\sigma} \hat{d}_{i,\sigma}^\dagger \hat{f}_{i,\sigma} \) is obtained from \(-\sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} \) as \(-\sum_{n=1}^{8} a_{n,d}^* a_{n,f} \sum_{i,\sigma} \hat{d}_{i,\sigma}^\dagger \hat{f}_{i,\sigma} \), implying \(-V_0 = \sum_{n=1}^{8} a_{n,d}^* a_{n,f} \). In the same way we obtain the coefficient of \(-\sum_{i,\sigma} \hat{b}_{i,\sigma}^\dagger \hat{b}_{i,\sigma} \) as \(-\sum_{n=1}^{8} |a_{n,b}|^2 = K_b \). Therefore the terms \(-\sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} + K_d \hat{N} \) in (A2) yield \(-(K_d \hat{N}_d + K_f \hat{N}_f) + K_d (\hat{N}_d + \hat{N}_f) = (K_d - K_f) \hat{N}_f \), where \( \hat{N} = \hat{N}_d + \hat{N}_f \). Taking into account the term \((U + E_f) \hat{N}_f \) in (A1) one obtains \( U + E_f = K_d - K_f \) [last relation in (8)].
APPENDIX B: THE CURRENT OPERATOR

In this appendix we derive the current operator as well as the charge conductivity sum rule for a general form of the PAM.

The charge density operator at site \( i \) is given by \( \hat{\rho}(i) = e \sum_{\sigma} (\hat{d}_{i,\sigma}^\dagger \hat{d}_{i,\sigma} + \hat{f}_{i,\sigma}^\dagger \hat{f}_{i,\sigma}) \), with \( e \) as the electron charge. The current operator \( \hat{\mathbf{j}} \) is defined as
\[
\hat{\mathbf{j}} = -\frac{ie}{\hbar V} \sum_i \sum_{\sigma} \sum_{b,b'=d,f} (\hat{J}_r^{bb'} d_{i+r,\sigma}^\dagger \hat{f}_{i,\sigma} - \hat{J}_r^{bb'} f_{i,\sigma}^\dagger \hat{d}_{i+r,\sigma}) \mathbf{r},
\]
where \( \hat{J}_r^{bb'} \) is defined in (S), and \( \mathbf{r} \) is restricted to the values presented in Sec.II.B.1. We note that only the itinerant part of the Hamiltonian, i.e., \( \hat{H}_{it} = \sum_r \hat{H}_{itin}(\mathbf{r}) = \hat{H} - \hat{H}_U - \sum_i [ (V_0 \hat{d}_{i,\sigma}^\dagger \hat{f}_{i,\sigma} + H.c.) + E_f \hat{n}_{i,\sigma}^f ] \), where
\[
\hat{H}_{itin}(\mathbf{r}) = \sum_{i,\sigma} \left[ \frac{(t_{i,r}^d \hat{d}_{i,\sigma}^\dagger \hat{d}_{i+\mathbf{r},\sigma} + t_{i,r}^f \hat{f}_{i,\sigma}^\dagger \hat{f}_{i+\mathbf{r},\sigma})}{2} + \frac{(V_{i,r}^d \hat{d}_{i,\sigma}^\dagger \hat{f}_{i,\sigma} + V_{i,r}^f \hat{f}_{i,\sigma}^\dagger \hat{d}_{i+\mathbf{r},\sigma})}{2} + H.c. \right]
\]
contributes to (B1).

Starting from the current operator in (B1), the Kubo formula for the charge conductivity at zero temperatures becomes \( \sigma_{\tau,\tau}(\omega) = iV \int_0^\infty dt e^{-i\omega t} \langle [\hat{q}_\tau(t), \hat{j}_\tau] \rangle \). The sum rule for the charge conductivity then has the form
\[
\int_0^\infty d\omega \text{Re} \sigma_{\tau,\tau}(\omega) = -\frac{ie^2}{\hbar V} \sum_{\mathbf{r}} \frac{(\mathbf{r} \cdot \mathbf{x}_\tau)^2}{|\mathbf{x}_\tau|^2} \langle \hat{H}_{itin}(\mathbf{r}) \rangle.
\]

APPENDIX C: LOCALIZED SOLUTION FOR THE NON-CUBIC CASE

In this appendix the matching conditions (28) from section III.B are solved for localized ground states in the case of non-cubic systems. We start from the observation that the coefficients \( a_{n,d} \) with \( n \geq 5 \) can be expressed by the unit cell diagonal hopping amplitudes and \( a_{n,d} \) with \( n < 5 \) as
\[
a_{5,d} = -t_{x_3-x_2-x_1}^d / a_{3,d}^*, \quad a_{6,d} = -t_{x_3-x_2+x_1}^d / a_{4,d}^*, \quad a_{7,d} = -t_{x_3+x_2+x_1}^d / a_{6,d}^*, \quad a_{8,d} = -t_{x_3+x_2-x_1}^d / a_{7,d}^*.
\]

With these relations and using the notations
\[
\tau_1 = \frac{4t_{x_3-x_2+x_1}^d t_{x_3-x_2-x_1}^d}{2t_{x_2+x_1}^d}, \quad \tau_2 = \frac{4t_{x_3-x_2+x_1}^d t_{x_3+x_2-x_1}^d}{2t_{x_3+x_2}^d}, \quad \tau_3 = \frac{4t_{x_3-x_2-x_1}^d t_{x_3+x_2+x_1}^d}{2t_{x_3+x_1}^d},
\]
\[ \tau_4 \equiv \frac{4t_{x_1-x_2}^d t_{x_3-x_2}^d t_{x_3-x_1}^d t_{x_3-x_1}^d}{t_{x_3-x_1}^d}, \quad \tau_5 \equiv \frac{4t_{x_1-x_3}^d t_{x_3-x_2}^d t_{x_3-x_1}^d t_{x_3-x_1}^d}{t_{x_3-x_2}^d}, \quad \tau_6 \equiv \frac{4t_{x_1-x_3}^d t_{x_3-x_1}^d t_{x_3-x_1}^d t_{x_3-x_1}^d}{t_{x_3-x_1}^d} \quad \text{(C1)} \]

(23) leads to

\[ |a_{1,d}|^2 = -\frac{t_{x_2-x_1}^d t_{x_3-x_2}^d}{2t_{x_1-x_1}^d} F(\tau_1) F(\tau_2) F(\tau_4), \quad |a_{2,d}|^2 = -\frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{2t_{x_3-x_2}^d} \frac{F(\tau_3) F(\tau_6)}{F(\tau_2)}, \]

\[ |a_{3,d}|^2 = -\frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{2t_{x_2-x_2}^d} \frac{\tau_1 F(\tau_1)}{F(\tau_2) F(\tau_4)}, \quad |a_{4,d}|^2 = -\frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{2t_{x_3-x_2}^d} \frac{\tau_3 F(\tau_2) F(\tau_6)}{F(\tau_2) F(\tau_3)}, \quad \text{(C2)} \]

where \( F(x) = 1 \pm \sqrt{1-x} \). The function required for the expression of \( E_g \) becomes

\[
\sum_{n=1}^8 |a_{n,d}|^2 = (|a_{1,d}|^2 + \frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{|a_{1,d}|^2}) + (|a_{2,d}|^2 + \frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{|a_{2,d}|^2}) + (|a_{3,d}|^2 + \frac{t_{x_2-x_1}^d t_{x_3-x_1}^d}{|a_{3,d}|^2}) \quad \text{(C3)}
\]

For the localized solution to be stable the quantities \( |a_{n,d}|^2 \) in (C2), and hence the function \( F(\tau_i) \), need to be real. When \( F(\tau_i) \) becomes complex the localized solution becomes unstable. At these points the derivative \( \partial F(x)/\partial x \) diverges. Except for accidental cancellations in (C2), this implies an infinite slope of \( E_g \) as a function of hopping amplitudes.

APPENDIX D: SECTOR OF MINIMAL SPIN OF THE ITINERANT SOLUTION

Here we present details of the calculation of spin expectation values in the itinerant case for minimum total spin (see Sec.IV.E.2).

In (I) the terms

\[ \left[ \prod_{i=k_{\sigma}}^{N_L/2} (\sum_{k \in D_{\sigma}} e^{i k \phi(k_{\sigma})} \hat{F}^\dagger_{f,(k_{\sigma})}) \right] = \sum_{\{k_i\}} \beta_{\{k_i\},\sigma} \hat{F}^\dagger_{f,(k_{\sigma})}, \quad \beta_{\{k_i\},\sigma} = \sum_{P_{\{k_i\}}} (-1)^p e^{i (\tilde{\phi} k_{i_1} + \cdots + i N_L/2 k_{i N_L/2})}, \quad \text{(D1)} \]

appear where \( \hat{F}^\dagger_{f,(k_{\sigma})} = \hat{F}^\dagger_{k_{i_1},\sigma} \hat{F}^\dagger_{k_{i_2},\sigma} \cdots \hat{F}^\dagger_{k_{N_L/2},\sigma} \). Here the sum over \( \{k_i\} \) extends over all sets of momentum with \( N_L/2 \) elements chosen from the first Brillouin zone, the sum \( \sum_{P_{\{k_i\}}} \) goes over all permutations \( P_{\{k_i\}} \) of the momenta in each set \( \{k_i\} = (k_1, \ldots, k_{N_L/2}) \), and \( \tilde{p} \) represents the parity of \( P_{\{k_i\}} \). Since for \( i_{n,\sigma} \in D_{\sigma} \) we have \( i_{n,\downarrow} = i_{n,\uparrow} + R \), one finds \( \beta_{\{k_i\},\downarrow} = e^{i \phi(k_i)} \beta_{\{k_i\},\uparrow} \), where \( \phi(k_i) = R \sum_{k \in \{k_i\}} k \). Thus, (I) becomes

\[ |\Psi_g \rangle = \sum_{\{k_i\}} \sum_{\{k_j\}} \alpha_{\{k_i\},\{k_j\}} |v_{\{k_i\},\{k_j\}} \rangle, \quad |v_{\{k_i\},\{k_j\}} \rangle = \left( \prod_{k} A_{k_{\uparrow},\downarrow} \hat{F}^\dagger_{f,(k_{\sigma})} \hat{F}^\dagger_{f,(k_{\sigma})} |0 \rangle \right), \quad \text{(D2)} \]
where \( \alpha_{\{k\},\{k\}} = \beta_{\{k\},\uparrow} \beta_{\{k\},\downarrow}, \) \( |\alpha_{\{k\},\{k\}}| = |\alpha_{\{k\},\{k\}}|, \) and \( |v_{\{k\},\{k\}}\) are orthogonal states. Using (D2) one finds

\[
\langle \hat{S}^z \rangle = \langle \sum_k \hat{S}_k^z \rangle = 0, \quad \langle \hat{S}^y \rangle = \langle \sum_k \hat{S}_k^y \rangle = 0, \quad \langle \hat{S}^z \rangle = \langle \sum_k \hat{S}_k^z \rangle = 0, \quad \langle \hat{S} \rangle = 0. \tag{D3}
\]

To calculate expectation values of the square of the spin we use normalized wave functions \( |w_{\{k\},\{k\}}\rangle = |v_{\{k\},\{k\}}\rangle / (|v_{\{k\},\{k\}}| |v_{\{k\},\{k\}}|)^{1/2}, \) in terms of which the ground state can be written as \( |\Psi_g\rangle = \sum_{\{k\}} \sum_{\{k\}} \alpha'_{\{k\},\{k\}} |w_{\{k\},\{k\}}\rangle, \) where \( \alpha'_{\{k\},\{k\}} \) are new numerical coefficients. Thereby one finds

\[
\langle (\hat{S}^z)^2 \rangle = \frac{1}{4} \langle \hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+ \rangle = 2N_A \left( N_A - d_{\{k\},\{k\}} \right) / 4 \sum_{\{k\}} \sum_{\{k\}} |\alpha'_{\{k\},\{k\}}|^2 < \frac{N_A}{4}, \tag{D4}
\]

where \( d_{\{k\},\{k\}} \) is the number of common elements of the sets \( \{k\} \) and \( \{k\}. \)

**APPENDIX E: EXPECTATION VALUES FOR THE FLAT BAND**

In this appendix we present details of the calculation of ground state expectation values for the itinerant solution in Sec.IV. The ground state wave vector (D2) is a superposition of states

\[
|\Psi_{g,\{\sigma\}}\rangle = \left[ \prod_k \hat{C}_{1,k}^\dagger \hat{C}_{1,k}^\dagger \right] \left[ \prod_{n=1}^{N_A} \left( \frac{1}{\sqrt{N_A}} \sum_{k_n} X_{k_n} e^{ik_n10} \hat{C}_{2,k_n1n}^\dagger \right) \right] |0\rangle, \tag{E1}
\]

where \( \{\sigma\} = \{\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_{N_A}\}. \) By modifying the \( \{\sigma\} \) sets in (E1) one obtains \( 2^{N_A} \) states, which obey \( \langle \Psi_{g,\{\sigma\}} | \Psi_{g,\{\sigma'\}} \rangle = Det[x_{i,j}(\{X_k^*\}, \{X_k\}, \sigma_i, \sigma'_j)], \) where \( x_{i,j}(\{V_k\}, \{W_k\}, \sigma_i, \sigma'_j) = \delta_{\sigma_i,\sigma'_j} (1/N_A) \sum_k V_k^* W_k e^{i(kd_{j-1})}. \) We see that for \( \{\sigma'\} \neq \{\sigma\} \) the states \( |\Psi_{g,\{\sigma\}}\rangle, \) and \( |\Psi_{g,\{\sigma'\}}\rangle \) are not necessarily orthogonal.

1. **The case \( X_k \neq 0 \)**

We first consider \( X_k \neq 0 \) for all \( k. \) Introducing the states

\[
|\Psi_g^{\{\sigma\}}\rangle = \left[ \prod_k \hat{C}_{1,k}^\dagger \hat{C}_{1,k}^\dagger \right] \left[ \prod_{n=1}^{N_A} \left( \frac{1}{\sqrt{N_A}} \sum_{k_n} X_{k_n} e^{ik_n10} \hat{C}_{2,k_n1n}^\dagger \right) \right] |0\rangle, \tag{E2}
\]

one finds \( \langle \Psi_g^{\{\sigma\}} | \Psi_{g,\{\sigma'\}} \rangle = Det[z_{i,j}(\sigma_i, \sigma'_j)], \) where \( z_{i,j}(\sigma_i, \sigma'_j) = x_{i,j}(\{1/X_k\}, \{X_k\}, \sigma_i, \sigma'_j) = \delta_{\sigma_i,\sigma'_j} \delta_{i,j}, \) such that \( Det[z_{i,j}(\sigma_i, \sigma'_j)] = \delta_{\{\sigma\},\{\sigma'\}}. \) This yields \( \langle \Psi_g^{\{\sigma\}} | \Psi_{g,\{\sigma'\}} \rangle = \delta_{\{\sigma\},\{\sigma'\}}, \) i.e., the

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An arbitrary state of the form of (42) can then be written as $|\Psi_g,\{\sigma\}\rangle = \sum_{\{\sigma\}} \alpha_{\{\sigma\}} |\Psi_{g,\{\sigma\}}\rangle$, where $\alpha_{\{\sigma\}}$ are numerical coefficients. Furthermore, one finds

$$\hat{C}_{2,k_1\sigma_1}^\dagger \hat{C}_{2,k_2\sigma_2} |\Psi_{g,\{\sigma'\}}\rangle = \sum_{n=1}^{N_A} \frac{1}{N_A} \sum_{k'} X_{k'} e^{i k_1 n} \hat{C}_{2,k_1\sigma_1}^\dagger \hat{C}_{2,k_2\sigma_2} = \sum_{n=1}^{N_A} \frac{1}{N_A} \sum_{k'} X_{k'} e^{i k_1 n} \hat{C}_{2,k_1\sigma_1}^\dagger \hat{C}_{2,k_2\sigma_2},$$

from which

$$\langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,k_1\sigma_1}^\dagger \hat{C}_{2,k_2\sigma_2} |\Psi_{g,\{\sigma'\}}\rangle = \sum_{n=1}^{N_A} Det[z_{ij}(n, \sigma''_i, \sigma'_j)]$$

(E4)

follows. Here, the matrix $z_{ij}(n, \sigma''_i, \sigma'_j)$ is the same as $z_{ij}(\sigma''_i, \sigma'_j)$, except for the matrix elements in the $n$-th column which are given by $z_{in} = (1/N_A)(X_{k_2}/X_{k_1})e^{i(k_2 n - k_1)} \delta_{\sigma''_i, \sigma'_{n}}$. From (E4) one finds that $\langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} |\Psi_{g,\{\sigma'\}}\rangle$ vanishes in the thermodynamic limit as $1/N_A$. In the case of $\sigma_1 = \sigma_2 = \sigma$, only $\{\sigma''\} = \{\sigma'\}$ components remain in (E4) yielding

$$\langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} |\Psi_{g,\{\sigma'\}}\rangle = \delta_{\sigma''_i, \sigma'_{i}} X_{k_2}/X_{k_1} \sum_{n=1}^{N_A} \delta_{\sigma, \sigma'_{i}} e^{i(k_2 n - k_1)} \langle \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} \rangle,$$

(E5)

where $\sum_{n=1}^{N_A} \delta_{\sigma, \sigma'_{i}}$ quantifies the number of $\sigma$ spins from $\{\sigma'\}$. Since $\sum_{n=1}^{N_A} \delta_{\sigma, \sigma'_{i}} = 1$ for arbitrary $\sigma'_{i}$, it follows that $\langle \Psi_g^{\{\sigma''\}} | \sum_{\sigma} \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} |\Psi_{g,\{\sigma'\}}\rangle = \delta_{k_2,k_1} \delta_{\sigma'', \{\sigma'\}}$. Using the notation $\langle \ldots \rangle = \langle \Psi_g | \ldots | \Psi_g \rangle / \langle \Psi_g | \Psi_g \rangle$, one finally obtains

$$\langle \sum_{\sigma} \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} \rangle = \delta_{k_2,k_1}.$$ 

(E6)

The spin dependent expectation value $\langle \hat{C}_{2,k_1\sigma}^\dagger \hat{C}_{2,k_2\sigma} \rangle$ may be calculated, for example, by taking the $T \rightarrow 0$ limit of $\langle \hat{C}_{2,k_0}^\dagger \hat{C}_{2,k_0} \rangle$ as

$$\langle \hat{A} \rangle = \lim_{T \rightarrow 0} \frac{Tr(\hat{A} e^{-\beta \hat{H}})}{Tr(e^{-\beta \hat{H}})} = \lim_{T \rightarrow 0} \frac{Tr(\hat{A} e^{-\beta \hat{H}})}{Tr(e^{-\beta \hat{H}})} = \frac{\sum_{\sigma} \langle \Psi_g^{\{\sigma}\} | \hat{A} |\Psi_{g,\{\sigma\}}\rangle}{\sum_{\sigma} \langle \Psi_g^{\{\sigma}\} |\Psi_{g,\{\sigma\}}\rangle}.$$ 

(E7)

where $\hat{A}$ is an arbitrary operator and $\hat{H}_g$ is defined in (36). The second equality in (E7) holds since for $N_A < \infty$ excited states of $\hat{H}$ are always separated by a finite energy from the ground state and thus give only exponentially small corrections to the contribution of $\hat{H}_g$. Eq.(E7) therefore yields

$$\langle \hat{C}_{2,k_1\sigma_1}^\dagger \hat{C}_{2,k_2\sigma_2} \rangle = \frac{1}{2} \delta_{k_2,k_1} \delta_{\sigma_1, \sigma_2}.$$ 

(E8)
2. The case $X_k = 0$

Here we consider the case $a_{k^*,d} = 0$ for a given vector $k = k^*$ which implies $X_k = 0$ (we note that the $C_{\delta,k\sigma}$ operators are then still well-defined and $R^{-1}_{k^*} \neq 0$), with $X_k \neq k^* = 0$. Such a situation arises, for example, in the case of the itinerant solution (see Sec.IV.B) for large next-nearest neighbor hopping amplitude $|t_{4d}^d/t_{3a}^d| \leq 3$. Except for $k^*$ remain valid the thermodynamic limit, and the ground state expectation values of the momentum occupation becomes

$$\langle \hat{C}^\dagger_{1,k\sigma} \hat{C}_{1,k\sigma} \rangle = 1, \quad \langle \hat{C}^\dagger_{2,k^*\sigma} \hat{C}_{2,k^*\sigma} \rangle = 0, \quad \langle \hat{C}^\dagger_{2,k\neq k^*\sigma} \hat{C}_{2,k\neq k^*\sigma} \rangle = \frac{1}{2}. \quad (E9)$$

We note that for one vector $k^*$ the maximum total spin decreases from $N_\Lambda/2$ to $N_\Lambda/2 - 1$ since in the sum over $k_n$ in (E1, E2) the term with $k^*$ is missing.

3. Expectation values for correlation functions

A key problem in the calculation of correlation functions is the evaluation of expectation values of products of four $\hat{C}_{2,k\sigma}$ operators. Using (E8) one finds

$$\hat{C}^\dagger_{2,k_3\sigma_3} \hat{C}_{2,k_3\sigma_3} \hat{C}^\dagger_{2,k_4\sigma_4} \hat{C}_{2,k_4\sigma_4} \vert \Psi_{g,\{\sigma'\}} \rangle = \delta_{k_1,k_4} \delta_{\sigma_1,\sigma_4} \sum_{n=1}^{N_\Lambda} \vert \Psi_{g,\{\sigma_1\}, \{\sigma_2\}, \{\sigma_3\}, n} \rangle +$$

$$(1 - \delta_{k_1,k_3} \delta_{\sigma_1,\sigma_3})(1 - \delta_{k_2,k_4} \delta_{\sigma_2,\sigma_4}) \sum_{n=1}^{N_\Lambda} \sum_{m=1, m \neq n}^{N_\Lambda} \vert \Psi_{g,\{\sigma_1\}, \{\sigma_2\}, \{\sigma_3\}, \{\sigma_4\}, m,n} \rangle, \quad (E10)$$

where $k_4 = k_3 + k_1 - k_2$. Here $\vert \Psi_{g,\{\sigma_1\}, \{\sigma_2\}} \rangle$ is defined in (E8), and

$$\vert \Psi_{g,\{\sigma_1\}, \{\sigma_2\}} \rangle = \left[ \prod_{k'} \hat{C}^\dagger_{1,k'} \hat{C}_{1,k'} \right] \left[ \frac{1}{\sqrt{N_\Lambda}} \sum_{k'} X_k e^{ik'_n} \hat{C}^\dagger_{2,k'_\sigma_{m-1}} \hat{C}_{2,k'_\sigma_{m-1}} \right] \left[ \frac{1}{\sqrt{N_\Lambda}} \sum_{k'} X_k e^{ik'_n} \hat{C}^\dagger_{2,k'_\sigma_{n-1}} \hat{C}_{2,k'_\sigma_{n-1}} \right] \left[ \frac{1}{\sqrt{N_\Lambda}} \sum_{k'} X_k e^{ik'_n} \hat{C}^\dagger_{2,k'_\sigma_{n+1}} \hat{C}_{2,k'_\sigma_{n+1}} \right] \cdots$$

$$\left( \frac{1}{\sqrt{N_\Lambda}} \sum_{k'} X_k e^{ik'_n} \hat{C}^\dagger_{2,k'_\sigma_{n+1}} \hat{C}_{2,k'_\sigma_{n+1}} \right) \left( \frac{1}{\sqrt{N_\Lambda}} \sum_{k'} X_k e^{ik'_n} \hat{C}^\dagger_{2,k'_\sigma_{n+1}} \hat{C}_{2,k'_\sigma_{n+1}} \right) \cdots$$

contains only contribution with $n \neq m$. The expectation value of the density–density correlation function can be calculated from (E10), with $\sigma_1 = \sigma_2 = \sigma_a$, $\sigma_3 = \sigma_4 = \sigma_b$, where a
summation $\sum_{\sigma_a} \sum_{\sigma_b}$ has to be included. Introducing the notations $\sigma_{k_3,k_1} = Z_{k_3,k_1}^{k_4,k_2}$, where $Z_{k_3,k_1} = X_{k_4} X_{k_2} / (X_{k_3} X_{k_1} N_A)$, and using the procedure leading to (E6) one then finds

$$\langle \sum_{\sigma_a,\sigma_b} \hat{C}^\dagger_{2,k_3,k_1} \hat{C}_{2,k_4,k_2} \hat{C}^\dagger_{2,k_1,k_3} \hat{C}_{2,k_2,k_4} \rangle = \delta_{k_1,k_4} \delta_{k_2,k_3} + \delta_{k_1,k_2} \delta_{k_3,k_4} - Z_{k_3,k_1} \delta_{k_4,k_3+k_1-k_2}. \quad (E12)$$

The same expression is obtained if we calculate the expectation value in the $T \to 0$ limit, as described in connection with (E7 - E8).

In the case of the spin-spin correlation function for the $S^z$ components one again has $\sigma_1 = \sigma_2 = \sigma_a$ and $\sigma_3 = \sigma_4 = \sigma_b$, but the sum over the spin indices must be separately performed for $\sigma_b = \sigma_a = \sigma$ and $\sigma_b = -\sigma_a = \sigma$. Using (E7 - E10), one finds in the $T \to 0$ limit

$$\langle \sum_{\sigma} \hat{C}^\dagger_{2,k_3,k_1} \hat{C}_{2,k_4,k_2} \hat{C}^\dagger_{2,k_1,k_3} \hat{C}_{2,k_2,k_4} \rangle = \delta_{k_1,k_4} \delta_{k_2,k_3} + \frac{1}{2} \delta_{k_1,k_2} \delta_{k_3,k_4} - \frac{1}{2} Z_{k_3,k_1} \delta_{k_4,k_3+k_1-k_2}.$$

$$\langle \sum_{\sigma} \hat{C}^\dagger_{2,k_3,k_1} \hat{C}_{2,k_4,k_2} \hat{C}^\dagger_{2,k_1,-\sigma} \hat{C}_{2,-\sigma,k_2} \rangle = \frac{1}{2} \delta_{k_1,k_2} \delta_{k_3,k_4} - \frac{1}{2} Z_{k_3,k_1} \delta_{k_4,k_3+k_1-k_2}. \quad (E13)$$

To calculate the spin-spin correlation functions for the $S^x, S^y$ components, (E10) must be evaluated for $\sigma_3 = \sigma_2 = -\sigma_1 = -\sigma_4 = \sigma$, and the summation $\sum_{\sigma}$ must be performed. In the $T \to 0$ limit one finds

$$\langle \sum_{\sigma} \hat{C}^\dagger_{2,k_3,k_1} \hat{C}_{2,k_4,-\sigma} \hat{C}^\dagger_{2,k_1,-\sigma} \hat{C}_{2,-\sigma,k_2} \rangle = \delta_{k_1,k_4} \delta_{k_2,k_3},$$

$$\langle \sum_{\sigma} \hat{C}^\dagger_{1,k_3,k_1} \hat{C}_{2,k_4,-\sigma} \hat{C}^\dagger_{2,k_1,-\sigma} \hat{C}_{1,-\sigma,k_2} \rangle \delta_{k_1,k_4+k_3-k_2} = \delta_{k_2,k_3} \delta_{k_1,k_4}. \quad (E14)$$

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24 As will be discussed in Sec.V. this is not the only possibility to cast the Hamiltonian into positive semi-definite form.
25 Special cases where $S_{\text{max}} < N_\Lambda/2$ will be mentioned in Appendix E.2.
26 Degenerate ground states with different total spin have been discussed before; see for example R. Arita and H. Aoki, Phys. Rev. B. 61, 12261, (2000).
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29 The total spin operator $\hat{S}$ is defined by $\hat{S}^\alpha = \sum_{i=1}^{N_\Lambda} \hat{S}^\alpha_i$, $\alpha = x, y, z$, where $\hat{S}^z_i = \frac{1}{2}(\hat{n}^{d\uparrow}_i - \hat{n}^{d\downarrow}_i + \hat{n}^{f\uparrow}_i - \hat{n}^{f\downarrow}_i)$, $\hat{S}^+_i = (\hat{S}^-_i)^\dagger = \hat{d}^\dagger_{i\uparrow}\hat{d}_{i\downarrow} + \hat{f}^\dagger_{i\uparrow}\hat{f}_{i\downarrow}$, $\hat{S}^{\pm}_i = \hat{S}^x_i \pm i\hat{S}^y_i$. By interchanging $i$ and $k$, similar expressions are obtained in $k$ space, where $\hat{S}^\alpha = \sum_{k=1}^{N_\Lambda} \hat{S}^\alpha_k$.
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31 Eq. 32 has solutions for real $(V_0V_1)$ with $t^d_2 < 0$ and $(V_0V_1)/t^d_1 < 0$, arbitrary $|t^d_1|, |t^d_2|, V_1 =
Using (35) one obtains \( \hat{\mathbf{P}} \) which have the form \( a_{2,d} = a_{4,d} = a_{5,d} \). In particular, one finds
\[
a_{1,d} = (|t_1^d|/|t_2^d|) e^{i\phi}, \quad a_{2,d} = -\text{sign}(t_1^d)|t_1^d| \sqrt{|t_2^d|} e^{-i\phi},
\]
where \( \phi \) is an arbitrary phase. For complex \( V_k \) a solution of the form \( V_k = V_0 + \sum_{\tau=1}^3 \exp(i k_{\tau}) \), emerges (see (33)) where \( k_{\tau} = \mathbf{k} \mathbf{x}_\tau \). Since \( t_{x+1}^d - t_{x-1}^d \neq 0 \), \( \tau > \tau' \), this requires anisotropic hopping parameters.

32 For the operators \( \hat{C}_{\delta,k,\sigma} \) to be well-defined, \( R_k^{-1} \) has to be nonzero for all \( k \). This holds for both itinerant solutions discussed in Sec.IV (see (33)). For example, for the solution obtained in Sec.IV.B., one finds \( |a_{k,f}|^2 = |a_{f}|^2 = |V_1|^2/|t_2^d| \), \( |a_{k,d}|^2 = |t_2^d||t_1^d|/|t_1^d| - \text{sign}(t_1^d)(\sum_{\tau=1}^3 \cos k_\tau)^2 + (\sum_{\tau=1}^3 \sin k_\tau)^2 \). Using (33) one obtains \( \hat{d}_{k,\sigma} = \sqrt{R_k} (a_{k,d} \hat{C}_{1,k,\sigma} + a_{k,f} \hat{C}_{2,k,\sigma}) \), \( \hat{f}_{k,\sigma} = \sqrt{R_k} (a_{k,f} \hat{C}_{1,k,\sigma} - a_{k,d} \hat{C}_{2,k,\sigma}) \).

34 The first equality in (35) leads to \( -\sum_{\sigma} \hat{d}_{i,\sigma} \hat{A}_{i,\sigma} = \sum_{\sigma} (1/R_k) \hat{C}_{1,k,\sigma} \hat{C}_{1,k,\sigma} \).

35 Using (33) this leads to \( -\sum_{\sigma} \hat{d}_{i,\sigma} \hat{A}_{i,\sigma} = \sum_{\delta=1,2} \hat{C}_{\delta,k,\sigma} \hat{C}_{\delta,k,\sigma} \).

36 For example, we can choose \( D_1 \) to be defined by the set \( \{x_1, x_2, 2x_3\} \) of primitive vectors, and \( \mathbf{R} = x_3 \).

37 The consequences of \( |a_{k,d}| = 0 \) with \( R_k \neq 0 \) are pointed out in Appendix E.2.

38 There exist special cases (see, e.g., Sec.IV.B for \( |t_1^d/t_2^d| < 3 \) and footnote (32)) where for some vector \( \mathbf{k}^* \) one has \( a_{k^*,d} = 0 \) and hence \( X_{k^*,k^*} = 0 \). Nevertheless, as long as \( R_k^{-1} \neq 0 \) for all \( k \), the operators \( \hat{C}_{\delta,k,\sigma} \) are well-defined, and itinerant solutions are still possible. In this case (see the second equality in (E9)), the momentum distribution function will have a discontinuity at a single point, i.e., \( \langle \hat{C}_{2,k,\sigma}^\dagger \hat{C}_{2,k,\sigma} \rangle \) is 1/2 for all \( k \), except for \( k^* \) where it is zero.

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Another possibility to define a cell operator is discussed in Ref.\[19\] for 2D. In this case a local-
ized phase is obtained without third neighbor contributions of the hopping and hybridization
amplitudes.

Eq.\((55)\) has solutions only for real \(V_{x_r}\), \(t_{2x_2}^d < 0\), with \(\text{sign}(V_{x_r})\text{sign}(Re(V_0)) = -\text{sign}(t_{2x_2}^d)\),
real or complex values of \(V_0 = |V_0|e^{i\phi_V}\), with \(Re(V_0) = -t_{1}^d V_1/|t_{2}^d|\) and arbitrary \(Im(V_0)\).

In the isotropic case when \(t_{1}^d = t_{x_1}^d = t_{x_2}^d = t_{x_3}^d, t_{2}^d = t_{x_r=0}^d\), \(V_1 = V_{x_1} = V_{x_2} = V_{x_3}\),
\(t_{2}^d = t_{2x_2}^d = t_{2x_3}^d\), one finds \(a_{1,d} = a_{2,d} = a_{3,d} = a_{4,d} = a_{5,d} = a_{7,d}\).

The \(a_{k,b}\) parameters presented in \[51\], are now defined by the Fourier transform of \(\hat{B}_{\delta_{1,\sigma}}\)
which have the form \(\hat{B}_{\delta_{1,\sigma}} = \sum_{b=d,f} a_{k,b,s}^* \hat{b}_{\delta_{1,\sigma}}\), where \(a_{k,f} = a_{6,f}\), and
\(a_{k,d} = a_{6,d} + a_{3,d}e^{-i\delta_{x_1}} + a_{2,d}e^{-i\delta_{x_2}} + a_{3,d}e^{+i\delta_{x_1}} + a_{4,d}e^{-i\delta_{x_2}} + a_{5,d}e^{-i\delta_{x_3}} + a_{5,d}e^{+i\delta_{x_3}}\). For the solution defined below
\[57\], one finds \(a_{k,d} = \sqrt{2|t_{2}^d|^2}e^{i\phi}([\sum_{\tau=1}^{3} \cos k_\tau] + (|V_0|/|2V_1|)e^{-i\phi_V})\) \(a_{k,f} = -V_1 \sqrt{2|t_{2}^d|^2}e^{i\phi}\). The
parameters \(R_{-1}^{-1}\), \(|a_{k,f}|\) are nonzero for all \(k\); (see \[55\]), so the operators \(\hat{C}_{\delta_{1,\sigma}}\) are well-defined.

For real \(V_0\) one finds \(|a_{k,d}| \neq 0\) for \(|t_{1}^d/t_{2}^d| > 6\), while for \(Im(V_0) \neq 0\) one always has \(|a_{k,d}| > 0\).
We note that \(a_{k,d} \neq 0\) implies \(X_k \neq 0\), where \(X_k\) has been defined in \[12\].

Complementary anti-commuting operators, but with additional constraints on lattice site, have
previously been employed in the construction of exact ground states corresponding to extended
spiral structures of the 1D Hubbard model\[52\], and for ferromagnetism on decorated lattices\[53\].

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The proof of the finite conductivity starts from the observation that the ground state \[61\] can
be generalized beyond quarter filling via \[65\] , see Sect.V.B.2. Using \(E'_g\) from \(58\), one finds
\(\mu^+ = E'_g(N) - E'_g(N-1) = K_d\) , \(\mu^- = E'_g(N-1) - E'_g(N-2) = K_d\), i.e. \(\mu^+ - \mu^- = 0\).
Consequently, the described state is conducting\[39\].

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FIG. 1: A unit cell $I_i$ connected to an arbitrary site $i$ showing the primitive vectors $x_r$ and indices $n$ of the sites in $I$. Arrows depict some of the hopping and hybridization amplitudes ($J = t, V$) defined within $I_i$. 
FIG. 2: Ground state energy per lattice site, $E_g/N_{\Lambda}$, in units of $U$ as a function of $y = |t_2^d/t_1^d|$ for the localized solution in a simple cubic crystal for $|t_1^f/t_1^d| = 0.01$. As seen from the plot, $E_g/N_{\Lambda}$ is finite at $y_c = 1/2$ but has infinite slope.
FIG. 3: Surface in parameter space representing the stability region of the conducting ground state discussed in Sec.IV.A.

FIG. 4: Tilted unit cell located at site i discussed in Sec.IV.B. Numbers represent the intra-cell numbering of lattice sites. Only those bonds are presented along which hopping of d electrons occurs.
FIG. 5: Surface in parameter space representing the stability region of the itinerant solution derived in the case of the conventional PAM, \textsuperscript{BM}. For \(|t_2^d/t_1^d| \rightarrow 0\), the surface asymptotically approaches the \((|V_1/t_1^d|, (U + E_f)/|t_1^d|)\) plane.
FIG. 6: Momentum distribution functions $n^d_{k,\sigma}$, $n^f_{k,\sigma}$ for the conducting solution discussed in Section IV.B, for $|t_1^d|/|t_2^d| = 5.0$, $|V_1|/|t_1^d| = 0.5$, $t_1^d > 0$, and $k_2 = k_3 = 0$, where $k_\tau = k x_\tau$. The plot presents the behavior in the first Brillouin zone for $k_1 \in [-\pi, \pi]$. For other $k$ directions a similar behavior is found.
FIG. 7: Density-density correlation function for $|t^d_1/t^d_2| = 4$, $|V_1/t^d_1| = 0.25$, $t^d_1 > 0$ for the itinerant case obtained from (49) in the thermodynamic limit. The nine-dimensional integration was performed by a Monte Carlo method using 69 points. The distance $r$ was taken in $\tau = 1$ direction, and is expressed in units of the lattice constant $a$. 
FIG. 8: Octahedral cell defined at lattice site $i$ as discussed in Section V.A. The $\tau = 1, 2, 3$ axes are represented by arrows with broken lines, $x_{\tau}$ are indicated by thick full line arrows, and $n$ represents the cell independent notation of sites inside the octahedron.
FIG. 9: Surfaces in parameter space above which the conducting phase discussed in Section V.A. is stable. a) $|V_1|/|t_1^d| < 0.5$; $(U + E_f)/|t_1^d|$ is seen to diverge as $|t_3^d|/|t_1^d|$ approaches zero. b) $|V_1|/|t_1^d| > 0.5$. In contrast to Fig.5 where $V_1$ is imaginary, $V_1$ is real here.
FIG. 10: Four neighboring unit cells in $D = 3$. Each cell (e.g., $I_i$) is denoted by one of the lattice sites at which it is located (e.g., $i$); see Sec. II.B.1. For simplicity, orthorhombic unit cells are used.