

Exact ground states of the periodic Anderson model in $D=3$ dimensions

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(Received 8 April 2005; published 23 August 2005)

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 nonlocal 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 semidefinite form using composite operators in combination with coupled nonlinear 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 nonlocal 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 nonmagnetic 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.

DOI: [10.1103/PhysRevB.72.075130](https://doi.org/10.1103/PhysRevB.72.075130)

PACS number(s): 71.10.Hf, 05.30.Fk, 67.40.Db, 71.10.Pm

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.¹ 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,²⁻⁴ (ii) nonlocal contributions to the hybridization, and (iii) hopping of the d electrons beyond nearest neighbors.⁵

Recently the PAM was employed to study the dramatic volume collapse at the $\alpha \rightarrow \gamma$ transition in cerium compounds.⁶⁻⁸ 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 hopping⁹ and the PAM with nearest-neighbor hybridization and d hopping⁹⁻¹² 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 situation exact results on the existence of insulating and metallic phases in the PAM and their dependence on the hopping, hybridization, and interaction parameters are particularly desirable—especially in three dimensions. So far exact results for the PAM were mostly limited to special regions of parameter space, namely, for infinite repulsion of the f electrons,¹³⁻¹⁵ and for finite repulsion in low dimensions $D=1, 2$.¹⁶⁻¹⁹

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,²⁰ (ii) explicitly present and analyze the nonlinear 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 semidefinite form, one arrives at exact ground states in different regions of the parameter space.

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

$$\hat{H} = \hat{H}_0 + \hat{H}_U, \quad (1a)$$

$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} [(\epsilon_{\mathbf{k}}^d \hat{n}_{\mathbf{k}\sigma}^d + \epsilon_{\mathbf{k}}^f \hat{n}_{\mathbf{k}\sigma}^f) + (V_{\mathbf{k}} \hat{d}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} + V_{\mathbf{k}}^* \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{d}_{\mathbf{k}\sigma})], \quad (1b)$$

$$\hat{H}_U = U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i},\uparrow}^f \hat{n}_{\mathbf{i},\downarrow}^f. \quad (1c)$$

We denote the two types of electrons by $b=d, f$, i.e., $\hat{b}_{\mathbf{k}\sigma}^\dagger$ creates a b ($=d, f$) electron with momentum \mathbf{k} and spin σ . The corresponding particle number operators are $\hat{n}_{\mathbf{k}\sigma}^b = \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma}$, and the dispersion relations of the b electrons are given by $\epsilon_{\mathbf{k}}^b$. Furthermore, the hybridization amplitude and the local (Hubbard) interaction are denoted by $V_{\mathbf{k}}$ 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 $\{\mathbf{x}_\tau\}$, $\tau=1, 2, 3$. The noninteracting part of the Hamiltonian \hat{H}_0 reads

$$\begin{aligned} \hat{H}_0 = \sum_{\mathbf{i}, \sigma} \left(\sum_{\mathbf{r}} [(t_{\mathbf{r}}^d \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma} + t_{\mathbf{r}}^f \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma}) + (V_{\mathbf{r}}^{d,f} \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma} \right. \\ \left. + V_{\mathbf{r}}^{f,d} \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma}) + \text{H.c.}] + (V_0 \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma} + \text{H.c.}) + E_f \hat{n}_{\mathbf{i},\sigma}^f \right), \end{aligned} \quad (2)$$

where $t_{\mathbf{r}}^b$ characterizes the hopping of b electrons between sites \mathbf{i} and $\mathbf{i}+\mathbf{r}$, $V_{\mathbf{r}}^{b,b'}$ is the hybridization of b and b' electrons at sites \mathbf{i} and $\mathbf{i}+\mathbf{r}$, V_0 is the on-site hybridization, and E_f is the local on-site f -electron energy. The separation between a site \mathbf{i} and its neighbors in the unit cell is denoted by \mathbf{r} , with $\mathbf{r} \neq \mathbf{0}$. While the amplitudes $t_{\mathbf{r}}^b$ are real, $V_0, V_{\mathbf{r}}^{b,b'}$ can, in principle, be complex (whether $V_{\mathbf{r}}^{b,b'}$ is real, imaginary, or complex depends on the linear combination of the corresponding electronic orbitals and hence on the lattice symmetry^{9,18,21–23}) and obey the relations

$$\epsilon_{\mathbf{k}}^b = E_f \delta_{b,f} + \sum_{\mathbf{r}} (t_{\mathbf{r}}^b e^{-i\mathbf{k}\mathbf{r}} + t_{\mathbf{r}}^{b*} e^{+i\mathbf{k}\mathbf{r}}), \quad (3)$$

$$V_{\mathbf{k}} = V_0 + \sum_{\mathbf{r}} (V_{\mathbf{r}}^{d,f} e^{-i\mathbf{k}\mathbf{r}} + V_{\mathbf{r}}^{f,d*} e^{+i\mathbf{k}\mathbf{r}}).$$

In particular, for $t_{\mathbf{r}}^f=0$, 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 \mathbf{i} in Eq. (2) is indicated by the vector \mathbf{r} which corresponds to neighboring sites located in different coordination spheres. In our investigation \mathbf{r} may

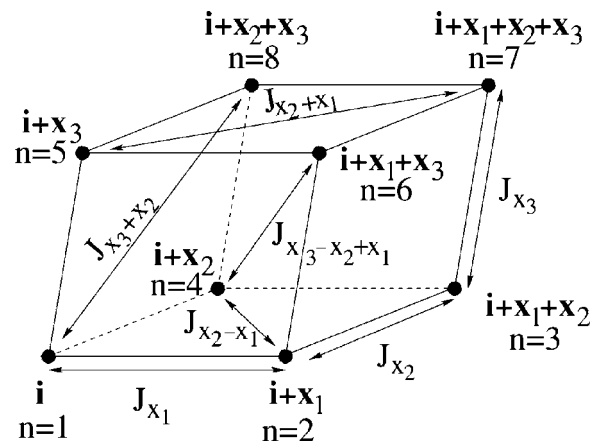


FIG. 1. A unit cell I_i connected to an arbitrary site \mathbf{i} showing the primitive vectors \mathbf{x}_τ and indices n of the sites in I . Arrows depict some of the hopping and hybridization amplitudes ($J=t, V$) defined within I_i .

extend over a *unit cell* I of a general Bravais lattice in $D=3$. This implies 26 different intersite hopping and nonlocal hybridization amplitudes. To avoid multiple counting of contributions by the H.c. term in Eq. (2) the vector \mathbf{r} must be properly defined. To this end the sites within I_i , the unit cell defined at site \mathbf{i} , are denoted by $\mathbf{r}_{I_i} = \mathbf{i} + \mathbf{r}_{\alpha\beta\gamma}$ with $\mathbf{r}_{\alpha\beta\gamma} = \alpha\mathbf{x}_1 + \beta\mathbf{x}_2 + \gamma\mathbf{x}_3$; $\alpha, \beta, \gamma=0, 1$. As shown in Fig. 1 the eight sites \mathbf{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 $\mathbf{r} = \mathbf{r}_{\alpha'\beta'\gamma'} - \mathbf{r}_{\alpha\beta\gamma}$ 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 $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_2 \pm \mathbf{x}_1, \mathbf{x}_3 \pm \mathbf{x}_1, \mathbf{x}_3 \pm \mathbf{x}_2, \mathbf{x}_3 \pm \mathbf{x}_2 \pm \mathbf{x}_1$. The remaining (negative) values of \mathbf{r} are taken into account in Eq. (2) by the H.c. contributions.

2. Transformation of \hat{H} into positive semidefinite form

To construct exact ground states the Hamiltonian \hat{H} needs to be rewritten in terms of positive semidefinite operators. This is made possible²⁴ 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” $\hat{A}_{I_i, \sigma}^\dagger$ which represents a superposition of fermionic operators creating d or f electrons with spin σ inside every unit cell I_i as

$$\begin{aligned} \hat{A}_{I_i, \sigma}^\dagger &= \sum_{n(\alpha, \beta, \gamma)=1}^8 (a_{n,d}^* \hat{d}_{\mathbf{i}+\mathbf{r}_{\alpha, \beta, \gamma}, \sigma}^\dagger + a_{n,f}^* \hat{f}_{\mathbf{i}+\mathbf{r}_{\alpha, \beta, \gamma}, \sigma}^\dagger) \\ &= (a_{1,d}^* \hat{d}_{\mathbf{i}, \sigma}^\dagger + a_{2,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_1, \sigma}^\dagger + a_{3,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_1+\mathbf{x}_2, \sigma}^\dagger + a_{4,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_2, \sigma}^\dagger \\ &\quad + \cdots + a_{8,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_2+\mathbf{x}_3, \sigma}^\dagger) + (a_{1,f}^* \hat{f}_{\mathbf{i}, \sigma}^\dagger + a_{2,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_1, \sigma}^\dagger \\ &\quad + a_{3,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_1+\mathbf{x}_2, \sigma}^\dagger + a_{4,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_2, \sigma}^\dagger + \cdots + a_{8,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_2+\mathbf{x}_3, \sigma}^\dagger). \end{aligned} \quad (4)$$

Because of the translational symmetry of the lattice, the nu-

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

$$(\hat{A}_{I, \sigma}^\dagger)^2 = 0, \quad (5a)$$

$$-\hat{A}_{I, \sigma}^\dagger \hat{A}_{I, \sigma} = \hat{A}_{I, \sigma} \hat{A}_{I, \sigma}^\dagger - (K_d + K_f). \quad (5b)$$

The second operator \hat{P} originates from the relation $\sum_i \hat{n}_{i, \uparrow}^f \hat{n}_{i, \downarrow}^f = \hat{P} + \sum_{i, \sigma} \hat{n}_{i, \sigma}^f - N_\Lambda$, where

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

and N_Λ is the number of lattice sites. The local operators \hat{P}_i are positive semidefinite 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 semidefinite 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 \mathbf{r} to take only the values discussed above, Eqs. (1a) and (2) may be written as

$$\hat{H} = \hat{P}_A + U\hat{P} + E_g, \quad (7)$$

where $\hat{P}_A = \sum_{i, \sigma} \hat{A}_{I_i, \sigma} \hat{A}_{I_i, \sigma}^\dagger$, $E_g = K_d N + U N_\Lambda - 2 N_\Lambda (2K_d - E_f)$, and N is the total number of particles, which is assumed to be fixed.

For Eq. (7) to reproduce Eq. (1a) prefactors $a_{n,b}^*$ in $\hat{A}_{I_i, \sigma}^\dagger$ must be expressed in terms of the microscopic parameters $t_{\mathbf{r}}^d$, $t_{\mathbf{r}}^f$, $V_{\mathbf{r}}$, $V_{\mathbf{r}}^*$, V_0 , V_0^* , E_f , and U , for all $\mathbf{r} \in I_i$, taking into account periodic boundary conditions. This leads to 55 coupled, non-linear matching conditions which can be written in compact notation as²⁰

$$\sum_{\beta_1, \beta_2, \beta_3 = -1}^1 \left(\prod_{\alpha=1}^3 D_{\beta, \alpha} \right) a_{n^+, b}^* a_{n^-, b'} = T_{\mathbf{r}, v}^{b, b'}.$$

These matching conditions have the explicit forms

$$J_{\mathbf{x}_1}^{b, b'} = a_{1, b}^* a_{2, b'} + a_{4, b}^* a_{3, b'} + a_{5, b}^* a_{6, b'} + a_{8, b}^* a_{7, b'},$$

$$J_{\mathbf{x}_2 + \mathbf{x}_1}^{b, b'} = a_{1, b}^* a_{3, b'} + a_{5, b}^* a_{7, b'},$$

$$J_{\mathbf{x}_2}^{b, b'} = a_{1, b}^* a_{4, b'} + a_{2, b}^* a_{3, b'} + a_{6, b}^* a_{7, b'} + a_{5, b}^* a_{8, b'},$$

$$J_{\mathbf{x}_3 + \mathbf{x}_1}^{b, b'} = a_{1, b}^* a_{6, b'} + a_{4, b}^* a_{7, b'},$$

$$J_{\mathbf{x}_3}^{b, b'} = a_{1, b}^* a_{5, b'} + a_{2, b}^* a_{6, b'} + a_{3, b}^* a_{7, b'} + a_{4, b}^* a_{8, b'},$$

$$J_{\mathbf{x}_3 + \mathbf{x}_2}^{b, b'} = a_{1, b}^* a_{8, b'} + a_{2, b}^* a_{7, b'},$$

$$J_{\mathbf{x}_2 - \mathbf{x}_1}^{b, b'} = a_{2, b}^* a_{4, b'} + a_{6, b}^* a_{8, b'},$$

$$J_{\mathbf{x}_3 - \mathbf{x}_1}^{b, b'} = a_{2, b}^* a_{5, b'} + a_{3, b}^* a_{8, b'},$$

$$J_{\mathbf{x}_3 - \mathbf{x}_2}^{b, b'} = a_{4, b}^* a_{5, b'} + a_{3, b}^* a_{6, b'},$$

$$J_{\mathbf{x}_3 + \mathbf{x}_2 + \mathbf{x}_1}^{b, b'} = a_{1, b}^* a_{7, b'}, \quad J_{\mathbf{x}_3 + \mathbf{x}_2 - \mathbf{x}_1}^{b, b'} = a_{2, b}^* a_{8, b'},$$

$$J_{\mathbf{x}_3 - \mathbf{x}_2 + \mathbf{x}_1}^{b, b'} = a_{4, b}^* a_{6, b'},$$

$$J_{\mathbf{x}_3 - \mathbf{x}_2 - \mathbf{x}_1}^{b, b'} = a_{3, b}^* a_{5, b'}, \quad V_0 = - \sum_{n=1}^8 a_{n,d}^* a_{n,f}, \quad U + E_f = K_d - K_f, \quad (8)$$

where $J_{\mathbf{r}}^{b, b'} = -[\delta_{b, b'} t_{\mathbf{r}}^b + (1 - \delta_{b, b'}) V_{\mathbf{r}}^{b, b'}]$, $b, b' = d, f$.

Details of this transformation are presented in Appendix A.

C. Construction of exact ground states

Apart from the constant term E_g in Eq. (7) \hat{H} is a positive semidefinite operator. A state $|\Psi_g\rangle$ which satisfies the conditions

$$\hat{P}_i |\Psi_g\rangle = 0, \quad (9a)$$

$$\hat{A}_{I_i, \sigma}^\dagger |\Psi_g\rangle = 0 \quad (9b)$$

for all i , and which contains all linearly independent states with properties (9a) and (9b), 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 (9a) and (9b) 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

$$\mathcal{H}_g = \ker(\hat{P}_A) \cap \ker(\hat{P}). \quad (10)$$

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 Eqs. (6) and (9a) it follows that $\ker(\hat{P})$ is defined by states $\hat{F}^\dagger |0\rangle = \prod_{i=1}^{N_\Lambda} \hat{F}_i^\dagger |0\rangle$, where $\hat{F}_i^\dagger = (\mu_{i, \uparrow} \hat{f}_{i, \uparrow}^\dagger + \mu_{i, \downarrow} \hat{f}_{i, \downarrow}^\dagger)$ and $\mu_{i, \sigma}$ are arbitrary coefficients. Obviously \hat{F}^\dagger creates one f

electron on every site \mathbf{i} . Furthermore, Eqs. (5a) and (9b) imply that $\ker(\hat{P}_A)$ is defined by states $\hat{G}^\dagger|0\rangle$, where $\hat{G}^\dagger = \prod_{\mathbf{i}=1}^{N_\Lambda} (\hat{A}_{I_{\mathbf{i},\uparrow}}^\dagger \hat{A}_{I_{\mathbf{i},\downarrow}}^\dagger)$ creates at most two (d or f) electrons on \mathbf{i} . Since \hat{G}^\dagger also creates contributions without f electrons, Eq. (10) implies the (unnormalized) ground state

$$|\Psi_g\rangle = \hat{G}^\dagger \hat{F}^\dagger |0\rangle = \prod_{\mathbf{i}=1}^{N_\Lambda} [\hat{A}_{I_{\mathbf{i},\uparrow}}^\dagger \hat{A}_{I_{\mathbf{i},\downarrow}}^\dagger \hat{F}_{\mathbf{i}}^\dagger] |0\rangle \quad (11)$$

at $N=3N_\Lambda$, 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 Eq. (7), i.e., the Hubbard interaction U , $|\Psi_g\rangle$ can only be a ground state for $U > 0$.

Equation (11) implies that (i) the linearly independent basis vectors of \mathcal{H}_g have the form $|\Psi_g\{\sigma_{\mathbf{i}}\}\rangle = \hat{G}^\dagger \hat{F}_{\{\sigma_{\mathbf{i}}\}}^\dagger |0\rangle$, where $\hat{F}_{\{\sigma_{\mathbf{i}}\}}^\dagger = \prod_{\mathbf{i}=1}^{N_\Lambda} \hat{f}_{\mathbf{i},\sigma_{\mathbf{i}}}^\dagger$, and (ii) \hat{G}^\dagger does not contribute to the total spin of the ground state. The overall degeneracy and total spin $S \in [0, N_\Lambda/2]$ of $|\Psi_g\rangle$ are then determined only by the (arbitrary) set of coefficients $\mu_{\mathbf{i},\sigma}$ (see also Secs. III A 2 and IV E and Ref. 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 nonmagnetic.²⁶

Exact ground states can also be constructed away from 3/4 filling. For example, the operator $\hat{V}_M^\dagger = \prod_{\mathbf{j}=1}^M (\sum_{\mathbf{i}=1}^{N_\Lambda} \sum_{b=d,f,\sigma} a_{\mathbf{i},\mathbf{j},\sigma}^b \hat{b}_{\mathbf{i},\sigma}^\dagger)$ with numerical coefficients $a_{\mathbf{i},\mathbf{j},\sigma}^b$ creates $M < N_\Lambda$ additional particles in the system such that

$$|\Psi_g\rangle = \prod_{\mathbf{i}=1}^{N_\Lambda} [\hat{A}_{I_{\mathbf{i},\uparrow}}^\dagger \hat{A}_{I_{\mathbf{i},\downarrow}}^\dagger \hat{F}_{\mathbf{i}}^\dagger] \hat{V}_M^\dagger |0\rangle \quad (12)$$

is a ground state for $U > 0$ and $N > 3N_\Lambda$.

III. EXACT LOCALIZED GROUND STATE

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

A. Derivation of the localized ground state

From Eq. (4) it follows that if $a_{n,d}^*$ and $a_{n,f}^*$ are proportional, i.e., $a_{n,d}^* = p a_{n,f}^*$ for all n , the operators $\hat{A}_{I_{\mathbf{i},\sigma}}^\dagger$ take the form

$$\hat{A}_{I_{\mathbf{i},\sigma}}^\dagger = \sum_{n(\alpha,\beta,\gamma)=1}^8 a_{n(\alpha,\beta,\gamma)}^* E_{\mathbf{i}+\mathbf{r}_{\alpha,\beta,\gamma},\sigma}^\dagger \quad (13)$$

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

$$|\Psi_{loc}\rangle = \prod_{\mathbf{i}=1}^{N_\Lambda} \left(\sum_{\sigma} \mu_{\mathbf{i},\sigma} (p \hat{d}_{\mathbf{i},\downarrow}^\dagger \hat{d}_{\mathbf{i},\uparrow}^\dagger \hat{f}_{\mathbf{i},\sigma}^\dagger + \hat{f}_{\mathbf{i},\uparrow}^\dagger \hat{f}_{\mathbf{i},\downarrow}^\dagger \hat{d}_{\mathbf{i},\sigma}^\dagger) \right) |0\rangle. \quad (14)$$

Since $\langle \Psi_{loc} | \Psi_{loc} \rangle = (1 + |p|^2)^{N_\Lambda} \prod_{\mathbf{i}=1}^{N_\Lambda} (|\mu_{\mathbf{i},\uparrow}|^2 + |\mu_{\mathbf{i},\downarrow}|^2) \neq 0$ 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 $\hat{n}_{\mathbf{i}} = \sum_{b=d,f} \sum_{\sigma} \hat{n}_{\mathbf{i},\sigma}^b$ one finds $\hat{n}_{\mathbf{i}} |\Psi_{loc}\rangle = 3 |\Psi_{loc}\rangle$. Denoting ground-state expectation values in terms of $|\Psi_{loc}\rangle$ by $\langle \dots \rangle$, one obtains

$$\begin{aligned} \langle \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{j},\sigma'} \rangle &= 0, & \langle \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{j},\sigma'} \rangle &= 0, \\ \langle \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{j},\sigma'} \rangle &= 0, & \langle \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{j},\sigma'} \rangle &= 0, \end{aligned} \quad (15)$$

for all σ, σ' and all $\mathbf{i} \neq \mathbf{j}$. Hence hopping or nonlocal hybridization does not occur.

By separating the Hamiltonian \hat{H} into an itinerant part $\hat{H}_{itin} = \sum_{\mathbf{r}} \hat{H}_{itin}(\mathbf{r})$ and a complementary localized part $\hat{H}_{loc} = \hat{H} - \hat{H}_{itin}$ (see Appendix B), and using Eq. (15), one finds $\langle \hat{H}_{itin}(\mathbf{r}) \rangle = 0$ for all \mathbf{r} , and $\langle \hat{H}_{loc} \rangle = E_g$. This clearly demonstrates the localized nature of the ground state. Furthermore, from Eq. (B3), 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 $\text{Re } \sigma_{\tau,\tau}(\omega) = 0$. In particular, $\text{Re } \sigma_{\tau,\tau}(0) = 0$, the dc conductivity, is also zero. The ground state (14) is therefore insulating.^{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 ($\hat{d}_{\mathbf{i},\uparrow}^\dagger \hat{d}_{\mathbf{i},\downarrow}^\dagger \hat{f}_{\mathbf{i},\sigma}^\dagger$) and two f and one d electron ($\hat{f}_{\mathbf{i},\uparrow}^\dagger \hat{f}_{\mathbf{i},\downarrow}^\dagger \hat{d}_{\mathbf{i},\sigma}^\dagger$) on every site \mathbf{i} .

A state with $\text{Re } \sigma_{\tau,\tau}(\omega) = 0$ for all ω 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 $\text{Re } \sigma_{\tau,\tau}(\omega) = 0$ 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 ω .

2. Global magnetic properties

The expectation value of the spin²⁹ in terms of the ground state (14) in Cartesian coordinates is found as

$$\begin{aligned} \langle \hat{\mathbf{S}} \rangle &= \mathbf{x} \sum_{\mathbf{i}=1}^{N_\Lambda} \frac{\mu_{\mathbf{i},\downarrow} \mu_{\mathbf{i},\uparrow}^* + \mu_{\mathbf{i},\uparrow} \mu_{\mathbf{i},\downarrow}^*}{2(|\mu_{\mathbf{i},\uparrow}|^2 + |\mu_{\mathbf{i},\downarrow}|^2)} + \mathbf{y} \sum_{\mathbf{i}=1}^{N_\Lambda} \frac{(-i)(\mu_{\mathbf{i},\downarrow} \mu_{\mathbf{i},\uparrow}^* - \mu_{\mathbf{i},\uparrow} \mu_{\mathbf{i},\downarrow}^*)}{2(|\mu_{\mathbf{i},\uparrow}|^2 + |\mu_{\mathbf{i},\downarrow}|^2)} \\ &\quad + \mathbf{z} \sum_{\mathbf{i}=1}^{N_\Lambda} \frac{|\mu_{\mathbf{i},\uparrow}|^2 - |\mu_{\mathbf{i},\downarrow}|^2}{2(|\mu_{\mathbf{i},\uparrow}|^2 + |\mu_{\mathbf{i},\downarrow}|^2)}, \end{aligned} \quad (16)$$

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

$$\langle \hat{\mathbf{S}}^2 \rangle = \frac{N_\Lambda}{2} \left(\frac{N_\Lambda}{2} + 1 \right), \quad \langle \hat{S}^z \rangle = \frac{N_\Lambda (|\mu_\uparrow|^2 - |\mu_\downarrow|^2)}{2 (|\mu_\uparrow|^2 + |\mu_\downarrow|^2)}, \quad (17)$$

which represents a ferromagnetic state with maximal total spin $S/N_\Lambda = 1/2$, leading to $\sqrt{\langle \hat{\mathbf{S}}^2 \rangle}/N_\Lambda = 1/2$ in the thermodynamic limit; μ_σ 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 $N_\Lambda/2$. Taking $\mu_{i,\sigma} = \mu_\sigma$, $\mu_{i,-\sigma} = 0$ in each subsystem one finds

$$\frac{\sqrt{\langle \hat{\mathbf{S}}^2 \rangle}}{N_\Lambda} = \frac{1}{\sqrt{2N_\Lambda}}, \quad \langle \hat{S}^x \rangle = \langle \hat{S}^y \rangle = \langle \hat{S}^z \rangle = 0, \quad (18)$$

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 $\langle \hat{n}_{i,\uparrow}^b \hat{n}_{i,\downarrow}^b \rangle = (\delta_{b,f} + |p|^2 \delta_{b,d}) / (1 + |p|^2)$. Consequently, each site carries a local moment. Indeed, irrespective of the values of $\mu_{i,\sigma}$ and p one has $\langle \hat{\mathbf{S}}_i^2 \rangle = 3/4$ on each site \mathbf{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

$$\begin{aligned} (\langle \hat{\mathbf{S}}_{i,f} \rangle + \langle \hat{\mathbf{S}}_{i,d} \rangle) \left(\sum_{\sigma} |\mu_{i,\sigma}|^2 \right) &= \mathbf{x} \operatorname{Re}(\mu_{i,\downarrow} \mu_{i,\uparrow}^*) + \mathbf{y} \operatorname{Im}(\mu_{i,\downarrow} \mu_{i,\uparrow}^*) \\ &+ \mathbf{z} \frac{|\mu_{i,\uparrow}|^2 - |\mu_{i,\downarrow}|^2}{2}, \end{aligned} \quad (19)$$

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

$$\langle \hat{S}_i^z \hat{S}_j^z \rangle = \frac{1}{4} \frac{|\mu_{i,\uparrow}|^2 - |\mu_{i,\downarrow}|^2}{|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2} \frac{|\mu_{j,\uparrow}|^2 - |\mu_{j,\downarrow}|^2}{|\mu_{j,\uparrow}|^2 + |\mu_{j,\downarrow}|^2}, \quad (20)$$

$$\langle \hat{S}_i^+ \hat{S}_j^- \rangle = \frac{\mu_{i,\downarrow} \mu_{i,\uparrow}^*}{|\mu_{i,\uparrow}|^2 + |\mu_{i,\downarrow}|^2} \frac{\mu_{j,\uparrow} \mu_{j,\downarrow}^*}{|\mu_{j,\uparrow}|^2 + |\mu_{j,\downarrow}|^2}.$$

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

B. Solutions of the matching conditions

The matching conditions (8) for the nonlocal hybridization amplitudes along the space diagonals of the unit cell read

$$\begin{aligned} -V_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1} &= a_{1,d}^* a_{7,f} = a_{1,f}^* a_{7,d}, \\ -V_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1} &= a_{2,d}^* a_{8,f} = a_{2,f}^* a_{8,d}, \\ -V_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1} &= a_{4,d}^* a_{6,f} = a_{4,f}^* a_{6,d}, \\ -V_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1} &= a_{3,d}^* a_{5,f} = a_{3,f}^* a_{5,d}. \end{aligned} \quad (21)$$

They hold for all $\{\mathbf{x}_\tau\}$, $\tau=1, 2, 3$, and hence imply $a_{n,d}^*/a_{n,f}^* = a_{n',d}/a_{n',f} = p = p^*$. Since for real p , Eq. (8) leads to the relations

$$t_{\mathbf{r}}^f = \frac{t_{\mathbf{r}}^d}{p^2}, \quad V_{\mathbf{r}} = \frac{t_{\mathbf{r}}^d}{p}, \quad \frac{U + E_f}{V_0} = \frac{1 - p^2}{p}, \quad (22)$$

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

$$\begin{aligned} -t_{\mathbf{x}_1}^d &= a_{1,d}^* a_{2,d} + a_{8,d}^* a_{7,d} + a_{4,d}^* a_{3,d} + a_{5,d}^* a_{6,d}, \\ -t_{\mathbf{x}_2}^d &= a_{1,d}^* a_{4,d} + a_{6,d}^* a_{7,d} + a_{2,d}^* a_{3,d} + a_{5,d}^* a_{8,d}, \\ -t_{\mathbf{x}_3}^d &= a_{1,d}^* a_{5,d} + a_{3,d}^* a_{7,d} + a_{2,d}^* a_{6,d} + a_{4,d}^* a_{8,d}, \\ -t_{\mathbf{x}_2+\mathbf{x}_1}^d &= a_{1,d}^* a_{3,d} + a_{5,d}^* a_{7,d}, \quad -t_{\mathbf{x}_2-\mathbf{x}_1}^d = a_{2,d}^* a_{4,d} + a_{6,d}^* a_{8,d}, \\ -t_{\mathbf{x}_3+\mathbf{x}_1}^d &= a_{1,d}^* a_{6,d} + a_{4,d}^* a_{7,d}, \quad -t_{\mathbf{x}_3-\mathbf{x}_1}^d = a_{2,d}^* a_{5,d} + a_{3,d}^* a_{8,d}, \\ -t_{\mathbf{x}_3+\mathbf{x}_2}^d &= a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d}, \quad -t_{\mathbf{x}_3-\mathbf{x}_2}^d = a_{4,d}^* a_{5,d} + a_{3,d}^* a_{6,d}, \\ -t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d &= a_{1,d}^* a_{7,d}, \quad -t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d = a_{2,d}^* a_{8,d}, \\ & -t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d = a_{4,d}^* a_{6,d}, \\ -t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d &= a_{3,d}^* a_{5,d}, \quad pV_0 = -\sum_{n=1}^8 |a_{n,d}|^2. \end{aligned} \quad (23)$$

They determine the unknown complex coefficients $a_{n,d}$ (i.e., 16 unknown real values) from the input parameters $t_{\mathbf{r}}^d$. 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., $|t_{\mathbf{x}_1}^f| < |t_{\mathbf{x}_1}^d|$, $|t_{\mathbf{x}_1+\mathbf{x}_2}^f| < |t_{\mathbf{x}_1}^d|$, $|t_{\mathbf{x}_1+\mathbf{x}_2}^f| < |t_{\mathbf{x}_1}^f|$. That is, they decrease with increasing distance, and the magnitudes of the amplitudes of the d electrons are larger than those of the almost localized f electrons.

Based on Eq. (7), the corresponding ground-state energy becomes $E_g/N_\Lambda = -U + (1 - 2/p^2) \sum_{n=1}^8 |a_{n,d}|^2$. Depending on the solution, E_g has a nontrivial structure which will be analyzed below.

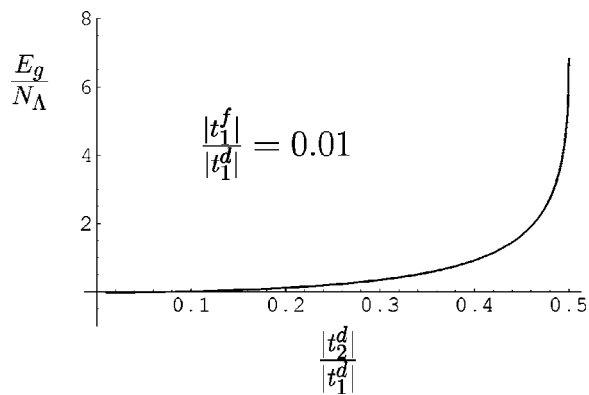


FIG. 2. Ground-state energy per lattice site, Eq. (25), in units of U as a function of $y=|t_2^d/t_1^d|$ for the localized solution in a simple cubic crystal for $|t_1^f/t_1^d|=0.01$. As seen from the plot, E_g/N_Λ is finite at $y_c=1/2$ but has infinite slope.

1. Solution for a cubic lattice

For a simple cubic lattice one has $t_{\mathbf{x}_1}^d = t_{\mathbf{x}_2}^d = t_{\mathbf{x}_3}^d = t_1^d$, $t_{\mathbf{x}_2 \pm \mathbf{x}_1}^d = t_{\mathbf{x}_3 \pm \mathbf{x}_1}^d = t_2^d$, $t_{\mathbf{x}_3 \pm \mathbf{x}_2}^d = t_3^d$. Then Eq. (23) has a solution

$$\begin{aligned} a_{1,d} &= a_1, & a_{2,d} &= a_{4,d} = a_{5,d} = u a_1, \\ a_{3,d} &= a_{6,d} = a_{8,d} = u^2 a_1, & a_{7,d} &= u^3 a_1, \end{aligned} \quad (24)$$

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 \hat{H} through Eqs. (23) and (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 $z \equiv |t_1^f/t_1^d| < 1/2$ the ground-state energy is given by

$$\frac{E_g}{UN_\Lambda} = -1 + \left(1 - 2 \frac{|t_1^f|}{|t_1^d|}\right) \left(1 + \frac{(1 - \sqrt{1 - 4y^2})^2}{4y^2}\right)^3, \quad (25)$$

where $u = (1 - \sqrt{1 - 4y^2})/(2y)$, and $y = |t_2^d/t_1^d| \in (0, 1/2]$ holds. We see that $|\Psi_{loc}\rangle$ 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.³⁰

2. Solutions for noncubic lattices

Similar results may be deduced for other lattice structures. In the most general case, i.e., when all hopping amplitudes $t_{\mathbf{r}}^d$ are different, the ground state energy for the localized solution becomes $E_g/N_\Lambda = -U + (1 - 2|t_{\mathbf{x}_1}^f|/|t_{\mathbf{x}_1}^d|) \sum_{n=1}^8 |a_{n,d}|^2$. When at least one of the terms $|a_{n,d}|^2$ [see Eq. (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 intersite hopping and hybridization will lead to a variable number of electrons on each site. In that case the ground state $|\Psi_g\rangle$, Eq. (11), becomes conducting. We will now describe solutions of this kind.

A. Solution for $a_{n,b} \neq 0$ for all n, b

To solve the matching conditions (8) for the case where $a_{n,b} \neq 0$ for all n, b , we define

$$p_n = \frac{a_{n,d}^*}{a_{n,f}}, \quad n = 1, 2, 3, 4, \quad (26a)$$

$$p_{n'} = \frac{a_{n',d}}{a_{n',f}}, \quad n' = 5, 6, 7, 8, \quad (26b)$$

and consider again $V_{\mathbf{r}}^{d,f} = V_{\mathbf{r}}^{f,d} = V_{\mathbf{r}}$. Equation (26b) is seen to contain coefficients $a_{n,b}$ instead of $a_{n,b}^*$ since Eq. (21) holds as well. An itinerant solution is obtained by choosing $p_n = p = -p^*$, i.e., imaginary p . For this choice Eq. (8) leads to

$$t_{\mathbf{r}_1}^f = \frac{t_{\mathbf{r}_1}^d}{|p|^2}, \quad t_{\mathbf{r}_2}^f = -\frac{t_{\mathbf{r}_2}^d}{|p|^2}, \quad V_{\mathbf{r}_2} = p t_{\mathbf{r}_2}^f, \quad V_{\mathbf{r}_1} = 0, \quad (27)$$

where $\mathbf{r}_1 = \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_2 \pm \mathbf{x}_1$, $\mathbf{r}_2 = \mathbf{x}_3, \mathbf{x}_3 \pm \mathbf{x}_2, \mathbf{x}_3 \pm \mathbf{x}_1, \mathbf{x}_3 \pm \mathbf{x}_2 \pm \mathbf{x}_1$, and $V_{\mathbf{r}_1} = 0$ follows from $V_{\mathbf{r}_1} = -V_{\mathbf{r}_1}$. As discussed earlier, imaginary p imply imaginary $V_{\mathbf{r}}$. 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 Eq. (8) are

$$-t_{\mathbf{x}_1}^d = a_{1,d}^* a_{2,d} + a_{8,d}^* a_{7,d} + a_{4,d}^* a_{3,d} + a_{5,d}^* a_{6,d},$$

$$-t_{\mathbf{x}_2}^d = a_{1,d}^* a_{4,d} + a_{6,d}^* a_{7,d} + a_{2,d}^* a_{3,d} + a_{5,d}^* a_{8,d},$$

$$-t_{\mathbf{x}_3}^d = a_{1,d}^* a_{5,d} + a_{3,d}^* a_{7,d} + a_{2,d}^* a_{6,d} + a_{4,d}^* a_{8,d},$$

$$-t_{\mathbf{x}_2 + \mathbf{x}_1}^d = a_{1,d}^* a_{3,d} + a_{5,d}^* a_{7,d}, \quad -t_{\mathbf{x}_2 - \mathbf{x}_1}^d = a_{2,d}^* a_{4,d} + a_{6,d}^* a_{8,d},$$

$$-t_{\mathbf{x}_3 + \mathbf{x}_1}^d = a_{1,d}^* a_{6,d} + a_{4,d}^* a_{7,d}, \quad -t_{\mathbf{x}_3 - \mathbf{x}_1}^d = a_{2,d}^* a_{5,d} + a_{3,d}^* a_{8,d},$$

$$-t_{\mathbf{x}_3 + \mathbf{x}_2}^d = a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d}, \quad -t_{\mathbf{x}_3 - \mathbf{x}_2}^d = a_{4,d}^* a_{5,d} + a_{3,d}^* a_{6,d},$$

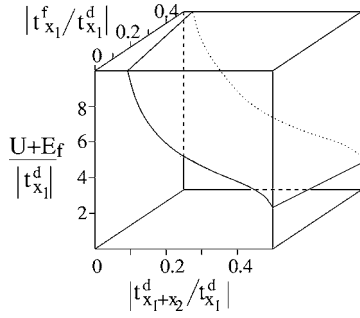


FIG. 3. Surface in parameter space representing the stability region of the conducting ground state discussed in Sec. IV A.

$$\begin{aligned}
 -t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d &= a_{1,d}^* a_{7,d}, & -t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d &= a_{2,d}^* a_{8,d}, \\
 -t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d &= a_{4,d}^* a_{6,d}, & -t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d &= a_{3,d}^* a_{5,d}.
 \end{aligned} \quad (29)$$

Furthermore, $V_{\mathbf{r}_1}=0$ implies

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

From Eqs. (29) and (30) it follows that

$$\begin{aligned}
 a_{1,d}^* &= a_1^*, & a_{2,d}^* &= u a_1^*, & a_{3,d}^* &= u^2 a_1^*, & a_{4,d}^* &= u a_1^*, \\
 a_{5,d}^* &= u a_1^*, & a_{6,d}^* &= u^2 a_1^*, & a_{7,d}^* &= u a_1^*, & a_{8,d}^* &= a_1^*,
 \end{aligned} \quad (31)$$

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 satisfied for *anisotropic* hopping and hybridization amplitudes, e.g., for vanishing hybridization in the basal (x, y) plane. Namely, Eqs. (29)–(31) yield $|u| = \sqrt{|t_{\mathbf{x}_3-\mathbf{x}_2}^d|/|t_{\mathbf{x}_3+\mathbf{x}_2}^d|}$ and $|t_{\mathbf{x}_\tau}^b| = |t_{\mathbf{x}_\tau}^a|$. 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, Eqs. (21)–(25) and (27)–(31), require the f electrons to be itinerant, i.e., $t_{\mathbf{r}}^f \neq 0$. We will now show that exact itinerant ground states can even be constructed for the *conventional* PAM, i.e., for $t_{\mathbf{r}}^f=0$. 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 $(t_{\mathbf{x}_2+\mathbf{x}_1}^d, t_{\mathbf{x}_3+\mathbf{x}_1}^d, t_{\mathbf{x}_3+\mathbf{x}_2}^d)$ 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 $(t_{\mathbf{x}_2-\mathbf{x}_1}^d, t_{\mathbf{x}_3-\mathbf{x}_1}^d, t_{\mathbf{x}_3-\mathbf{x}_2}^d)$. For this reason the former hopping elements are neglected (i.e., put to zero). In this case

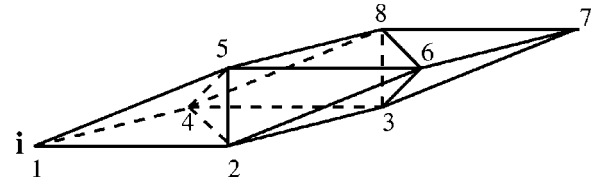


FIG. 4. Tilted unit cell located at site \mathbf{i} discussed in Sec. IV B. Number represent the intracell numbering of lattice sites. Only those bonds are presented along which hopping of d electrons occurs.

Eq. (8) reduces to the following 11 equations:

$$\begin{aligned}
 t_{\mathbf{x}_1}^d &= -a_{1,d}^* a_{2,d}, & t_{\mathbf{x}_2}^d &= -a_{1,d}^* a_{4,d}, & t_{\mathbf{x}_3}^d &= -a_{1,d}^* a_{5,d}, \\
 t_{\mathbf{x}_2-\mathbf{x}_1}^d &= -a_{2,d}^* a_{4,d}, & t_{\mathbf{x}_3-\mathbf{x}_1}^d &= -a_{2,d}^* a_{5,d}, & t_{\mathbf{x}_3-\mathbf{x}_2}^d &= -a_{4,d}^* a_{5,d}, \\
 V_{\mathbf{x}_1}^{f,d} &= -a_{1,f}^* a_{2,d}, & V_{\mathbf{x}_2}^{f,d} &= -a_{1,f}^* a_{4,d}, & V_{\mathbf{x}_3}^{f,d} &= -a_{1,f}^* a_{5,d},
 \end{aligned}$$

$$V_0 = -a_{1,d}^* a_{1,f}, \quad U + E_f = K_d - |a_{1,f}|^2, \quad (32)$$

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., $t_1^d = t_{\mathbf{x}_\tau}^d$, $V_1 = V_{\mathbf{x}_\tau}^{f,d}$, $\tau=1, 2, 3$, and $t_2^d = t_{\mathbf{x}_\tau-\mathbf{x}_\tau'}^d$, $\tau > \tau'$, with real hopping amplitudes,³¹ the corresponding stability region corresponds to the surface in parameter space (see Fig. 5) described by

$$\frac{U + E_f}{|t_1^d|} = x + \frac{1}{x}(1 - y^2), \quad (33)$$

where $x = |t_2^d|/|t_1^d|$ and $y = |V_1|/|t_1^d|$. Further properties of the solution are discussed in Refs. 31 and 32. The fact that $a_{n,d}^* = p a_{n,f}^*$ with $p = p^*$ does not hold for all $n=1, 2, \dots, 8$, implies a variable number of electrons at each site, i.e., an itinerant ground state.

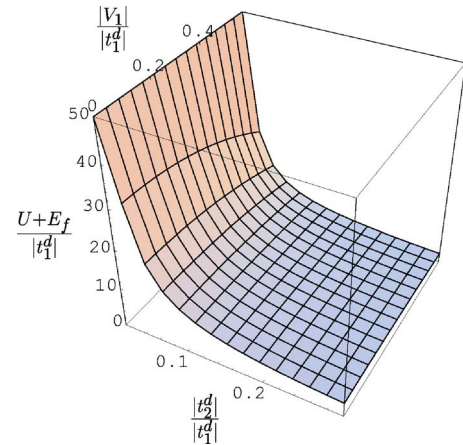


FIG. 5. (Color online) Surface in parameter space representing the stability region of the itinerant solution derived in the case of the conventional PAM, Eq. (33). For $|t_2^d|/|t_1^d| \rightarrow 0$, the surface asymptotically approaches the $(|V_1|/|t_1^d|, (U+E_f)/|t_1^d|)$ plane.

C. Diagonalization of the Hamiltonian

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

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

$$a_{\mathbf{k},b}^* = a_{1,b}^* + a_{2,b}^* e^{ikx_1} + a_{3,b}^* e^{ik(x_1+x_2)} + a_{4,b}^* e^{ikx_2} + a_{5,b}^* e^{ikx_3} + a_{6,b}^* e^{ik(x_1+x_3)} + a_{7,b}^* e^{ik(x_1+x_2+x_3)} + a_{8,b}^* e^{ik(x_2+x_3)}, \quad (34)$$

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

$$\hat{C}_{1,\mathbf{k}\sigma} = \sqrt{R_{\mathbf{k}}} \hat{A}_{\mathbf{k}\sigma} = \sqrt{R_{\mathbf{k}}} (a_{\mathbf{k},d} \hat{d}_{\mathbf{k}\sigma} + a_{\mathbf{k},f} \hat{f}_{\mathbf{k}\sigma}), \quad (35)$$

$$\hat{C}_{2,\mathbf{k}\sigma} = \sqrt{R_{\mathbf{k}}} (a_{\mathbf{k},d}^* \hat{d}_{\mathbf{k}\sigma} - a_{\mathbf{k},f}^* \hat{f}_{\mathbf{k}\sigma}),$$

where $R_{\mathbf{k}}^{-1} = \sum_{b=d,f} |a_{\mathbf{k},b}|^2$. Then the Hamiltonian becomes³⁴

$$\begin{aligned} \hat{H} &= \hat{H}_g + U\hat{P} - UN_\Lambda, \\ \hat{H}_g &= \sum_{\mathbf{k},\sigma} [(K_d - R_{\mathbf{k}}^{-1}) \hat{C}_{1,\mathbf{k}\sigma}^\dagger \hat{C}_{1,\mathbf{k}\sigma} + K_d \hat{C}_{2,\mathbf{k}\sigma}^\dagger \hat{C}_{2,\mathbf{k}\sigma}]. \end{aligned} \quad (36)$$

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 $\xi_{1,\mathbf{k}} = K_d - R_{\mathbf{k}}^{-1}$, while the upper one is dispersionless, i.e., flat, since $\xi_{2,\mathbf{k}} = K_d = \text{const}$. The lower (upper) diagonalized band contains fermions created by $\hat{C}_{1,\mathbf{k}\sigma}^\dagger$ ($\hat{C}_{2,\mathbf{k}\sigma}^\dagger$), 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.³⁵⁻³⁷

D. Conductivity of the itinerant state

The ground-state expectation value of \hat{H}_{iim} , the itinerant part of \hat{H} , is obtained as

$$\langle \hat{H}_{iim} \rangle = - \sum_{\mathbf{k}} \frac{K_d |a_{\mathbf{k},d}|^2 + K_f |a_{\mathbf{k},f}|^2}{|a_{\mathbf{k},d}|^2 + |a_{\mathbf{k},f}|^2} < 0. \quad (37)$$

This is in contrast to the localized case where $\langle \hat{H}_{iim} \rangle = 0$.³⁸

Since $\langle \hat{H}_{iim}(\mathbf{r}) \rangle \neq 0$ the charge sum rule (B3) implies $\int_0^\infty d\omega \text{Re } \sigma_{\tau,\tau}(\omega) \neq 0$, i.e., the (dynamic) conductivity is in general nonzero. 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 Eq. (11) can be generalized to fillings beyond 3/4 via Eq. (12). Using Eq. (7) 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.³⁹

E. Magnetic properties

Using \mathbf{k} -space notation the unnormalized ground state (11) can be written as⁴⁰

$$|\Psi_g\rangle = \left(\prod_{\mathbf{k}} \hat{A}_{\mathbf{k}\uparrow}^\dagger \hat{A}_{\mathbf{k}\downarrow}^\dagger \right) \left[\prod_{\mathbf{i}} \left(\sum_{\mathbf{k}} e^{ik\mathbf{i}} (\mu_{\mathbf{i},\uparrow} \hat{f}_{\mathbf{k}\uparrow}^\dagger + \mu_{\mathbf{i},\downarrow} \hat{f}_{\mathbf{k}\downarrow}^\dagger) \right) \right] |0\rangle, \quad (38)$$

where the sum and product over \mathbf{k} extend over the first Brillouin zone, and the set $\{\mu_{\mathbf{i},\sigma}\}$ is arbitrary. Using Eq. (38) we will now calculate ground-state expectation values of the spin for different sets of $\{\mu_{\mathbf{i},\sigma}\}$.²⁹

1. Maximum total spin

As in the localized case $\mu_{\mathbf{i},\sigma} = \mu_{\sigma}$ corresponds to maximum total spin. Defining $\hat{F}_{\mathbf{k},b}^\dagger = (\mu_{\uparrow} \hat{b}_{\mathbf{k}\uparrow}^\dagger + \mu_{\downarrow} \hat{b}_{\mathbf{k}\downarrow}^\dagger)$ and employing $(\hat{F}_{\mathbf{k},b}^\dagger)^2 = 0$ the product over sites \mathbf{i} in Eq. (38) may be written as $\prod_{\mathbf{i}}^{\Lambda} (\sum_{\mathbf{k}} e^{ik\mathbf{i}} \hat{F}_{\mathbf{k},f}^\dagger) = Z \prod_{\mathbf{k}}^{\Lambda} \hat{F}_{\mathbf{k},f}^\dagger$, where Z is defined in Ref. 40. Then the normalized ground state becomes

$$|\Psi_g\rangle = \prod_{\mathbf{k}} \frac{a_{\mathbf{k},d}^* \hat{d}_{\mathbf{k}\uparrow}^\dagger \hat{d}_{\mathbf{k}\downarrow}^\dagger \hat{F}_{\mathbf{k},f}^\dagger + a_{\mathbf{k},f}^* \hat{f}_{\mathbf{k}\uparrow}^\dagger \hat{f}_{\mathbf{k}\downarrow}^\dagger \hat{F}_{\mathbf{k},d}^\dagger}{\sqrt{(|\mu_{\uparrow}|^2 + |\mu_{\downarrow}|^2)(|a_{\mathbf{k},d}|^2 + |a_{\mathbf{k},f}|^2)}} |0\rangle. \quad (39)$$

The spin expectation value then follows as

$$\frac{2\langle \hat{S} \rangle}{N_\Lambda} = \mathbf{x} \frac{\mu_{\uparrow} \mu_{\uparrow}^* + \mu_{\downarrow} \mu_{\downarrow}^*}{|\mu_{\uparrow}|^2 + |\mu_{\downarrow}|^2} + \mathbf{y} \frac{i(\mu_{\uparrow} \mu_{\downarrow}^* - \mu_{\downarrow} \mu_{\uparrow}^*)}{|\mu_{\uparrow}|^2 + |\mu_{\downarrow}|^2} + \mathbf{z} \frac{|\mu_{\uparrow}|^2 - |\mu_{\downarrow}|^2}{(|\mu_{\uparrow}|^2 + |\mu_{\downarrow}|^2)}, \quad (40)$$

resulting in $|\langle \hat{S} \rangle / N_\Lambda|^2 = 1/4$, and $\langle \hat{S}^2 \rangle = (N_\Lambda/2)(N_\Lambda/2 + 1)$. Thus we recover Eq. (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.²⁵

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 \mathcal{D}_\uparrow and \mathcal{D}_\downarrow containing both $N_\Lambda/2$ lattice sites, such that for all $\mathbf{i}_n \in \mathcal{D}_\uparrow$ and $\mathbf{j}_n \in \mathcal{D}_\downarrow$ we have $\mathbf{j}_n = \mathbf{i}_n + \mathbf{R}$, where \mathbf{R} is a fixed Bravais vector.⁴¹ Choosing $\mu_{\mathbf{i},\sigma} = \mu_\sigma$, $\mu_{\mathbf{i},-\sigma} = 0$ for \mathcal{D}_σ in Eq. (38) the unnormalized ground state becomes

$$|\Psi_g\rangle = \left(\prod_{\mathbf{k}} \hat{A}_{\mathbf{k}\uparrow}^\dagger \hat{A}_{\mathbf{k}\downarrow}^\dagger \right) \left[\prod_{\mathbf{i} \in \mathcal{D}_1} \left(\sum_{\mathbf{k}} e^{ik\mathbf{i}} \hat{f}_{\mathbf{k}\uparrow}^\dagger \right) \right] \times \left[\prod_{\mathbf{j} \in \mathcal{D}_2} \left(\sum_{\mathbf{k}} e^{ik\mathbf{j}} \hat{f}_{\mathbf{k}\downarrow}^\dagger \right) \right] |0\rangle. \quad (41)$$

Details of the calculation of ground-state expectation values

in terms of Eq. (41) are presented in Appendix D. Based on Eq. (D3) one finds $\langle \hat{S} \rangle = 0$, and using Eq. (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 Eq. (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, Eq. (35), we need to express $|\Psi_g\rangle$, Eq. (38), in terms of $\hat{C}_{\delta,\mathbf{k},\sigma}^\dagger$ too. For the unnormalized ground state one finds

$$|\Psi_g\rangle = \left(\prod_{\mathbf{k}} \hat{C}_{1,\mathbf{k}\uparrow}^\dagger \hat{C}_{1,\mathbf{k}\downarrow}^\dagger \right) \times \left[\prod_{\mathbf{i}} \left(\sum_{\mathbf{k}} X_{\mathbf{k}} e^{i\mathbf{k}\mathbf{i}} (\mu_{i,\uparrow} \hat{C}_{2,\mathbf{k}\uparrow}^\dagger + \mu_{i,\downarrow} \hat{C}_{2,\mathbf{k}\downarrow}^\dagger) \right) \right] |0\rangle, \quad (42)$$

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

$$\hat{C}_{1,\mathbf{k}\sigma}^\dagger \hat{C}_{1,\mathbf{k}'\sigma'} |\Psi_g\rangle = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} |\Psi_g\rangle, \quad \hat{C}_{1,\mathbf{k}\sigma}^\dagger \hat{C}_{2,\mathbf{k}'\sigma'} |\Psi_g\rangle = 0. \quad (43)$$

Details of the calculation of ground-state expectation values of $\hat{C}_{2,\mathbf{k}\sigma}^\dagger \hat{C}_{2,\mathbf{k}\sigma}$ operators are presented in Appendix E. Using Eqs. (43) and (E8), one finds in particular

$$\langle \hat{C}_{\delta,\mathbf{k}\sigma}^\dagger \hat{C}_{\delta,\mathbf{k}\sigma} \rangle = \delta_{1,\delta} + \frac{1}{2} \delta_{2,\delta} \quad (44)$$

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 Eq. (44) the momentum distribution of $b=d,f$ electrons is then obtained as³³

$$n_{\mathbf{k}\sigma}^b = \langle \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma} \rangle = \frac{1}{2} + \frac{1}{2} R_{\mathbf{k}} |a_{\mathbf{k},b}|^2, \quad (45)$$

which implies $n_{\mathbf{k}\sigma} = \sum_{b=d,f} n_{\mathbf{k}\sigma}^b = 3/2$. Since the coefficients $R_{\mathbf{k}} |a_{\mathbf{k},b}|^2 = |a_{\mathbf{k},b}|^2 / (|a_{\mathbf{k},d}|^2 + |a_{\mathbf{k},f}|^2)$ are regular functions of \mathbf{k} , this is also the case for $n_{\mathbf{k},\sigma}^b$ and $n_{\mathbf{k},\sigma}$ (see Fig. 6).⁴³ 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 \mathbf{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 theorem⁴⁴ does not apply. Non-

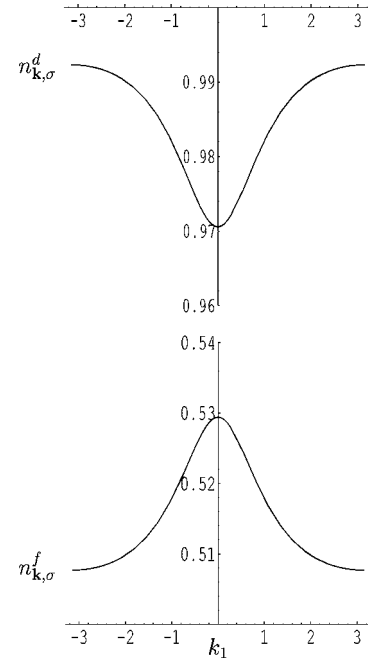


FIG. 6. Momentum distribution functions $n_{\mathbf{k},\sigma}^d, n_{\mathbf{k},\sigma}^f$ for the conducting solution discussed in Sec. IV B, for $|t_1^d|/|t_2^d|=5.0$, $|V_1|/|t_1^d|=0.5$, $t_1^d > 0$, and $k_2=k_3=0$, where $k_\tau = \mathbf{k}\mathbf{x}_\tau$. The plot presents the behavior in the first Brillouin zone for $k_1 \in [-\pi, \pi]$. For other \mathbf{k} directions a similar behavior is found.

Fermi-liquid properties connected to a flat band have also been observed in other investigations.^{45–47}

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 Eq. (43) the density-density correlation function

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

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

$$\begin{aligned} \rho_{n,n}(\mathbf{r}) = & \frac{1}{N_\Lambda} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} e^{i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}} \sqrt{R_{\mathbf{k}_1} R_{\mathbf{k}_2} R_{\mathbf{k}_3} R_{\mathbf{k}_4}} [(a_{\mathbf{k}_3,d}^* a_{\mathbf{k}_4,d} \\ & + a_{\mathbf{k}_3,f}^* a_{\mathbf{k}_4,f}) (a_{\mathbf{k}_1,d}^* a_{\mathbf{k}_2,d} + a_{\mathbf{k}_1,f}^* a_{\mathbf{k}_2,f}) \\ & \times (\langle \hat{C}_{2,\mathbf{k}_3\sigma'}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma'} \hat{C}_{2,\mathbf{k}_1\sigma}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma} \rangle - \langle \hat{C}_{2,\mathbf{k}_3\sigma'}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma'} \rangle \\ & \times \langle \hat{C}_{2,\mathbf{k}_1\sigma}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma} \rangle) + (a_{\mathbf{k}_3,d} a_{\mathbf{k}_4,f} - a_{\mathbf{k}_3,f} a_{\mathbf{k}_4,d}) (a_{\mathbf{k}_1,f}^* a_{\mathbf{k}_2,d} \\ & - a_{\mathbf{k}_1,d}^* a_{\mathbf{k}_2,f}) \langle \hat{C}_{1,\mathbf{k}_3\sigma'}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma'} \hat{C}_{2,\mathbf{k}_1\sigma}^\dagger \hat{C}_{1,\mathbf{k}_2\sigma} \rangle], \quad (47) \end{aligned}$$

where $\mathbf{k}_4 = \mathbf{k}_3 + \mathbf{k}_1 - \mathbf{k}_2$. Employing Eqs. (E6) and (E12) in the first term and Eqs. (43) and (E6) in the second term of Eq. (47) one finds

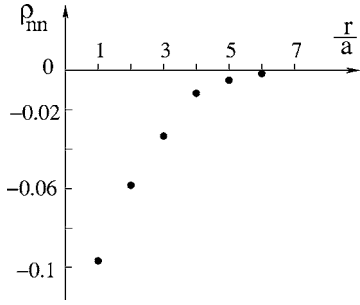


FIG. 7. Density-density correlation function for $|t_1^d/t_2^d|=4$, $|V_1/t_1^d|=0.25$, $t_1^d > 0$ for the itinerant case obtained from Eq. (49) in the thermodynamic limit. The nine-dimensional integration was performed by a Monte Carlo method using 69 points. The distance \mathbf{r} was taken in the $\tau=1$ direction, and is expressed in units of the lattice constant a .

$$\begin{aligned} & \sum_{\sigma, \sigma'} \langle \langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma'} \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle - \langle \hat{C}_{2, \mathbf{k}_3 \sigma'}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma'} \rangle \\ & \quad \times \langle \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle \rangle \\ & = \delta_{\mathbf{k}_1, \mathbf{k}_4} \delta_{\mathbf{k}_2, \mathbf{k}_3} - \frac{1}{N_\Lambda} \frac{X_{\mathbf{k}_4 \neq \mathbf{k}_2} X_{\mathbf{k}_2}}{X_{\mathbf{k}_3 \neq \mathbf{k}_1} X_{\mathbf{k}_1}} \delta_{\mathbf{k}_4, \mathbf{k}_3 + \mathbf{k}_1 - \mathbf{k}_2}, \\ & \sum_{\sigma, \sigma'} \langle \langle \hat{C}_{1, \mathbf{k}_3 \sigma'}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma'} \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{1, \mathbf{k}_2 \sigma} \rangle \rangle = \delta_{\mathbf{k}_4, \mathbf{k}_1} \delta_{\mathbf{k}_3, \mathbf{k}_2}. \end{aligned} \quad (48)$$

Then the density-density correlation function becomes

$$\begin{aligned} \rho_{n,n}(\mathbf{r}) & = \delta_{\mathbf{r},0} - \frac{1}{N_\Lambda^3} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2)\mathbf{r}} \frac{a_{\mathbf{k}_4 \neq \mathbf{k}_2, d} a_{\mathbf{k}_2, d}}{a_{\mathbf{k}_3 \neq \mathbf{k}_1, d} a_{\mathbf{k}_1, d}} \\ & \quad \times \frac{(a_{\mathbf{k}_3, d}^* a_{\mathbf{k}_4, d} + a_{\mathbf{k}_3, f}^* a_{\mathbf{k}_4, f})(a_{\mathbf{k}_1, d}^* a_{\mathbf{k}_2, d} + a_{\mathbf{k}_1, f}^* a_{\mathbf{k}_2, f})}{(|a_{\mathbf{k}_2, d}|^2 + |a_{\mathbf{k}_2, f}|^2)(|a_{\mathbf{k}_4, d}|^2 + |a_{\mathbf{k}_4, f}|^2)} \\ & \quad \times \delta_{\mathbf{k}_4, \mathbf{k}_3 + \mathbf{k}_1 - \mathbf{k}_2}. \end{aligned} \quad (49)$$

In the thermodynamic limit the contributions from $\mathbf{k}_4 = \mathbf{k}_2$ and $\mathbf{k}_3 = \mathbf{k}_1$ in the second term have zero measure. Hence all \mathbf{k} sums can be calculated without restriction. $\rho_{n,n}(\mathbf{r})$ is seen to vanish for all \mathbf{r} whenever the \mathbf{k} dependence of the $a_{\mathbf{k},b}$ coefficients is negligible (for example in the case $|t_1^d/t_2^d| \gg 1$ for the solution from Sec. IV B). It also vanishes in the limit $|\mathbf{r}| \rightarrow \infty$, where the $\mathbf{k} \rightarrow 0$ limit of the coefficients $a_{\mathbf{k},b}$ gives the dominant contribution to Eq. (49); this behavior is indeed seen in Fig. 7.

2. Spin-spin correlation function

Similarly, the spin-spin correlation function

$$\rho_{S,S}(\mathbf{r}) = \frac{1}{N_\Lambda} \sum_{\mathbf{i}} (\langle \hat{S}_{\mathbf{i}} \hat{S}_{\mathbf{i}+\mathbf{r}} \rangle - \langle \hat{S}_{\mathbf{i}} \rangle \langle \hat{S}_{\mathbf{i}+\mathbf{r}} \rangle) \quad (50a)$$

$$= \rho_{S_z, S_z}(\mathbf{r}) + \rho_{S_\perp, S_\perp}(\mathbf{r}) \quad (50b)$$

is given by

$$\rho_{S_z, S_z}(\mathbf{r}) = \frac{1}{N_\Lambda} \sum_{\mathbf{i}} (\langle \hat{S}_{\mathbf{i}}^z \hat{S}_{\mathbf{i}+\mathbf{r}}^z \rangle - \langle \hat{S}_{\mathbf{i}}^z \rangle \langle \hat{S}_{\mathbf{i}+\mathbf{r}}^z \rangle) \quad (51a)$$

$$\begin{aligned} & = \frac{1}{4N_\Lambda^2} \sum_{\sigma} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2)\mathbf{r}} \sqrt{R_{\mathbf{k}_1} R_{\mathbf{k}_2} R_{\mathbf{k}_3} R_{\mathbf{k}_4}} \{ (a_{\mathbf{k}_3, d}^* a_{\mathbf{k}_4, d} \\ & \quad + a_{\mathbf{k}_3, f}^* a_{\mathbf{k}_4, f}) (a_{\mathbf{k}_1, d}^* a_{\mathbf{k}_2, d} + a_{\mathbf{k}_1, f}^* a_{\mathbf{k}_2, f}) \\ & \quad \times [(\langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma} \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle - \langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma} \rangle \\ & \quad \times \langle \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle) - (\langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma} \hat{C}_{2, \mathbf{k}_1 - \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 - \sigma} \rangle \\ & \quad - \langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma} \rangle \langle \hat{C}_{2, \mathbf{k}_1 - \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 - \sigma} \rangle)] + (a_{\mathbf{k}_3, d} a_{\mathbf{k}_4, f} - a_{\mathbf{k}_3, f} a_{\mathbf{k}_4, d}) \\ & \quad \times (a_{\mathbf{k}_1, f}^* a_{\mathbf{k}_2, d} - a_{\mathbf{k}_1, d}^* a_{\mathbf{k}_2, f}) \\ & \quad \times \langle \hat{C}_{1, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 \sigma} \hat{C}_{2, \mathbf{k}_1 \sigma}^\dagger \hat{C}_{1, \mathbf{k}_2 \sigma} \rangle \} \delta_{\mathbf{k}_4, \mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3}, \end{aligned} \quad (51b)$$

$$\rho_{S_\perp, S_\perp}(\mathbf{r}) = \frac{1}{N_\Lambda} \sum_{\mathbf{i}} [\langle \hat{S}_{\mathbf{i}}^x \hat{S}_{\mathbf{i}+\mathbf{r}}^x + \hat{S}_{\mathbf{i}}^y \hat{S}_{\mathbf{i}+\mathbf{r}}^y \rangle - (\langle \hat{S}_{\mathbf{i}}^x \rangle \langle \hat{S}_{\mathbf{i}+\mathbf{r}}^x \rangle + \langle \hat{S}_{\mathbf{i}}^y \rangle \langle \hat{S}_{\mathbf{i}+\mathbf{r}}^y \rangle)] \quad (52a)$$

$$\begin{aligned} & = \frac{1}{2N_\Lambda^2} \sum_{\sigma} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2)\mathbf{r}} \sqrt{R_{\mathbf{k}_1} R_{\mathbf{k}_2} R_{\mathbf{k}_3} R_{\mathbf{k}_4}} \\ & \quad \times \{ (a_{\mathbf{k}_3, d}^* a_{\mathbf{k}_4, d} + a_{\mathbf{k}_3, f}^* a_{\mathbf{k}_4, f}) (a_{\mathbf{k}_1, d}^* a_{\mathbf{k}_2, d} + a_{\mathbf{k}_1, f}^* a_{\mathbf{k}_2, f}) \\ & \quad \times (\langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 - \sigma} \hat{C}_{2, \mathbf{k}_1 - \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle - \langle \hat{C}_{2, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 - \sigma} \rangle \\ & \quad \times \langle \hat{C}_{2, \mathbf{k}_1 - \sigma}^\dagger \hat{C}_{2, \mathbf{k}_2 \sigma} \rangle) + (a_{\mathbf{k}_3, d} a_{\mathbf{k}_4, f} - a_{\mathbf{k}_3, f} a_{\mathbf{k}_4, d}) \\ & \quad \times (a_{\mathbf{k}_1, f}^* a_{\mathbf{k}_2, d} - a_{\mathbf{k}_1, d}^* a_{\mathbf{k}_2, f}) \\ & \quad \times \langle \hat{C}_{1, \mathbf{k}_3 \sigma}^\dagger \hat{C}_{2, \mathbf{k}_4 - \sigma} \hat{C}_{2, \mathbf{k}_1 - \sigma}^\dagger \hat{C}_{1, \mathbf{k}_2 \sigma} \rangle \} \delta_{\mathbf{k}_4, \mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3}. \end{aligned} \quad (52b)$$

Thus one finds $\rho_{S_z, S_z}(\mathbf{r}) = \delta_{\mathbf{r},0}/4$ and $\rho_{S_\perp, S_\perp}(\mathbf{r}) = \delta_{\mathbf{r},0}/2$ in the thermodynamic limit. Consequently, the spins are uncorrelated at distances $|\mathbf{r}| \neq 0$. 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 semidefinite form in terms of composite operators (the unit cell operators $\hat{A}_{\mathbf{i},\sigma}$ in Sec. 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 Eq. (7). The corresponding matching conditions are similar to Eq. (8) but are now satisfied in a different region of parameter space. In this way

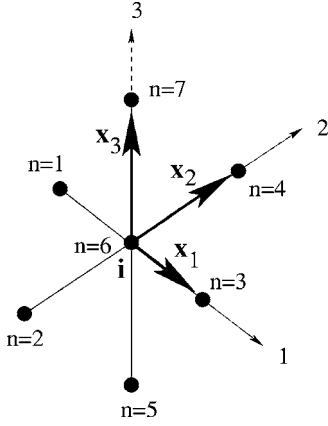


FIG. 8. Octahedral cell defined at lattice site \mathbf{i} as discussed in Sec. V A. The $\tau=1, 2, 3$ axes are represented by arrows with broken lines, \mathbf{x}_τ are indicated by thick full line arrows, and n represents the cell-independent notation of sites inside the octahedron.

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.⁴⁸ This clearly shows that a transformation of the PAM Hamiltonian into positive semidefinite form is not linked to finite f -electron hopping amplitudes in the PAM as one might have suspected from the steps performed in Sec. 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 noninteracting bands.

We consider an octahedral cell $B_{\mathbf{i}}$ at each lattice site \mathbf{i} . The seven sites within $B_{\mathbf{i}}$ are denoted by $\mathbf{r}_{B_{\mathbf{i}}} = \mathbf{i} + \mathbf{r}_{\alpha_1, \alpha_2, \alpha_3}$, where $\mathbf{r}_{\alpha_1, \alpha_2, \alpha_3} = \alpha_1(1 - |\alpha_2|)(1 - |\alpha_3|)\mathbf{x}_1 + \alpha_2(1 - |\alpha_1|)(1 - |\alpha_3|)\mathbf{x}_2 + \alpha_3(1 - |\alpha_1|)(1 - |\alpha_2|)\mathbf{x}_3$, $\alpha_\tau = -1, 0, 1$. Here \mathbf{x}_τ are the primitive vectors of the unit cell of the lattice. As seen from Fig. 8, the seven sites $\mathbf{r}_{B_{\mathbf{i}}}$ can be numbered by the indices $n_{\alpha_1, \alpha_2, \alpha_3} = (1 - |\alpha_2|)(1 - |\alpha_3|)(|\alpha_1|\alpha_1 + 2) + (1 - |\alpha_1|) \times (1 - |\alpha_3|)(\alpha_2|\alpha_2| + |\alpha_2| + 2) + (1 - |\alpha_1|)(1 - |\alpha_2|)(\alpha_3|\alpha_3| + 4|\alpha_3| + 2)$ without reference to $B_{\mathbf{i}}$. The separation vector \mathbf{r} between a site \mathbf{i} and its neighbors in the cell $B_{\mathbf{i}}$ 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 Eqs. (2) and (3) must be performed. Instead of Eq. (4) the cell operator is now defined as

$$\hat{B}_{B_{\mathbf{i}}, \sigma}^\dagger = a_{6f}^* \hat{f}_{\mathbf{i}, \sigma}^\dagger + \sum_{n_{\alpha_1, \alpha_2, \alpha_3}=1}^7 a_{n,d}^* \hat{d}_{\mathbf{i} + \mathbf{r}_{\alpha_1, \alpha_2, \alpha_3}}^\dagger, \quad (53)$$

where $n = n_{\alpha_1, \alpha_2, \alpha_3}$, and the seven vectors $\mathbf{r}_{\alpha_1, \alpha_2, \alpha_3} \equiv \mathbf{r}_{n_{\alpha_1, \alpha_2, \alpha_3}} \equiv \mathbf{r}_n$ in the sum are, in increasing order of the index n , $-\mathbf{x}_1, -\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_2, -\mathbf{x}_3, \mathbf{0}, \mathbf{x}_3$, (see Fig. 8.). We note that $a_{n,f} \neq 0$ only on the central site (e.g., $n=6$) of the cell $B_{\mathbf{i}}$. Consequently the product $\hat{B}_{B_{\mathbf{i}}, \sigma}^\dagger \hat{B}_{B_{\mathbf{i}}, \sigma}$ 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 Eq. (7) the transformed Hamiltonian then becomes

$$\hat{H} = \sum_{\mathbf{i}, \sigma} \hat{B}_{B_{\mathbf{i}}, \sigma} \hat{B}_{B_{\mathbf{i}}, \sigma}^\dagger + U \hat{P} + E_{g,b}, \quad (54)$$

where $E_{g,b} = K\hat{N} - UN_\Lambda - 2N_\Lambda(|a_{6,f}|^2 + K)$, $K = \sum_{n=1}^7 |a_{n,d}|^2$. Furthermore, the matching conditions from Eq. (8) transform into the following nonlinear system of 19 coupled complex algebraic equations:

$$-t_{\mathbf{x}_1}^d = a_{6,d}^* a_{3,d} + a_{1,d}^* a_{6,d}, \quad -t_{\mathbf{x}_2}^d = a_{6,d}^* a_{4,d} + a_{2,d}^* a_{6,d},$$

$$-t_{\mathbf{x}_3}^d = a_{6,d}^* a_{7,d} + a_{5,d}^* a_{6,d},$$

$$-t_{\mathbf{x}_2 + \mathbf{x}_1}^d = a_{2,d}^* a_{3,d} + a_{1,d}^* a_{4,d}, \quad -t_{\mathbf{x}_2 - \mathbf{x}_1}^d = a_{3,d}^* a_{4,d} + a_{2,d}^* a_{1,d},$$

$$-t_{\mathbf{x}_3 + \mathbf{x}_1}^d = a_{5,d}^* a_{3,d} + a_{1,d}^* a_{7,d},$$

$$-t_{\mathbf{x}_3 - \mathbf{x}_1}^d = a_{3,d}^* a_{7,d} + a_{5,d}^* a_{1,d}, \quad -t_{\mathbf{x}_3 + \mathbf{x}_2}^d = a_{2,d}^* a_{7,d} + a_{5,d}^* a_{4,d},$$

$$-t_{\mathbf{x}_3 - \mathbf{x}_2}^d = a_{4,d}^* a_{7,d} + a_{5,d}^* a_{2,d},$$

$$-t_{2\mathbf{x}_1}^d = a_{1,d}^* a_{3,d}, \quad -t_{2\mathbf{x}_2}^d = a_{2,d}^* a_{4,d}, \quad -t_{2\mathbf{x}_3}^d = a_{5,d}^* a_{7,d},$$

$$-V_0 = a_{6,d}^* a_{6,f},$$

$$-V_{\mathbf{x}_1} = a_{1,d}^* a_{6,f} = a_{6,f}^* a_{3,d}, \quad -V_{\mathbf{x}_2} = a_{2,d}^* a_{6,f} = a_{6,f}^* a_{4,d},$$

$$-V_{\mathbf{x}_3} = a_{5,d}^* a_{6,f} = a_{6,f}^* a_{7,d}, \quad (55)$$

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

$$|\Psi_{g,b}\rangle = \prod_{\mathbf{i}=1}^{N_\Lambda} (\hat{B}_{B_{\mathbf{i}}, \uparrow}^\dagger \hat{B}_{B_{\mathbf{i}}, \downarrow}^\dagger \hat{F}_{\mathbf{i}}^\dagger) \hat{V}_M^\dagger |0\rangle, \quad (56)$$

where, for $N = 3N_\Lambda$, $\hat{V}_M^\dagger = 1$ holds. Since $a_{n,d}/a_{n,f}$ cannot be constant for all $n=1, 2, \dots, 7$ (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 for⁴⁹

$$a_{1,d} = \sqrt{\frac{|t_{2\mathbf{x}_1}^d|}{2}} e^{i\phi}, \quad a_{6,d} = \frac{|V_0|}{V_1} \sqrt{\frac{|t_{2\mathbf{x}_3}^d|}{2}} e^{i(\phi - \phi_{V_0})}, \quad (57)$$

$$a_{6,f} = -V_1 \sqrt{\frac{2}{|t_{2\mathbf{x}_1}^d|}} e^{i\phi},$$

where ϕ is an arbitrary phase and ϕ_{V_0} is the phase³¹ of the hybridization amplitude V_0 . Introducing the notation

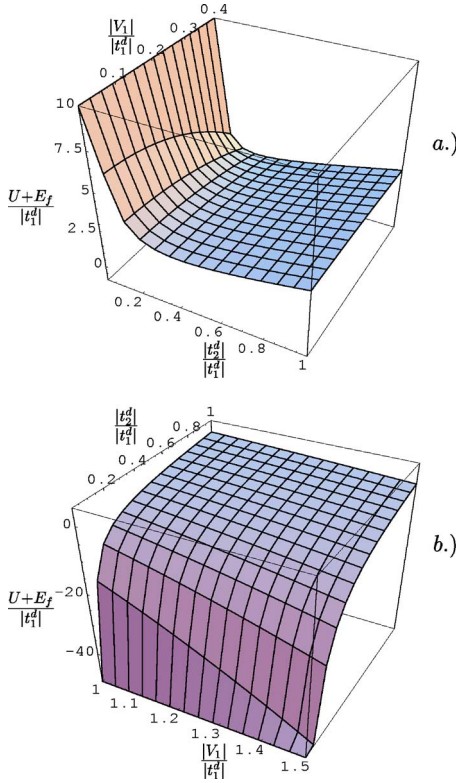


FIG. 9. (Color online) Surfaces in parameter space above which the conducting phase discussed in Sec. V A. is stable. (a) $|V_1|/|t_1^d| < 0.5$; $(U+E_f)/|t_1^d|$ is seen to diverge as $|t_2^d|/|t_1^d|$ approaches zero. (b) $|V_1|/|t_1^d| > 0.5$. In contrast to Fig. 5 where V_1 is imaginary, V_1 is real here.

$t = |t_2^d|/|t_1^d|$, $v = |V_1|/|t_1^d|$, 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 $\text{Im}(V_0)$ is in principle arbitrary, Eq. (58) defines an entire region in the parameter space where the solution exists (see Fig. 9). For $\text{Im}(V_0) \neq 0$, or real V_0 at $|t_1^d|/|t_2^d| > 6$, the properties presented in Sec. IV remain valid.⁵⁰

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 $\hat{A}_{I,\sigma}$ are used, alternative decompositions are possible which lead to qualitatively different ground states in other regions of the parameter space. For example, instead of Eq. (7) the Hamiltonian \hat{H} defined by Eqs. (1a), (1c), and (2) can also be cast into the form

$$\hat{H} = \sum_{\mathbf{i},\sigma} \hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i},\uparrow} \hat{n}_{\mathbf{i},\downarrow} + E'_g. \quad (59)$$

For periodic boundary conditions the matching conditions can then be obtained from Eq. (8) by (i) replacing $J_{\mathbf{r}}^{b,b'}$ by $\bar{J}_{\mathbf{r}}^{b,b'} = -J_{\mathbf{r}}^{b,b'}$, 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 $a_{n,d}/a_{n,f} = p$ 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 $\hat{f}_{\mathbf{i},\sigma} + p \hat{d}_{\mathbf{i},\sigma}$ for all \mathbf{i} and σ . Introducing $\hat{I}_{\mathbf{i}}^\dagger(\mu_{\mathbf{i}}) = [\hat{f}_{\mathbf{i},\uparrow}^\dagger - (1/p) \hat{d}_{\mathbf{i},\uparrow}^\dagger] + \mu_{\mathbf{i}} [\hat{f}_{\mathbf{i},\downarrow}^\dagger - (1/p) \hat{d}_{\mathbf{i},\downarrow}^\dagger]$, where $\mu_{\mathbf{i}}$ is an arbitrary site-dependent constant, one observes that

$$\{\hat{f}_{\mathbf{j},\sigma} + p \hat{d}_{\mathbf{j},\sigma}, \hat{I}_{\mathbf{j}'}^\dagger(\mu_{\mathbf{j}'})\} = 0, \quad \forall \mathbf{j}, \mathbf{j}', \mu_{\mathbf{j}'}, \sigma. \quad (60)$$

Since the operator $\hat{I}_{\mathbf{i}}^\dagger(\mu_{\mathbf{i}})$ acts only on site \mathbf{i} , the operator $\hat{I}^\dagger = \prod_{\mathbf{i}} \hat{I}_{\mathbf{i}}^\dagger(\mu_{\mathbf{i}})$ does not introduce f -electron double occupancies. Consequently, $\sum_{\mathbf{i},\sigma} \hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} \hat{I}^\dagger |0\rangle = 0$, $U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i},\uparrow}^\dagger \hat{n}_{\mathbf{i},\downarrow}^\dagger \hat{I}^\dagger |0\rangle = 0$, and the ground state becomes

$$|\Psi_g\rangle = \prod_{\mathbf{i}=1}^{N_A} \left[\left(\hat{f}_{\mathbf{i},\uparrow}^\dagger - \frac{1}{p} \hat{d}_{\mathbf{i},\uparrow}^\dagger \right) + \mu_{\mathbf{i}} \left(\hat{f}_{\mathbf{i},\downarrow}^\dagger - \frac{1}{p} \hat{d}_{\mathbf{i},\downarrow}^\dagger \right) \right] |0\rangle. \quad (61)$$

The ground state (61) has exactly one electron per site, and is degenerate, localized, and globally nonmagnetic. 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 $a_{n,d}/a_{n,f}$ depends on n , $\hat{A}_{I,\sigma}$ does not anticommute with $\hat{I}_{\mathbf{i}}^\dagger(\mu_{\mathbf{i}})$; hence $\sum_{\mathbf{i},\sigma} \hat{A}_{I,\sigma}^\dagger \hat{A}_{I,\sigma} \hat{I}_{\mathbf{i}}^\dagger |0\rangle = 0$ does not hold. In this case one may introduce a complementary unit cell operator⁵¹

$$\begin{aligned} \hat{Q}_{I,\sigma}^\dagger &= \sum_{n(\alpha,\beta,\gamma)=1}^8 (q_{n,d}^* \hat{d}_{\mathbf{i}+\mathbf{r}}^\dagger_{\alpha,\beta,\gamma,\sigma} + q_{n,f}^* \hat{f}_{\mathbf{i}+\mathbf{r}}^\dagger_{\alpha,\beta,\gamma,\sigma}) = (q_{1,d}^* \hat{d}_{\mathbf{i},\sigma}^\dagger \\ &+ q_{2,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_1,\sigma}^\dagger + q_{3,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_1+\mathbf{x}_2,\sigma}^\dagger + q_{4,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_2,\sigma}^\dagger + \dots \\ &+ q_{8,d}^* \hat{d}_{\mathbf{i}+\mathbf{x}_2+\mathbf{x}_3,\sigma}^\dagger) + (q_{1,f}^* \hat{f}_{\mathbf{i},\sigma}^\dagger + q_{2,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_1,\sigma}^\dagger + q_{3,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_1+\mathbf{x}_2,\sigma}^\dagger \\ &+ q_{4,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_2,\sigma}^\dagger + \dots + q_{8,f}^* \hat{f}_{\mathbf{i}+\mathbf{x}_2+\mathbf{x}_3,\sigma}^\dagger), \end{aligned} \quad (62)$$

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

$$\begin{aligned} q_{1,d}^* &= wa_{7,f}, & q_{2,d}^* &= wa_{8,f}, & q_{3,d}^* &= wa_{5,f}, & q_{4,d}^* &= wa_{6,f}, \\ q_{5,d}^* &= wa_{3,f}, & q_{6,d}^* &= wa_{4,f}, & q_{7,d}^* &= wa_{1,f}, & q_{8,d}^* &= wa_{2,f}, \end{aligned}$$

$$\begin{aligned}
 q_{1,f}^* &= -wa_{7,d}, & q_{2,f}^* &= -wa_{8,d}, & q_{3,f}^* &= -wa_{5,d}, \\
 q_{4,f}^* &= -wa_{6,d}, \\
 q_{5,f}^* &= -wa_{3,f}, & q_{6,f}^* &= -wa_{4,d}, & q_{7,f}^* &= -wa_{1,d}, \\
 q_{8,f}^* &= -wa_{2,d},
 \end{aligned} \tag{63}$$

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

$$|\Psi_g\rangle = \prod_{i=1}^{N_\Lambda} \hat{Q}_{i, \sigma}^\dagger |0\rangle, \quad \sigma = \uparrow, \downarrow. \tag{64}$$

This corresponds to a fully saturated, nondegenerate *ferromagnetic* phase, which is metallic since in Eq. (64) double occupancies (e.g., $\hat{d}_{i, \uparrow}^\dagger \hat{f}_{i, \uparrow}^\dagger$), empty sites, and single occupancies are simultaneously present.⁵²

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-Hartmann⁵³ ferromagnetic phases in the PAM itself were found by Dorin and Schlottmann⁵⁴ in the limit $U \rightarrow \infty$, and at finite U by Möller and Wölfle⁵⁵ within a slave-boson approach. Subsequently, ferromagnetic solutions of the PAM at and near quarter filling were obtained within various other approximation schemes.^{56–64} Exact results were derived in $D=1$ for $U=\infty$ by Yanagisawa.⁶⁵

In the exact solution discussed here ferromagnetism emerges when the lower diagonalized band of Eq. (2) becomes nondispersive (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 $N < N_\Lambda$, i.e., below quarter filling. For the two cases discussed in Secs. V B 1 and V B 2 they have the same form as Eqs. (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

$$|\Psi_g\rangle = \sum_{\mathcal{D}_N} \sum_{\{\mathcal{D}_{N,m}\}} \sum_{\{\sigma_m\}} \alpha_{\mathcal{D}_N, \{\mathcal{D}_{N,m}\}, \{\sigma_m\}} \prod_m \left(\prod_{\mathbf{i} \in \mathcal{D}_{N,m}} \hat{Q}_{\mathbf{i}, \sigma_m}^\dagger \right) |0\rangle \tag{65}$$

where \mathcal{D}_N denotes an arbitrary domain (a subset of lattice points) of the full lattice containing $N < N_\Lambda$ lattice sites. A given domain \mathcal{D}_N consists of disjoint subdomains (clusters) denoted by $\mathcal{D}_{N,m}$ where m enumerates the clusters in \mathcal{D}_N ;

the maximum of m is denoted by N_m . Clearly one has $\mathcal{D}_N = \mathcal{D}_{N,1} \cup \mathcal{D}_{N,2} \cup \dots \cup \mathcal{D}_{N,N_m}$, and $\mathcal{D}_{N,m_1} \cap \mathcal{D}_{N,m_2} = 0$ for $m_1 \neq m_2$. Furthermore, $\sigma_m = \pm 1/2$ represents a fixed, but arbitrary, spin index in the subdomain $\mathcal{D}_{N,m}$, and $\alpha_{\mathcal{D}_N, \{\mathcal{D}_{N,m}\}, \{\sigma_m\}}$ are arbitrary coefficients. From a physical point of view Eq. (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

$$\begin{aligned}
 |\Psi_g\rangle = \sum_{\mathcal{D}_N} \sum_{\{\mathcal{D}_{N,m}\}} \alpha_{\mathcal{D}_N, \{\mathcal{D}_{N,m}\}} \prod_m \left\{ \prod_{\mathbf{i} \in \mathcal{D}_{N,m}} \left[\left(\hat{f}_{\mathbf{i}, \uparrow}^\dagger - \frac{1}{p} \hat{d}_{\mathbf{i}, \uparrow}^\dagger \right) \right. \right. \\
 \left. \left. + \mu_{\mathbf{i}} \left(\hat{f}_{\mathbf{i}, \downarrow}^\dagger - \frac{1}{p} \hat{d}_{\mathbf{i}, \downarrow}^\dagger \right) \right] \right\} |0\rangle
 \end{aligned} \tag{66}$$

containing again clusters of arbitrary shape and size. But now the clusters are insulating and nonmagnetic, 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 $t_{\mathbf{r}}^b \rightarrow -t_{\mathbf{r}}^b$, $V_{\mathbf{r}} \rightarrow -V_{\mathbf{r}}$, $U \rightarrow 0$. 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, including the conventional PAM, on regular Bravais lattices. First the Hamiltonian is cast into positive semidefinite form with the help of composite fermionic operators in combination with a set of coupled, nonlinear matching conditions for the microscopic parameters of the Hamiltonian. Then a nonlocal product state of these composite operators in position space, corresponding to 3/4 filling, is constructed, which yields exact ground states 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 semidefinite 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, nonmagnetic 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 nonmagnetic and has vanishing nonlocal 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 nonlinearity it is 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, on the level of both 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.

ACKNOWLEDGMENTS

This work was supported in part by the Hungarian Scientific Research Fund through Contract No. OTKA-T-037212, and by the Deutsche Forschungsgemeinschaft through SFB 484. The numerical calculations were performed at the Supercomputing Laboratory of the Faculty of Natural Sciences, University of Debrecen, and supported by Grant No. OTKA-M-041537. One of us (Z.G.) acknowledges valuable discussions with Ferenc Kun regarding numerical multidimensional integrations.

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 Eqs. (1), (2), and (6)]

$$\begin{aligned} \hat{H} = \sum_{\mathbf{i},\sigma} \left(\sum_{\mathbf{r}} \left[(t_{\mathbf{r}}^d \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma} + t_{\mathbf{r}}^f \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma}) + (V_{\mathbf{r}}^{df} \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma} \right. \right. \\ \left. \left. + V_{\mathbf{r}}^{fd} \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma}) + \text{H.c.} \right] + (V_0 \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma} + \text{H.c.}) \right) \\ + (E_f + U) \hat{n}_{\mathbf{i},\sigma}^f + U \hat{P} - U N_\Lambda, \end{aligned} \quad (\text{A1})$$

into the form with unit cell operators, Eq. (7),

$$\hat{H} = - \sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma} + K_d \hat{N} + U \hat{P} - U N_\Lambda, \quad (\text{A2})$$

and explain how the matching conditions (8) arise in this process.

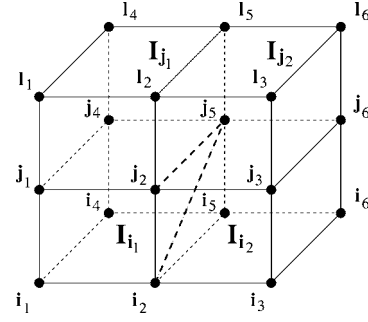


FIG. 10. Four neighboring unit cells in $D=3$. Each cell (e.g., I_i) is denoted by one of the lattice sites at which it is located (e.g., \mathbf{i}); see Sec. II B 1. For simplicity, orthorhombic unit cells are used.

One first calculates all terms in the sum $-\sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}$ from Eq. (A2). To identify the contributions generated thereby with those defined by Eq. (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—are depicted. Since the precise shape of the unit cells is unimportant here we use orthorhombic cells for simplicity.

Nearest-neighbor contributions. First we analyze a nearest-neighbor amplitude, e.g., $t_{\mathbf{j}_2, \mathbf{j}_5}^d$, which appears in the kinetic energy of Eq. (A1) as $t_{\mathbf{j}_2, \mathbf{j}_5}^d \hat{d}_{\mathbf{j}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$. This term acts along the bond $(\mathbf{j}_2, \mathbf{j}_5)$ represented by the horizontal, thick dashed line in Fig. 10. In Eq. (A2) this term originates from $-\sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}$, but only for sites $\mathbf{i}=\mathbf{i}_1, \mathbf{i}_2, \mathbf{j}_1, \mathbf{j}_2$ in $\Sigma_{\mathbf{i}}$. To calculate $-\sum_{\mathbf{i}=\mathbf{i}_1, \mathbf{i}_2, \mathbf{j}_1, \mathbf{j}_2} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}$ one must write down the unit cell operators $\hat{A}_{\mathbf{i},\sigma}^\dagger$, Eq. (4), corresponding to the aforementioned four unit cells. For example, one finds

$$\begin{aligned} \hat{A}_{\mathbf{i}_1, \sigma}^\dagger = \sum_{b=d,f} [a_{1,b}^* \hat{b}_{\mathbf{i}_1, \sigma}^\dagger + a_{2,b}^* \hat{b}_{\mathbf{i}_2, \sigma}^\dagger + a_{3,b}^* \hat{b}_{\mathbf{i}_5, \sigma}^\dagger + a_{4,b}^* \hat{b}_{\mathbf{i}_4, \sigma}^\dagger \\ + a_{5,b}^* \hat{b}_{\mathbf{j}_1, \sigma}^\dagger + a_{6,b}^* \hat{b}_{\mathbf{j}_2, \sigma}^\dagger + a_{7,b}^* \hat{b}_{\mathbf{j}_5, \sigma}^\dagger + a_{8,b}^* \hat{b}_{\mathbf{j}_4, \sigma}^\dagger], \end{aligned}$$

$$\begin{aligned} \hat{A}_{\mathbf{i}_2, \sigma}^\dagger = \sum_{b=d,f} [a_{1,b}^* \hat{b}_{\mathbf{i}_2, \sigma}^\dagger + a_{2,b}^* \hat{b}_{\mathbf{i}_3, \sigma}^\dagger + a_{3,b}^* \hat{b}_{\mathbf{i}_6, \sigma}^\dagger + a_{4,b}^* \hat{b}_{\mathbf{i}_5, \sigma}^\dagger \\ + a_{5,b}^* \hat{b}_{\mathbf{j}_2, \sigma}^\dagger + a_{6,b}^* \hat{b}_{\mathbf{j}_3, \sigma}^\dagger + a_{7,b}^* \hat{b}_{\mathbf{j}_6, \sigma}^\dagger + a_{8,b}^* \hat{b}_{\mathbf{j}_5, \sigma}^\dagger]. \end{aligned}$$

Thereby one obtains contributions of the form $-a_{6,d}^* a_{7,d} \hat{d}_{\mathbf{j}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$, $-a_{5,d}^* a_{8,d} \hat{d}_{\mathbf{j}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$, $-a_{2,d}^* a_{3,d} \hat{d}_{\mathbf{j}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$, and $-a_{1,d}^* a_{4,d} \hat{d}_{\mathbf{j}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$ implying $t_{\mathbf{j}_2, \mathbf{j}_5}^d = -(a_{1,d}^* a_{4,d} + a_{2,d}^* a_{3,d} + a_{5,d}^* a_{8,d} + a_{6,d}^* a_{7,d})$. Since (i) $t_{\mathbf{j}_2, \mathbf{j}_5}^d$ is a specific example of the general hopping amplitude $t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_2}^d$, (ii) all amplitudes $t_{\mathbf{r}}^d$ have the same form (i.e., $t_{\mathbf{x}_2}^d = t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_2}^d$), and (iii) this also holds for the f electrons, i.e., $t_{\mathbf{x}_2}^f = t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_2}^f$, one finds $-t_{\mathbf{x}_2}^b = a_{1,b}^* a_{4,b} + a_{2,b}^* a_{3,b} + a_{5,b}^* a_{8,b} + a_{6,b}^* a_{7,b}$, where $b=d, f$.

The same analysis applies to the hybridization amplitudes. Hence, for the terms $V_{\mathbf{x}_2}^{d,f} \hat{d}_{\mathbf{i}, \sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{x}_2, \sigma}$ and $V_{\mathbf{x}_2}^{f,d} \hat{f}_{\mathbf{i}, \sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{x}_2, \sigma}$ one finds $-V_{\mathbf{x}_2}^{b,b'} = a_{1,b}^* a_{4,b'} + a_{2,b}^* a_{3,b'} + a_{5,b}^* a_{8,b'} + a_{6,b}^* a_{7,b'}$.

Thus we have derived the matching condition $J_{\mathbf{x}_2}^{b,b'}$
 $= -[\delta_{b,b'} t_{\mathbf{x}_2}^b + (1 - \delta_{b,b'}) V_{\mathbf{x}_2}^{b,b'}]$ [the third relation in Eq. (8)].

It should be noted that the sum $-\sum_{\mathbf{i},\sigma} \hat{A}_{I_{\mathbf{i},\sigma}}^\dagger \hat{A}_{I_{\mathbf{i},\sigma}}$ also produces the Hermitian conjugates of the terms represented by Eq. (A1). Therefore, in addition to the result for $t_{\mathbf{j}_2, \mathbf{j}_5}^d$ one also finds $t_{\mathbf{j}_5, \mathbf{j}_2}^d = -(a_{4,d}^* a_{1,d} + a_{3,d}^* a_{2,d} + a_{8,d}^* a_{5,d} + a_{7,d}^* a_{6,d})$, where $t_{\mathbf{j}_5, \mathbf{j}_2}^d = t_{\mathbf{i}, \mathbf{i}-\mathbf{x}_2}^d = t_{-\mathbf{x}_2}^d = t_{\mathbf{x}_2}^d$.

Second-nearest-neighbor contributions. We now consider a plaquette-diagonal next-nearest-neighbor term, namely, $t_{\mathbf{i}_2, \mathbf{j}_5}^d$, acting on the oblique thick dashed line in Fig. 10. Since the bond $(\mathbf{i}_2, \mathbf{j}_5)$ appears only in the unit cells $I_{\mathbf{i}_1}$ and $I_{\mathbf{i}_2}$, only the contributions from $-\sum_{\mathbf{i},\sigma} \hat{A}_{I_{\mathbf{i},\sigma}}^\dagger \hat{A}_{I_{\mathbf{i},\sigma}}$ in Eq. (A2) with $\mathbf{i} = \mathbf{i}_1, \mathbf{i}_2$ give rise to $t_{\mathbf{i}_2, \mathbf{j}_5}^d \hat{d}_{\mathbf{i}_2, \mathbf{j}_5, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$ in Eq. (A1). The sum $-\sum_{\mathbf{i}=\mathbf{i}_1, \mathbf{i}_2} \hat{A}_{I_{\mathbf{i},\sigma}}^\dagger \hat{A}_{I_{\mathbf{i},\sigma}}$ leads to the expressions $-a_{2,d}^* a_{7,d} \hat{d}_{\mathbf{i}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$ and $-a_{1,d}^* a_{8,d} \hat{d}_{\mathbf{i}_2, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$, implying $t_{\mathbf{i}_2, \mathbf{j}_5}^d = -(a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d})$. Since (i) $t_{\mathbf{i}_2, \mathbf{j}_5}^d$ is a specific example of the general hopping amplitude $t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_3+\mathbf{x}_2}^d$, and (ii) all the amplitudes $t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_3+\mathbf{x}_2}^d$ have the same form (i.e., $t_{\mathbf{i}, \mathbf{i}+\mathbf{x}_3+\mathbf{x}_2}^d = t_{\mathbf{x}_3+\mathbf{x}_2}^d$) one finds $-t_{\mathbf{x}_3+\mathbf{x}_2}^d = a_{1,d}^* a_{8,d} + a_{2,d}^* a_{7,d}$. These relations also hold for the f electrons. Therefore we arrive at the matching condition $J_{\mathbf{x}_3+\mathbf{x}_2}^{b,b'} = a_{1,b}^* a_{8,b'} + a_{2,b}^* a_{7,b'}$ [the sixth relation in Eq. (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 $(\mathbf{j}_1, \mathbf{j}_5)$ of the cell $I_{\mathbf{i}_1}$, the product $-\hat{A}_{I_{\mathbf{i}_1, \sigma}}^\dagger \hat{A}_{I_{\mathbf{i}_1, \sigma}}$ leads to the term $-a_{1,d}^* a_{7,d} \hat{d}_{\mathbf{i}_1, \sigma}^\dagger \hat{d}_{\mathbf{j}_5, \sigma}$. Hence one finds $t_{\mathbf{i}_1, \mathbf{j}_5}^d = t_{\mathbf{i}_1+\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d = t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d = -a_{1,d}^* a_{7,d}$ and, consequently, $J_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^{b,b'} = a_{1,d}^* a_{7,d}$ [the tenth relation in Eq. (8)].

Single-site contributions. Since any site is common to eight unit cells, single-site contributions require the consideration of eight neighboring unit cells. For example, the term $V_0 \sum_{\mathbf{i},\sigma} \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma}$ is obtained from $-\sum_{\mathbf{i},\sigma} \hat{A}_{I_{\mathbf{i},\sigma}}^\dagger \hat{A}_{I_{\mathbf{i},\sigma}}$ as $-(\sum_{n=1}^8 a_{n,d}^* a_{n,f}) \sum_{\mathbf{i},\sigma} \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma}$, implying $-V_0 = \sum_{n=1}^8 a_{n,d}^* a_{n,f}$. In the same way we obtain the coefficient of $-\sum_{\mathbf{i},\sigma} \hat{b}_{\mathbf{i},\sigma}^\dagger \hat{b}_{\mathbf{i},\sigma}$ as $\sum_{n=1}^8 |a_{n,b}|^2 = K_b$. Therefore the terms $-\sum_{\mathbf{i},\sigma} \hat{A}_{I_{\mathbf{i},\sigma}}^\dagger \hat{A}_{I_{\mathbf{i},\sigma}} + K_d \hat{N}$ in Eq. (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 Eq. (A1) one obtains $U + E_f = K_d - K_f$ [last relation in Eq. (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 \mathbf{i} is given by $\hat{\rho}(\mathbf{i}) = e \sum_{\sigma} (\hat{d}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i},\sigma} + \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma})$, with e as the electron charge. The current operator $\hat{\mathbf{j}}$ is defined as²⁸ $\hat{\mathbf{j}} = -(i/\hbar) [\hat{\mathbf{q}}, \hat{H}]$, where V is the volume of the system, $\hat{\mathbf{q}} = (1/V) \sum_{\mathbf{i}} \hat{\rho}(\mathbf{i})$ is the charge polarization operator, and \hat{H} is the Hamiltonian. With \hat{H} from

Eq. (A1) the current operator of the PAM is found as

$$\hat{\mathbf{j}} = \frac{ie}{\hbar V} \sum_{\mathbf{i}} \sum_{\mathbf{r}} \sum_{\sigma} \sum_{b,b'=d,f} (J_{\mathbf{r}}^{b,b'} \hat{b}_{\mathbf{i}+\mathbf{r},\sigma}^\dagger \hat{b}_{\mathbf{i},\sigma} - J_{\mathbf{r}}^{b,b'} \hat{b}_{\mathbf{i},\sigma}^\dagger \hat{b}_{\mathbf{i}+\mathbf{r},\sigma}) \mathbf{r}, \quad (\text{B1})$$

where $J_{\mathbf{r}}^{b,b'}$ is defined in Eq. (8), 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., $\hat{H}_{\text{itin}} = \sum_{\mathbf{r}} \hat{H}_{\text{itin}}(\mathbf{r}) = \hat{H} - \hat{H}_U - \sum_{\mathbf{i},\sigma} [(V_0 \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma} + \text{H.c.}) + E_f \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i},\sigma}]$, where

$$\hat{H}_{\text{itin}}(\mathbf{r}) = \sum_{\mathbf{i},\sigma} [(t_{\mathbf{r}}^d \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma} + t_{\mathbf{r}}^f \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma}) + (V_{\mathbf{r}}^{df} \hat{d}_{\mathbf{i},\sigma}^\dagger \hat{f}_{\mathbf{i}+\mathbf{r},\sigma} + V_{\mathbf{r}}^{fd} \hat{f}_{\mathbf{i},\sigma}^\dagger \hat{d}_{\mathbf{i}+\mathbf{r},\sigma}) + \text{H.c.}], \quad (\text{B2})$$

contributes to Eq. (B1).

Starting from the current operator in Eq. (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 form²⁸ $\int_0^\infty d\omega \text{Re} \sigma_{\tau,\tau}(\omega) = -(i\pi V/2) \langle [\hat{q}_\tau, \hat{j}_\tau] \rangle$, where $\hat{q}_\tau = \hat{\mathbf{q}} \cdot \mathbf{x}_\tau / |\mathbf{x}_\tau|$ and $\hat{j}_\tau = \hat{\mathbf{j}} \cdot \mathbf{x}_\tau / |\mathbf{x}_\tau|$ represent the τ components of $\hat{\mathbf{q}}$ and $\hat{\mathbf{j}}$, respectively; here \mathbf{x}_τ are the primitive vectors of the unit cell. For the Hamiltonian under investigation one finds

$$\int_0^\infty d\omega \text{Re} \sigma_{\tau,\tau}(\omega) = -\frac{\pi e^2}{2\hbar V} \sum_{\mathbf{r}} \frac{(\mathbf{r} \cdot \mathbf{x}_\tau)^2}{|\mathbf{x}_\tau|^2} \langle \hat{H}_{\text{itin}}(\mathbf{r}) \rangle. \quad (\text{B3})$$

APPENDIX C: LOCALIZED SOLUTION FOR THE NONCUBIC CASE

In this appendix the matching conditions (23) from Sec. III B are solved for localized ground states in the case of noncubic 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 $a_{5,d} = -t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d / a_{3,d}^*$, $a_{6,d} = -t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d / a_{4,d}^*$, $a_{7,d} = -t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d / a_{1,d}^*$, $a_{8,d} = -t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d / a_{2,d}^*$. With these relations and using the notations

$$\tau_1 \equiv \frac{4t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d}{t_{\mathbf{x}_2+\mathbf{x}_1}^d{}^2}, \quad \tau_2 \equiv \frac{4t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d}{t_{\mathbf{x}_3+\mathbf{x}_2}^d{}^2}, \quad (\text{C1})$$

$$\tau_3 \equiv \frac{4t_{\mathbf{x}_3+\mathbf{x}_2+\mathbf{x}_1}^d t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d}{t_{\mathbf{x}_3+\mathbf{x}_1}^d{}^2},$$

$$\tau_4 \equiv \frac{4t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d}{t_{\mathbf{x}_3-\mathbf{x}_1}^d{}^2}, \quad \tau_5 \equiv \frac{4t_{\mathbf{x}_3-\mathbf{x}_2-\mathbf{x}_1}^d t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d}{t_{\mathbf{x}_3-\mathbf{x}_2}^d{}^2},$$

$$\tau_6 \equiv \frac{4t_{\mathbf{x}_3-\mathbf{x}_2+\mathbf{x}_1}^d t_{\mathbf{x}_3+\mathbf{x}_2-\mathbf{x}_1}^d}{t_{\mathbf{x}_2-\mathbf{x}_1}^d{}^2},$$

Eq. (23) leads to

$$\begin{aligned}
|a_{1,d}|^2 &= -\frac{t_{x_2+x_1}^d t_{x_3+x_2}^d}{2t_{x_3-x_1}^d \tau_4} F(\tau_1)F(\tau_2)F(\tau_4), \\
|a_{2,d}|^2 &= -\frac{t_{x_2-x_1}^d t_{x_3+x_2}^d \tau_2}{2t_{x_3+x_1}^d} \frac{F(\tau_3)F(\tau_6)}{\tau_3 F(\tau_2)}, \\
|a_{3,d}|^2 &= -\frac{t_{x_2+x_1}^d t_{x_3-x_1}^d}{2t_{x_3+x_2}^d} \frac{\tau_4 F(\tau_1)}{F(\tau_2)F(\tau_4)}, \\
|a_{4,d}|^2 &= -\frac{t_{x_2-x_1}^d t_{x_3+x_1}^d \tau_3}{2t_{x_3+x_2}^d} \frac{F(\tau_2)F(\tau_6)}{\tau_2 F(\tau_3)},
\end{aligned} \tag{C2}$$

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

$$\begin{aligned}
\sum_{n=1}^8 |a_{n,d}|^2 &= \left(|a_{1,d}|^2 + \frac{t_{x_2+x_2+x_1}^{d2}}{|a_{1,d}|^2} \right) + \left(|a_{2,d}|^2 + \frac{t_{x_3+x_2-x_1}^{d2}}{|a_{2,d}|^2} \right) \\
&+ \left(|a_{3,d}|^2 + \frac{t_{x_3-x_2-x_1}^{d2}}{|a_{3,d}|^2} \right) + \left(|a_{4,d}|^2 + \frac{t_{x_3-x_2+x_1}^{d2}}{|a_{4,d}|^2} \right).
\end{aligned} \tag{C3}$$

For the localized solution to be stable the quantities $|a_{n,d}|^2$ in Eq. (C2), and hence the function $F(\tau_i)$, Eq. (C3), 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 Eq. (C3), 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 Eq. (41) the terms

$$\begin{aligned}
\left[\prod_{\mathbf{i} \in \mathcal{D}_\sigma} \left(\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{i}} \hat{f}_{\mathbf{k}\sigma}^\dagger \right) \right] &= \sum_{\{\mathbf{k}_i\}} \beta_{\{\mathbf{k}_i, \sigma\}} \hat{F}_{f, \{\mathbf{k}_i, \sigma\}}^\dagger \beta_{\{\mathbf{k}_i, \sigma\}} \\
&= \sum_{P_{\{\mathbf{k}_i\}}} (-1)^{\bar{p}} e^{i(\mathbf{i}_1 \mathbf{k}_1 + \dots + \mathbf{i}_{N_\Lambda/2} \mathbf{k}_{N_\Lambda/2})}
\end{aligned} \tag{D1}$$

appear where $\hat{F}_{f, \{\mathbf{k}_i, \sigma\}}^\dagger = (\hat{f}_{\mathbf{k}_1, \sigma}^\dagger \hat{f}_{\mathbf{k}_2, \sigma}^\dagger \dots \hat{f}_{\mathbf{k}_{N_\Lambda/2}, \sigma}^\dagger)$. Here the sum over $\{\mathbf{k}_i\}$ extends over all sets of momentum with $N_\Lambda/2$ elements chosen from the first Brillouin zone, the sum $\sum_{P_{\{\mathbf{k}_i\}}}$ goes over all permutations $P_{\{\mathbf{k}_i\}}$ of the momenta in each set $\{\mathbf{k}_i\} = (\mathbf{k}_1, \dots, \mathbf{k}_{N_\Lambda/2})$, and \bar{p} represents the parity of $P_{\{\mathbf{k}_i\}}$. Since for $\mathbf{i}_{n, \sigma} \in \mathcal{D}_\sigma$ we have $\mathbf{i}_{n, \downarrow} = \mathbf{i}_{n, \uparrow} + \mathbf{R}$, one finds $\beta_{\{\mathbf{k}_i, \downarrow\}} = e^{i\phi_{\{\mathbf{k}_i\}}} \beta_{\{\mathbf{k}_i, \uparrow\}}$, where $\phi_{\{\mathbf{k}_i\}} = \mathbf{R} \sum_{\mathbf{k} \in \{\mathbf{k}_i\}} \mathbf{k}$. Thus, Eq. (41) becomes

$$|\Psi_g\rangle = \sum_{\{\mathbf{k}_i\}} \sum_{\{\mathbf{k}_j\}} \alpha_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}} |v_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}\rangle, \tag{D2}$$

$$|v_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}\rangle = \left(\prod_{\mathbf{k}} \hat{A}_{\mathbf{k}, \uparrow}^\dagger \hat{A}_{\mathbf{k}, \downarrow}^\dagger \right) \hat{F}_{f, \{\mathbf{k}_i, \uparrow\}}^\dagger \hat{F}_{f, \{\mathbf{k}_i, \downarrow\}}^\dagger |0\rangle,$$

where $\alpha_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}} = \beta_{\{\mathbf{k}_i, \uparrow\}} \beta_{\{\mathbf{k}_i, \downarrow\}}$, $|\alpha_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}}| = |\alpha_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}}|$, and $|v_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}\rangle$ are orthogonal states. Using Eq. (D2) one finds²⁹

$$\langle \hat{S}^x \rangle = \left\langle \sum_{\mathbf{k}} \hat{S}_{\mathbf{k}}^x \right\rangle = 0, \tag{D3}$$

$$\langle \hat{S}^y \rangle = \left\langle \sum_{\mathbf{k}} \hat{S}_{\mathbf{k}}^y \right\rangle = 0, \quad \langle \hat{S}^z \rangle = \left\langle \sum_{\mathbf{k}} \hat{S}_{\mathbf{k}}^z \right\rangle = 0, \quad \langle \hat{\mathbf{S}} \rangle = 0.$$

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

$$\begin{aligned}
\langle (\hat{S}^z)^2 \rangle &= \frac{1}{4} \langle (\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+) \rangle \\
&= \frac{\sum_{\{\mathbf{k}_i\}} \sum_{\{\mathbf{k}_j\}} |\alpha'_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}}|^2 (N_\Lambda - d_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}})}{4 \sum_{\{\mathbf{k}_i\}} \sum_{\{\mathbf{k}_j\}} |\alpha'_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}}|^2} < \frac{N_\Lambda}{4},
\end{aligned} \tag{D4}$$

where $d_{\{\mathbf{k}_i, \{\mathbf{k}_j\}\}}$ is the number of common elements of the sets $\{\mathbf{k}_i\}$ and $\{\mathbf{k}_j\}$.

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 (42) is a superposition of states

$$|\Psi_{g, \{\sigma\}}\rangle = \left(\prod_{\mathbf{k}} \hat{C}_{1, \mathbf{k}, \uparrow}^\dagger \hat{C}_{1, \mathbf{k}, \downarrow}^\dagger \right) \left[\prod_{n=1}^{N_\Lambda} \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}_n} X_{\mathbf{k}_n} e^{i\mathbf{k}_n \mathbf{i}_n} \hat{C}_{2, \mathbf{k}_n, \sigma_{i_n}}^\dagger \right) \right] \times |0\rangle, \tag{E1}$$

where $\{\sigma\} = (\sigma_{i_1}, \sigma_{i_2}, \sigma_{i_3}, \dots, \sigma_{i_{N_\Lambda}})$. By modifying the $\{\sigma\}$ sets in Eq. (E1) one obtains 2^{N_Λ} states, which obey $\langle \Psi_{g, \{\sigma\}} | \Psi_{g, \{\sigma'\}} \rangle = \text{Det}[x_{i,j}(\{X_{\mathbf{k}}^*, \{X_{\mathbf{k}}\}, \sigma_i, \sigma_j')]$, where $x_{i,j}(\{X_{\mathbf{k}}^*, \{X_{\mathbf{k}}\}, \sigma_i, \sigma_j') = \delta_{\sigma_i, \sigma_j'} (1/N_\Lambda) \sum_{\mathbf{k}} V_{\mathbf{k}}^* W_{\mathbf{k}} e^{i\mathbf{k}(j-i)}$. 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 $X_{\mathbf{k}} \neq 0$ for all \mathbf{k} . Introducing the states

$$|\Psi_g^{\{\sigma\}}\rangle = \left(\prod_{\mathbf{k}} \hat{C}_{1,\mathbf{k}\uparrow}^\dagger \hat{C}_{1,\mathbf{k}\downarrow}^\dagger \right) \left[\prod_{n=1}^{N_\Lambda} \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}_n} \frac{1}{X_{\mathbf{k}_n}^*} e^{i\mathbf{k}_n i_n} \hat{C}_{2,\mathbf{k}_n \sigma_{i_n}}^\dagger \right) \right] \times |0\rangle, \quad (\text{E2})$$

one finds $\langle \Psi_g^{\{\sigma\}} | \Psi_g^{\{\sigma'\}} \rangle = \text{Det}[z_{i,j}(\sigma_i, \sigma'_j)]$, where $z_{i,j}(\sigma_i, \sigma'_j) = x_{i,j}(\{1/X_{\mathbf{k}_j}\}, \{X_{\mathbf{k}_j}\}, \sigma_i, \sigma'_j) = \delta_{\sigma_i, \sigma'_i} \delta_{i,j}$, such that

$\text{Det}[z_{i,j}(\sigma_i, \sigma'_j)] = \delta_{\{\sigma\}, \{\sigma'\}}$. This yields $\langle \Psi_g^{\{\sigma\}} | \Psi_g^{\{\sigma'\}} \rangle = \delta_{\{\sigma\}, \{\sigma'\}}$, i.e., the set $\{|\Psi_g^{\{\sigma\}}\rangle\}$ is linearly independent and for $N = 3N_\Lambda$ provides a basis for \mathcal{H}_g [see Eq. (10)]. An arbitrary state of the form of (42) can then be written as $|\Psi_g\rangle = \sum_{\{\sigma\}} \alpha_{\{\sigma\}} |\Psi_g^{\{\sigma\}}\rangle$, where $\alpha_{\{\sigma\}}$ are numerical coefficients.¹⁸ Furthermore, one finds

$$\begin{aligned} \hat{C}_{2,\mathbf{k}_1 \sigma_1}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma_2} |\Psi_g^{\{\sigma'\}}\rangle &= \sum_{n=1}^{N_\Lambda} |\Psi_{g,\{\sigma'\},n}^{(\mathbf{k}_1 \sigma_1), (\mathbf{k}_2 \sigma_2)}\rangle, \quad |\Psi_{g,\{\sigma'\},n}^{(\mathbf{k}_1 \sigma_1), (\mathbf{k}_2 \sigma_2)}\rangle = \left(\prod_{\mathbf{k}'} \hat{C}_{1,\mathbf{k}'\uparrow}^\dagger \hat{C}_{1,\mathbf{k}'\downarrow}^\dagger \right) \\ &\times \left[\left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}' i_1} \hat{C}_{2,\mathbf{k}' \sigma'_{i_1}}^\dagger \right) \cdots \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}' i_{n-1}} \hat{C}_{2,\mathbf{k}' \sigma'_{i_{n-1}}}^\dagger \right) \left(\frac{1}{\sqrt{N_\Lambda}} X_{\mathbf{k}_2} e^{i\mathbf{k}_2 i_n} \hat{C}_{2,\mathbf{k}_1 \sigma_1}^\dagger \delta_{\sigma'_{i_n}, \sigma_2} \right) \right. \\ &\left. \times \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}' i_{n+1}} \hat{C}_{2,\mathbf{k}' \sigma'_{i_{n+1}}}^\dagger \right) \cdots \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}' i_{N_\Lambda}} \hat{C}_{2,\mathbf{k}' \sigma'_{i_{N_\Lambda}}}^\dagger \right) \right] |0\rangle, \quad (\text{E3}) \end{aligned}$$

from which

$$\langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,\mathbf{k}_1 \sigma_1}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma_2} |\Psi_g^{\{\sigma'\}}\rangle = \sum_{n=1}^{N_\Lambda} \text{Det}[\bar{z}_{i,j}(n, \sigma''_i, \sigma'_j)] \quad (\text{E4})$$

follows. Here, the matrix $\bar{z}_{i,j}(n, \sigma''_i, \sigma'_j)$ is the same as $z_{i,j}(\sigma''_i, \sigma'_j)$, except for the matrix elements in the n th column which are given by $\bar{z}_{i,n} = (1/N_\Lambda) \times (X_{\mathbf{k}_2}/X_{\mathbf{k}_1}) e^{i(\mathbf{k}_2 i_n - \mathbf{k}_1 i)} \delta_{\sigma''_i, \sigma_1} \delta_{\sigma'_i, \sigma_2}$. From Eq. (E4) one finds that $\langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,\mathbf{k}_1 \sigma_1}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma_2} |\Psi_g^{\{\sigma'\}}\rangle$ vanishes in the thermodynamic limit as $1/N_\Lambda$. In the case of $\sigma_1 = \sigma_2 = \sigma$, only $\{\sigma''\} = \{\sigma'\}$ components remain in Eq. (E4), yielding

$$\begin{aligned} \langle \Psi_g^{\{\sigma''\}} | \hat{C}_{2,\mathbf{k}_1 \sigma}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma} |\Psi_g^{\{\sigma'\}}\rangle \\ = \delta_{\{\sigma''\}, \{\sigma'\}} \frac{X_{\mathbf{k}_2}}{X_{\mathbf{k}_1}} \frac{1}{N_\Lambda} \sum_{n=1}^{N_\Lambda} \delta_{\sigma, \sigma'_i} e^{i(\mathbf{k}_2 - \mathbf{k}_1) i_n}, \quad (\text{E5}) \end{aligned}$$

where $\sum_{n=1}^{N_\Lambda} \delta_{\sigma, \sigma'_i}$ quantifies the number of σ spins from $\{\sigma'\}$. Since $\sum_{\sigma} \delta_{\sigma, \sigma'_i} = 1$ for arbitrary σ'_i , it follows that $\langle \Psi_g^{\{\sigma''\}} | \sum_{\sigma} \hat{C}_{2,\mathbf{k}_1 \sigma}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma} |\Psi_g^{\{\sigma'\}}\rangle = \delta_{\mathbf{k}_2, \mathbf{k}_1} \delta_{\{\sigma''\}, \{\sigma'\}}$. Using the notation $\langle \cdots \rangle = \langle \Psi_g | \cdots | \Psi_g \rangle / \langle \Psi_g | \Psi_g \rangle$, one finally obtains

$$\left\langle \sum_{\sigma} \hat{C}_{2,\mathbf{k}_1 \sigma}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma} \right\rangle = \delta_{\mathbf{k}_2, \mathbf{k}_1}. \quad (\text{E6})$$

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

$$\begin{aligned} \langle \hat{A} \rangle &= \lim_{T \rightarrow 0} \frac{\text{Tr}(\hat{A} e^{-\beta \hat{H}})}{\text{Tr}(e^{-\beta \hat{H}})} = \lim_{T \rightarrow 0} \frac{\text{Tr}(\hat{A} e^{-\beta \hat{H}_g})}{\text{Tr}(e^{-\beta \hat{H}_g})} \\ &= \frac{\sum_{\{\sigma\}} \langle \Psi_g^{\{\sigma\}} | \hat{A} | \Psi_g^{\{\sigma\}} \rangle}{\sum_{\{\sigma\}} \langle \Psi_g^{\{\sigma\}} | \Psi_g^{\{\sigma\}} \rangle}, \quad (\text{E7}) \end{aligned}$$

where \hat{A} is an arbitrary operator and \hat{H}_g is defined in Eq. (36). The second equality in Eq. (E7) holds since for $N_\Lambda < \infty$ 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 . Equation (E7) therefore yields

$$\langle \hat{C}_{2,\mathbf{k}_1 \sigma_1}^\dagger \hat{C}_{2,\mathbf{k}_2 \sigma_2} \rangle = \frac{1}{2} \delta_{\mathbf{k}_2, \mathbf{k}_1} \delta_{\sigma_2, \sigma_1}. \quad (\text{E8})$$

2. The case $X_{\mathbf{k}} = 0$

Here we consider the case $a_{\mathbf{k}^*, d} = 0$ for a given vector $\mathbf{k} = \mathbf{k}^*$ which implies $X_{\mathbf{k}^*} = 0$ (we note that the $\hat{C}_{\delta, \mathbf{k}\sigma}$ operators are then still well defined and $R_{\mathbf{k}^*}^{-1} \neq 0$), with $X_{\mathbf{k} \neq \mathbf{k}^*} \neq 0$. Such a situation arises, for example, in the case of the itinerant solution (see Sec. IV B) for large next-nearest-neighbor hopping amplitude $|t_1^d/t_2^d| \leq 3$. Except for \mathbf{k}^* Eqs. (E6) and (E8) remain valid in the thermodynamic limit, and the ground-state expectation values of the momentum occupation becomes

$$\langle \hat{C}_{1,\mathbf{k}\sigma}^\dagger \hat{C}_{1,\mathbf{k}\sigma} \rangle = 1, \quad \langle \hat{C}_{2,\mathbf{k}^* \sigma}^\dagger \hat{C}_{2,\mathbf{k}^* \sigma} \rangle = 0, \quad (\text{E9})$$

$$\langle \hat{C}_{2,\mathbf{k}\neq\mathbf{k}^*}^\dagger \hat{C}_{2,\mathbf{k}\neq\mathbf{k}^*} \rangle = \frac{1}{2}.$$

We note that for one vector \mathbf{k}^* the maximum total spin decreases from $N_\Lambda/2$ to $N_\Lambda/2-1$ since in the sum over \mathbf{k}_n in Eqs. (E1) and (E2) the term with \mathbf{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 $\hat{C}_{2,\mathbf{k}\sigma}$ operators. Using Eq. (E3) one finds

$$\begin{aligned} & \hat{C}_{2,\mathbf{k}_3\sigma_3}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma_4} \hat{C}_{2,\mathbf{k}_1\sigma_1}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma_2} |\Psi_{g,\{\sigma'\}}\rangle \\ &= \delta_{\mathbf{k}_1,\mathbf{k}_4} \delta_{\sigma_1,\sigma_4} \sum_{n=1}^{N_\Lambda} |\Psi_{g,\{\sigma'\},n}^{(\mathbf{k}_3\sigma_3),(\mathbf{k}_2\sigma_2)}\rangle + (1 - \delta_{\mathbf{k}_1,\mathbf{k}_3} \delta_{\sigma_1,\sigma_3}) (1 \\ & \quad - \delta_{\mathbf{k}_2,\mathbf{k}_4} \delta_{\sigma_2,\sigma_4}) \sum_{n=1}^{N_\Lambda} \sum_{m=1, m \neq n}^{N_\Lambda} |\Psi_{g,\{\sigma'\},m,n}^{[(\mathbf{k}_3\sigma_3),(\mathbf{k}_4\sigma_4)];[(\mathbf{k}_1\sigma_1),(\mathbf{k}_2\sigma_2)]}\rangle, \end{aligned} \quad (\text{E10})$$

where $\mathbf{k}_4 = \mathbf{k}_3 + \mathbf{k}_1 - \mathbf{k}_2$. Here $|\Psi_{g,\{\sigma'\},n}^{(\mathbf{k}_3\sigma_3),(\mathbf{k}_2\sigma_2)}\rangle$ is defined in Eq. (E3), and

$$\begin{aligned} |\Psi_{g,\{\sigma'\},m,n}^{[(\mathbf{k}_3\sigma_3),(\mathbf{k}_4\sigma_4)];[(\mathbf{k}_1\sigma_1),(\mathbf{k}_2\sigma_2)]}\rangle &= \left(\prod_{\mathbf{k}'}^{N_\Lambda} \hat{C}_{1,\mathbf{k}'\uparrow}^\dagger \hat{C}_{1,\mathbf{k}'\downarrow}^\dagger \right) \left[\left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_1} \hat{C}_{2,\mathbf{k}'\sigma'_1}^\dagger \right) \times \dots \times \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_{m-1}} \hat{C}_{2,\mathbf{k}'\sigma'_{m-1}}^\dagger \right) \right. \\ & \quad \times \left(\frac{1}{\sqrt{N_\Lambda}} X_{\mathbf{k}_4} e^{i\mathbf{k}_4\cdot\mathbf{i}_m} \hat{C}_{2,\mathbf{k}_3\sigma_3}^\dagger \delta_{\sigma'_m,\sigma_4} \right) \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_{m+1}} \hat{C}_{2,\mathbf{k}'\sigma'_{m+1}}^\dagger \right) \times \dots \\ & \quad \times \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_{n-1}} \hat{C}_{2,\mathbf{k}'\sigma'_{n-1}}^\dagger \right) \left(\frac{1}{\sqrt{N_\Lambda}} X_{\mathbf{k}_2} e^{i\mathbf{k}_2\cdot\mathbf{i}_n} \hat{C}_{2,\mathbf{k}_1\sigma_1}^\dagger \delta_{\sigma'_n,\sigma_2} \right) \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_{n+1}} \hat{C}_{2,\mathbf{k}'\sigma'_{n+1}}^\dagger \right) \\ & \quad \left. \times \dots \times \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{k}'} X_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{i}_{N_\Lambda}} \hat{C}_{2,\mathbf{k}'\sigma'_{N_\Lambda}}^\dagger \right) \right] |0\rangle \end{aligned} \quad (\text{E11})$$

contains only contributions with $n \neq m$. The expectation value of the density-density correlation function can be calculated from Eq. (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 $\bar{Z}_{\mathbf{k}_3,\mathbf{k}_1}^{\mathbf{k}_4,\mathbf{k}_2} = Z_{\mathbf{k}_3 \neq \mathbf{k}_1, \mathbf{k}_1}^{\mathbf{k}_4 \neq \mathbf{k}_2, \mathbf{k}_2}$, where $Z_{\mathbf{k}_3,\mathbf{k}_1}^{\mathbf{k}_4,\mathbf{k}_2} = X_{\mathbf{k}_4} X_{\mathbf{k}_2} / (X_{\mathbf{k}_3} X_{\mathbf{k}_1} N_\Lambda)$ and using the procedure leading to Eq. (E6) one then finds

$$\begin{aligned} & \left\langle \sum_{\sigma_a, \sigma_b} \hat{C}_{2,\mathbf{k}_3\sigma_b}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma_b} \hat{C}_{2,\mathbf{k}_1\sigma_a}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma_a} \right\rangle \\ &= \delta_{\mathbf{k}_1,\mathbf{k}_4} \delta_{\mathbf{k}_2,\mathbf{k}_3} + \delta_{\mathbf{k}_1,\mathbf{k}_2} \delta_{\mathbf{k}_3,\mathbf{k}_4} - \bar{Z}_{\mathbf{k}_3,\mathbf{k}_1}^{\mathbf{k}_4,\mathbf{k}_2} \delta_{\mathbf{k}_4,\mathbf{k}_3+\mathbf{k}_1-\mathbf{k}_2}. \end{aligned} \quad (\text{E12})$$

The same expression is obtained if we calculate the expectation value in the $T \rightarrow 0$ limit, as described in connection with Eqs. (E7) and (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 Eqs. (E7), (E8), and (E10), one finds in the $T \rightarrow 0$ limit

$$\begin{aligned} & \left\langle \sum_{\sigma} \hat{C}_{2,\mathbf{k}_3\sigma}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma} \hat{C}_{2,\mathbf{k}_1\sigma}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma} \right\rangle \\ &= \delta_{\mathbf{k}_1,\mathbf{k}_4} \delta_{\mathbf{k}_2,\mathbf{k}_3} + \frac{1}{2} \delta_{\mathbf{k}_1,\mathbf{k}_2} \delta_{\mathbf{k}_3,\mathbf{k}_4} - \frac{1}{2} \bar{Z}_{\mathbf{k}_3,\mathbf{k}_1}^{\mathbf{k}_4,\mathbf{k}_2} \delta_{\mathbf{k}_4,\mathbf{k}_3+\mathbf{k}_1-\mathbf{k}_2}, \\ & \left\langle \sum_{\sigma} \hat{C}_{2,\mathbf{k}_3\sigma}^\dagger \hat{C}_{2,\mathbf{k}_4\sigma} \hat{C}_{2,\mathbf{k}_1-\sigma}^\dagger \hat{C}_{2,\mathbf{k}_2-\sigma} \right\rangle \\ &= \frac{1}{2} \delta_{\mathbf{k}_1,\mathbf{k}_2} \delta_{\mathbf{k}_3,\mathbf{k}_4} - \frac{1}{2} \bar{Z}_{\mathbf{k}_3,\mathbf{k}_1}^{\mathbf{k}_4,\mathbf{k}_2} \delta_{\mathbf{k}_4,\mathbf{k}_3+\mathbf{k}_1-\mathbf{k}_2}. \end{aligned} \quad (\text{E13})$$

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

$$\begin{aligned} & \left\langle \sum_{\sigma} \hat{C}_{2,\mathbf{k}_3\sigma}^\dagger \hat{C}_{2,\mathbf{k}_4-\sigma} \hat{C}_{2,\mathbf{k}_1-\sigma}^\dagger \hat{C}_{2,\mathbf{k}_2\sigma} \right\rangle = \delta_{\mathbf{k}_1,\mathbf{k}_4} \delta_{\mathbf{k}_2,\mathbf{k}_3}, \\ & \left\langle \sum_{\sigma} \hat{C}_{1,\mathbf{k}_3\sigma}^\dagger \hat{C}_{2,\mathbf{k}_4-\sigma} \hat{C}_{2,\mathbf{k}_1-\sigma}^\dagger \hat{C}_{1,\mathbf{k}_2\sigma} \right\rangle \delta_{\mathbf{k}_4,\mathbf{k}_3+\mathbf{k}_1-\mathbf{k}_2} = \delta_{\mathbf{k}_2,\mathbf{k}_3} \delta_{\mathbf{k}_1,\mathbf{k}_4}. \end{aligned} \quad (\text{E14})$$

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- ³²For the operators $\hat{C}_{\delta,\mathbf{k},\sigma}$ to be well defined, $R_{\mathbf{k}}^{-1}$ has to be nonzero for all \mathbf{k} . This holds for both itinerant solutions discussed in Sec. IV [see Eq. (34)]. For example, for the solution obtained in Sec. IV B, one finds $|a_{\mathbf{k},f}|^2 = |a_f|^2 = |V_1|^2/|t_2^d|$, $|a_{\mathbf{k},d}|^2 = |t_2^d| \{ [|t_1^d|/|t_2^d| - \text{sgn}(t_1^d)(\sum_{\tau=1}^3 \cos k_{\tau})]^2 + (\sum_{\tau=1}^3 \sin k_{\tau})^2 \}$.
- ³³Using Eq. (35) one obtains $\hat{a}_{\mathbf{k},\sigma} = \sqrt{R_{\mathbf{k}}}(a_{\mathbf{k},d}^* \hat{C}_{1,\mathbf{k},\sigma} + a_{\mathbf{k},f} \hat{C}_{2,\mathbf{k},\sigma})$, $\hat{f}_{\mathbf{k},\sigma} = \sqrt{R_{\mathbf{k}}}(a_{\mathbf{k},f}^* \hat{C}_{1,\mathbf{k},\sigma} - a_{\mathbf{k},d} \hat{C}_{2,\mathbf{k},\sigma})$.
- ³⁴The first equality in (35) leads to $-\sum_{i,\sigma} \hat{A}_{i,\sigma}^{\dagger} \hat{A}_{i,\sigma} = \sum_{\mathbf{k},\sigma} (-1/R_{\mathbf{k}}) \hat{C}_{1,\mathbf{k},\sigma}^{\dagger} \hat{C}_{1,\mathbf{k},\sigma}$. With $\sum_{\delta=1,2} \hat{C}_{\delta,\mathbf{k},\sigma}^{\dagger} \hat{C}_{\delta,\mathbf{k},\sigma} = \sum_{b=d,f} \hat{C}_{b,\mathbf{k},\sigma}^{\dagger} \hat{C}_{b,\mathbf{k},\sigma}$ this leads to $\hat{N} = \sum_{\mathbf{k}} \sum_{\delta=1,2} \hat{C}_{\delta,\mathbf{k},\sigma}^{\dagger} \hat{C}_{\delta,\mathbf{k},\sigma}$.
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- ⁴¹For example, we can choose \mathcal{D}_{\uparrow} to be defined by the set $(\mathbf{x}_1, \mathbf{x}_2, 2\mathbf{x}_3)$ of primitive vectors, and $\mathbf{R} = \mathbf{x}_3$.
- ⁴²The consequences of $|a_{\mathbf{k},d}| = 0$ with $R_{\mathbf{k}} \neq 0$ are pointed out in Appendix E 2.
- ⁴³There exist special cases (see, e.g., Sec. IV B for $|t_1^d/t_2^d| < 3$ and Ref. 32) where for some vector \mathbf{k}^* one has $a_{\mathbf{k}^*,d} = 0$ and hence $X_{\mathbf{k}=\mathbf{k}^*} = 0$. Nevertheless, as long as $R_{\mathbf{k}}^{-1} \neq 0$ for all \mathbf{k} the operators $\hat{C}_{\delta,\mathbf{k},\sigma}$ 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., $\langle \hat{C}_{2,\mathbf{k},\sigma}^{\dagger} \hat{C}_{2,\mathbf{k},\sigma} \rangle$ is $1/2$ for all \mathbf{k} , except for \mathbf{k}^* where it is zero.
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- ⁵⁰The $a_{k,b}$ parameters presented in Eq. (34), are now defined by the Fourier transform of $\hat{B}_{B_i, \sigma}^\dagger$ which has the form $\hat{B}_{k, \sigma}^\dagger = \sum_{b=d,f} a_{k, \sigma}^* \hat{B}_{k, \sigma}^*$, where $a_{k, f} = a_{6, f}$, and $a_{k, d} = a_{6, d} + a_{1, d} e^{-ikx_1} + a_{2, d} e^{-ikx_2} + a_{3, d} e^{+ikx_1} + a_{4, d} e^{+ikx_2} + a_{5, d} e^{-ikx_3} + a_{7, d} e^{+ikx_3}$. For the solution defined below Eq. (57), one finds $a_{k, d} = \sqrt{2} |t_2^d| e^{i\phi} [(\sum_{\tau=1}^3 \cos k_\tau) + (|V_0|/2V_1) e^{-i\phi_{V_0}}]$, $a_{k, f} = -V_1 \sqrt{2} |t_2^d| e^{i\phi}$. The parameters $R_{\mathbf{k}}^{-1}$, $|a_{k, f}|$ are nonzero for all \mathbf{k} [see Eq. (35)], so the operators $\hat{C}_{\delta \mathbf{k}, \sigma}$ are well defined. For real V_0 one finds $|a_{k, d}| \neq 0$ for $|t_1^d / t_2^d| > 6$, while for $\text{Im}(V_0) \neq 0$ one always has $|a_{k, d}| > 0$. We note that $a_{k, d} \neq 0$ implies $X_{\mathbf{k}} \neq 0$, where $X_{\mathbf{k}}$ has been defined in Eq. (42).
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