Exact Insulating and Conducting Ground States of a Periodic Anderson Model in Three Dimensions

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We present a class of exact ground states of a three-dimensional periodic Anderson model at 3/4 filling. Hopping and hybridization of d and f electrons extend over the unit cell of a general Bravais lattice. Employing novel composite operators combined with 55 matching conditions the Hamiltonian is cast into positive semidefinite form. A product wave function in position space allows one to identify stability regions of an insulating and a conducting ground state. The metallic phase is a non-Fermi liquid with one dispersing and one flat band.

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The periodic Anderson model (PAM) is the basic microscopic model for the investigation of heavy-fermion and intermediate valence systems, e.g., compounds containing elements with incompletely filled f shells such as cerium or uranium [1]. In its simplest form the PAM describes strongly correlated, dispersionless f electrons which couple, via a local hybridization, to noninteracting conduction (d) electrons hopping between nearest-neighbor sites. For real systems this is certainly an oversimplification since there is experimental evidence for (i) a weak, but finite, dispersion of the f electrons (especially in uranium compounds) [2], (ii) nonlocal contributions to the hybridization, and (iii) hopping of the d electrons beyond nearest neighbors [3].

Recently, investigations into the origin of the dramatic volume collapse at the $\alpha \rightarrow \gamma$ transition in cerium have drawn attention to the possibility of a Mott metal-insulator transition in the PAM [4–6]. Although such a transition is usually associated with the half-filled Hubbard model with nearest-neighbor hopping, there exist remarkable similarities between the two models [7], especially if both the d electron hopping and $d-f$ hybridization in the PAM connect nearest-neighbor sites [7–10]. These results show that the spatial range of the hopping and hybridization in the PAM are very important, even on a qualitative level.

In this situation exact results on the existence of insulating and metallic phases in the PAM and their dependence on a general set of hopping, hybridization, and interaction parameters are particularly desirable. Exact results for the PAM are very rare since, in contrast to the Hubbard model, there does not even exist an exact solution of the PAM in dimension $D = 1$. On the other hand, it has been possible to construct exact ground states of the PAM in certain regions of parameter space, namely, for infinite repulsion of the f electrons [11–13]and for finite repulsion in low dimensions ($D = 1, 2$) [14,15].

In this Letter we show that it is possible to construct exact ground state wave functions describing metallic and insulating phases of the PAM at noninteger electron filling *even in dimension* $D = 3$. In particular, we explicitly demonstrate (i) the insulating and conducting nature of the solutions, (ii) the presence of strong variations in the compressibility of the system when leaving the insulating phase, and (iii) the non-Fermi liquid nature of the metallic phase.

We consider a general Bravais lattice in $D = 3$ with a unit cell I defined by the primitive vectors $\{\mathbf{x}_\tau\}$, $\tau = 1, 2, 3$. The Hamiltonian of the PAM has the form $\hat{H} = \hat{H}_0 + U\hat{D}^f$, where $\hat{D}^f = \sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i}\uparrow}\hat{n}^f_{\mathbf{i}\downarrow}$ describes the local Coulomb repulsion between the f electrons ($U > 0$). The one-particle part may, in general, be written as

$$\hat{H}_0 = \sum_{\mathbf{i},\sigma}\Big\{\sum_{\mathbf{r}}[t^d_{\mathbf{r}}\hat{d}^\dagger_{\mathbf{i}\sigma}\hat{d}_{\mathbf{i}+\mathbf{r},\sigma} + t^f_{\mathbf{r}}\hat{f}^\dagger_{\mathbf{i}\sigma}\hat{f}_{\mathbf{i}+\mathbf{r},\sigma} + V_{\mathbf{r}}(\hat{d}^\dagger_{\mathbf{i}\sigma}\hat{f}_{\mathbf{i}+\mathbf{r},\sigma} + \hat{f}^\dagger_{\mathbf{i}\sigma}\hat{d}_{\mathbf{i}+\mathbf{r},\sigma}) + \text{H.c.}] + V_0(\hat{d}^\dagger_{\mathbf{i}\sigma}\hat{f}_{\mathbf{i}\sigma} + \text{H.c.}) + E_f\hat{n}^f_{\mathbf{i}\sigma}\Big\}, \quad (1)$$

where the terms with $t^{d,f}_{\mathbf{r}}$ represent the kinetic energy of d and f electrons due to hopping between two sites $\mathbf{i}$ and $\mathbf{i}+\mathbf{r}$, $V_{\mathbf{r}}$ is the hybridization of d and f electrons at sites $\mathbf{i}$ and $\mathbf{i}+\mathbf{r}$, V_0 is the local hybridization, and E_f is the local f electron energy; here $\mathbf{r} \neq 0$. The amplitudes $t^{d,f}_{\mathbf{r}}$ are real, but $V_{\mathbf{r}}, V_0$ can, in principle, be complex. In our investigation the hopping and hybridization of the d and f electrons extend over the unit cell of a general Bravais lattice (Fig. 1). To avoid multiple counting of contributions to (1) by the H.c. term, the vector $\mathbf{r}$ must be properly defined. To this end the sites within $I_{\mathbf{i}}$, the unit cell defined at site $\mathbf{i}$, are denoted by $\mathbf{r}_{I_{\mathbf{i}}} = \mathbf{i} + \mathbf{r}_{\alpha\beta\gamma}$, 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 $\mathbf{r}_{I_{\mathbf{i}}}$ can be numbered by the indices $n(\alpha, \beta, \gamma) = 1 + \alpha + 3\beta + 4\gamma - 2\alpha\beta$ without reference to $I_{\mathbf{i}}$. In the following we use orthogonal $\mathbf{x}_\tau$ vectors for simplicity. 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 [16].

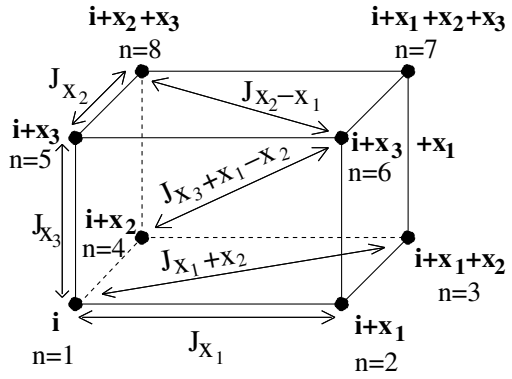

FIG. 1. Unit cell (I) of an orthorhombic lattice at an arbitrary site $\mathbf{i}$ showing the primitive vectors $\mathbf{x}_\tau$ and indices n of the sites in I. Arrows depict some of the hopping and hybridization matrix elements ($J = t, V$) extending over I.

We now introduce a superposition of operators creating b ($=d$ or f) electrons inside every unit cell $I_\mathbf{i}$ as

$$\hat{A}^\dagger_{I_\mathbf{i}\sigma} = \sum_{b=d,f} \sum_{\alpha,\beta,\gamma=0}^{1} a^*_{n(\alpha,\beta,\gamma),b} \hat{b}^\dagger_{\mathbf{i}+\mathbf{r}_{\alpha\beta\gamma},\sigma} = \sum_{b=d,f} (a^*_{1,b}\hat{b}^\dagger_{\mathbf{i}\sigma} + a^*_{2,b}\hat{b}^\dagger_{\mathbf{i}+\mathbf{x}_1,\sigma} + \ldots + a^*_{8,b}\hat{b}^\dagger_{\mathbf{i}+\mathbf{x}_2+\mathbf{x}_3,\sigma}), \tag{2}$$

with $a^*_{n,b} \neq 0$ for all n. Although $\{\hat{A}^\dagger_{I\sigma}, \hat{A}^\dagger_{I'\sigma'}\} = \{\hat{A}_{I\sigma}, \hat{A}_{I'\sigma'}\} = 0$ and $\{\hat{A}_{I\sigma}, \hat{A}^\dagger_{I\sigma}\} = K_d + K_f$, where $K_b = \sum_{n=1}^{8} |a_{n,b}|^2$ and $n \equiv n(\alpha, \beta, \gamma)$, the composite operator $\hat{A}^\dagger_{I\sigma}$ does not obey canonical anticommutation rules since $\{\hat{A}_{I\sigma}, \hat{A}^\dagger_{I'\sigma'}\} \neq 0$ for $I \neq I'$. Because of the translational symmetry of the lattice the prefactors $a^*_{n,b}$ *are the same* in every unit cell. Making use of this fact, $\hat{H}$ can be cast into the form

$$\hat{H} = \sum_{\mathbf{i},\sigma} \hat{A}_{I_\mathbf{i}\sigma}\hat{A}^\dagger_{I_\mathbf{i}\sigma} + U\sum_{\mathbf{i}} \hat{P}_\mathbf{i} + E_g, \tag{3}$$

where $\hat{P}_\mathbf{i} = \hat{n}^f_{\mathbf{i}\uparrow}\hat{n}^f_{\mathbf{i}\downarrow} - \hat{n}^f_{\mathbf{i}\uparrow} - \hat{n}^f_{\mathbf{i}\downarrow} + 1$, $E_g = K_d N + UN_\Lambda - 2N_\Lambda(2K_d - E_f)$, and N and N_Λ are the number of electrons and lattice sites, respectively. For (3) to reproduce (1) the prefactors $a^*_{n,b}$ in $\hat{A}^\dagger_{I_\mathbf{i}\sigma}$ must be expressed in terms of the microscopic parameters $t^d_\mathbf{r}$, $t^f_\mathbf{r}$, $V_\mathbf{r}$, $V^*_\mathbf{r}$, V_0, V^*_0, E_f, U, for all $\mathbf{r} \in I_\mathbf{i}$, taking into account periodic boundary conditions. This leads to 55 coupled, nonlinear matching conditions [17] which can be written in compact notation, with $b, b' = d, f$, as [18]

$$\sum_{\beta_1,\beta_2,\beta_3=-1}^{1} \left(\prod_{i=1}^{3} D_{\beta_i,\alpha_i}\right) a^*_{n^+,b} a_{n^-,b'} = T^{b,b'}_{\bar{\mathbf{r}},\nu}. \tag{4}$$

Apart from the constant term E_g in (3) $\hat{H}$ is a positive semidefinite operator. A state $|\Psi_g\rangle$ fulfilling the conditions $\hat{P}_\mathbf{i}|\Psi_g\rangle = 0$ and $\hat{A}^\dagger_{I_\mathbf{i}\sigma}|\Psi_g\rangle = 0$ for all $\mathbf{i}$ will then be an *exact ground state* of $\hat{H}$ with energy E_g. We note that $\hat{P}_\mathbf{i}$ assumes its lowest eigenvalue, 0, when there is at least one f electron on site $\mathbf{i}$. Therefore, a state of the form $|\Psi_g\rangle \sim \prod_{\mathbf{i}=1}^{N_\Lambda} \hat{F}^\dagger_\mathbf{i}|0\rangle$, where the operator $\hat{F}^\dagger_\mathbf{i} = \mu_{\mathbf{i}\uparrow}\hat{f}^\dagger_{\mathbf{i}\uparrow} + \mu_{\mathbf{i}\downarrow}\hat{f}^\dagger_{\mathbf{i}\downarrow}$ (with arbitrary coefficients $\mu_{\mathbf{i}\sigma}$) creates one f electron on every site $\mathbf{i}$, fulfills the first condition. Further, a state of the form $|\Psi_g\rangle \sim \prod_{\mathbf{i}=1}^{N_\Lambda}(\hat{A}^\dagger_{I_\mathbf{i}\uparrow}\hat{A}^\dagger_{I_\mathbf{i}\downarrow})|0\rangle$ fulfills the second condition. Consequently, the (unnormalized) product state

$$|\Psi_g\rangle = \prod_{\mathbf{i}=1}^{N_\Lambda} [\hat{A}^\dagger_{I_\mathbf{i}\uparrow}\hat{A}^\dagger_{I_\mathbf{i}\downarrow}\hat{F}^\dagger_\mathbf{i}]|0\rangle \tag{5}$$

has at least one f electron on every site $\mathbf{i}$, the product $\prod_{\mathbf{i}=1}^{N_\Lambda} \hat{A}^\dagger_{I_\mathbf{i}\uparrow}\hat{A}^\dagger_{I_\mathbf{i}\downarrow}$ creating at most two more (d or f) electrons on $\mathbf{i}$. Clearly, $|\Psi_g\rangle$ has the desired property $\hat{H}|\Psi_g\rangle = E_g|\Psi_g\rangle$ and is thus an exact ground state of $\hat{H}$ with energy E_g. Although $|\Psi_g\rangle$ is a product state over sites i it is actually *nonlocal* because the operator $\hat{A}^\dagger_{I_i\sigma}$ creates electrons also at the boundaries of the unit cell I_i with neighboring unit cells. This leads to a genuine dependence of $|\Psi_g\rangle$ on the lattice structure and hence on the spatial dimension.

Since the product of the three operators in $|\Psi_g\rangle$ creates $N = 3N_\Lambda$ electrons, the ground state is 3/4 filled; i.e., there are on average three electrons per site. The arbitrariness of $\mu_{\mathbf{i},\sigma}$ implies a large spin degeneracy of $|\Psi_g\rangle$ which is globally paramagnetic (for $\mu_{\mathbf{i}\sigma} = \mu_\sigma$ it would be ferromagnetic). Neglecting the trivial $2S + 1$ multiplicity of the spin orientation, the ground state is $N_\Lambda/2$-fold degenerate [19]; all degeneracies are still contained in (5). We note that a ground state solution $|\Psi_g\rangle$ for a particular value of the interaction $U = U_1$ is not connected in any simple way to a solution for a different value $U = U_2$ since the constraint (4) requires all other parameters to adjust when U is changed. In particular, $|\Psi_g\rangle$ is not a ground state at $U = 0$.

The physical nature of $|\Psi_g\rangle$ depends on the values of the coefficients $a^*_{n,b}$ in (2) which are solutions of (4) for given microscopic parameters. We now identify localized and itinerant ground states and discuss their physical properties.

(i) *Localized ground state.*—The coefficients $a_{n,b}$ may be chosen in such a way that $|\Psi_g\rangle$ has *exactly* three electrons per site. To see how this can be achieved we take a look at a typical factor $\hat{A}^\dagger_{I_\mathbf{j}\uparrow}\hat{A}^\dagger_{I_\mathbf{j}\downarrow}\hat{A}^\dagger_{I_{\mathbf{j}'}\uparrow}\hat{A}^\dagger_{I_{\mathbf{j}'}\downarrow}\hat{F}^\dagger_{\mathbf{j}''}$ entering in $|\Psi_g\rangle$, where $\mathbf{j}''$ is a common site of the two unit cells $I_\mathbf{j}$, $I_{\mathbf{j}'}$. Since $\hat{F}^\dagger_{\mathbf{j}''}$ always creates one f electron on $\mathbf{j}''$, the product of the four unit cell operators should create only two more electrons (one $\uparrow$ and one $\downarrow$) on $\mathbf{j}''$. Therefore, terms of the form $\hat{d}^\dagger_{\mathbf{j}''\uparrow}\hat{f}^\dagger_{\mathbf{j}''\uparrow}\hat{d}^\dagger_{\mathbf{j}''\downarrow}\hat{f}^\dagger_{\mathbf{j}''\downarrow}(a^*_{n_1,d}a^*_{n_2,f} - a^*_{n_1,f}a^*_{n_2,d})^2$ which are also generated and which lead to more than two additional electrons on this site must be prohibited. This can be achieved by choosing $a^*_{n,d}/a^*_{n,f} = p_n \equiv p$ for all n. It follows from (4) that along the diagonal of a unit cell with end points n, n' the relation $a^*_{n,f}a_{n',d} = a^*_{n,d}a_{n',f}$ holds, implying p and therefore also the hybridization

amplitudes to be real. A solution of (4) of this form is obtained for $t^b_{\mathbf{r}} = t^b_v$, i.e., for equal hopping along x, y, z. In this case the ground state takes the form

$$|\Psi_{\rm loc}\rangle = \prod_{\mathbf{i}}\Big[\sum_{\sigma}\mu_{\mathbf{i}\sigma}(p\hat{d}^{\dagger}_{\mathbf{i}\downarrow}\hat{d}^{\dagger}_{\mathbf{i}\uparrow}\hat{f}^{\dagger}_{\mathbf{i}\sigma} + \hat{f}^{\dagger}_{\mathbf{i}\uparrow}\hat{f}^{\dagger}_{\mathbf{i}\downarrow}\hat{d}^{\dagger}_{\mathbf{i}\sigma})\Big]|0\rangle. \quad (6)$$

Denoting ground state expectation values by $\langle\ldots\rangle$ the local f, d-electron occupations are found as $\langle\hat{n}^f_{\mathbf{i}}\rangle = (1+2z)/(1+z), \langle\hat{n}^d_{\mathbf{i}}\rangle = (2+z)/(1+z)$, where $z = |t^f_1/t^d_1|$ is a measure of the nearest-neighbor hopping amplitude of the f electrons. Since the latter can be expected to be much smaller than that of the d electrons ($z \ll 1$), the f (d) electron occupation per site is found to be close to one (two). Hence there exist local moments on most of the f sites. We see that $\langle\hat{n}_{\mathbf{i}}\rangle = \langle\hat{n}^f_{\mathbf{i}}\rangle + \langle\hat{n}^d_{\mathbf{i}}\rangle = 3$ for all $\mathbf{i}$; i.e., the electron distribution is indeed uniform. The localization is due to a subtle quantum mechanical interference between the hopping and hybridization processes of the electrons. Therefore, the nature of this localized state is quite nontrivial.

By separating the Hamiltonian $\hat{H}$ into an itinerant part $\hat{H}_{\rm itin} \equiv \hat{H}_0 - \sum_{\mathbf{i},\sigma}[V_0(\hat{d}^{\dagger}_{\mathbf{i}\sigma}\hat{f}_{\mathbf{i}\sigma} + \text{H.c.}) + E_f\hat{n}^f_{\mathbf{i}\sigma}] \equiv \sum_{\mathbf{r}}\hat{H}_{\rm itin}(\mathbf{r})$ and a complementary localized part $\hat{H}_{\rm loc} \equiv \hat{H} - \hat{H}_{\rm itin}$, and using $\langle\hat{b}^{\dagger}_{\mathbf{i}\sigma}\hat{b}'_{\mathbf{j}\sigma'}\rangle = 0$ for $\mathbf{i} \neq \mathbf{j}$ and $b, b' = d, f$, one finds $\langle\hat{H}_{\rm itin}(\mathbf{r})\rangle = 0$ and $\langle\hat{H}_{\rm loc}\rangle = E_g$. This clearly illustrates the localized, and thus insulating, nature of the ground state whose energy is obtained as $E_g = N_\Lambda[(1-2z)K_f/z - U]$ (Fig. 2). The parameter space in which the localized ground state $|\Psi_{\rm loc}\rangle$ is stable is represented in terms of the variables E_f, U, t^f_1/t^d_1, t^d_2/t^d_1 by the surfaces I_1, I_2 in Fig. 3. The stability region is seen to extend through the phase diagram from weak to strong interactions U.

For $y = |t^d_2/t^d_1| > 1/2$, i.e., rather large next-nearest neighbor hopping of d electrons, the localized state $|\Psi_{\rm loc}\rangle$ ceases to be the ground state. Apparently, at $y_c = 1/2$ a different, most probably itinerant, phase becomes stable. We note that the ground state energy $E_g(y)$ has a finite value at y_c, but *infinite* slope (see Fig. 2). This exact result has a direct physical interpretation. Namely, 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 compressibility at a critical pressure P_c. Such a feature is indeed observed in some heavy-fermion systems [20].

(ii) *Itinerant ground state.*—The localized ground state discussed above has exactly three electrons per site. In general, the intersite hopping and hybridization will lead to a variable number of electrons per site and hence to a conducting state. An itinerant ground state is obtained, for example, by choosing $p^*_n = -p_n$, $|p_n| = |p|$, corresponding to imaginary p and, hence, imaginary hybridization amplitudes $V_{\mathbf{r}}$. Whether $V_{\mathbf{r}}$ is real, complex, or imaginary depends on the linear combination of the corresponding electronic orbitals [7,15,21–23] and hence on the lattice symmetry. For example, $V_{\mathbf{r}}$ may be tuned from real to imaginary by introducing axial distortions of D_{4h} symmetry to an underlying O_h lattice symmetry [22]. Therefore, such a solution requires anisotropic hopping and hybridization amplitudes. The itinerant ground state discussed here emerges if the hybridization on the same site and in the basal (xy) plane vanish. The anisotropy in the hopping starts at the level of next-nearest neighbor amplitudes.

To show that this state is indeed conducting the solution is generalized to fillings beyond 3/4 by inserting the operator $\hat{V}^{\dagger}_M = \prod_{j=1}^{M}[\sum_{i=1}^{N_\Lambda} a_{ji}(\sum_{b=d,f;\sigma}\epsilon_{b\sigma}\hat{b}^{\dagger}_{i\sigma})]$ into (5) next to $|0\rangle$; here a_{ji}, $\epsilon_{b\sigma}$ are numerical coefficients. This operator introduces $M < N_\Lambda$ additional particles into the ground state. It allows one to calculate the energy E_g for different particle numbers. In particular, one finds $\mu^+ \equiv E_g(N+2) - E_g(N+1) = K_d$, $\mu^- \equiv E_g(N+1) - E_g(N) = K_d$, i.e., $\mu^+ - \mu^- = 0$. Therefore, the solution is conducting [24]. The stability region of the conducting state corresponds to the surface C in Fig. 3.

To describe the itinerant case a $\mathbf{k}$-type representation is more suitable. Denoting the Fourier transforms of $\hat{A}_{\mathbf{i}_1\sigma}$

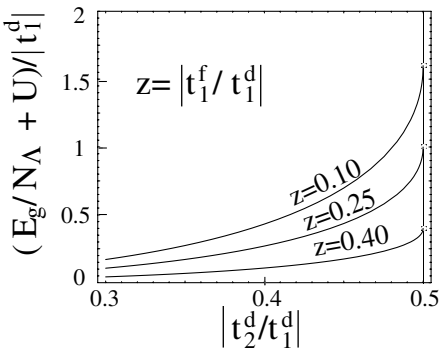

FIG. 2. Ground-state energy of the localized state expressed in terms of $(E_g/N_\Lambda + U)/|t^d_1|$ as a function of next-nearest neighbor hopping of d electrons, $|t^d_2/t^d_1|$, for different values of f hopping $z = |t^f_1/t^d_1|$; here $|V_1/V_0| \gg 1/2$.

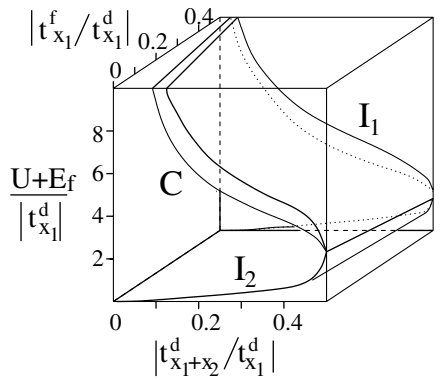

FIG. 3. Surfaces in parameter space representing stability regions of the insulating ground state (I_1 for $|V_1/V_0| < 1/2$, I_2 for $|V_1/V_0| \gg 1/2$) and the conducting ground state (C).

and $\hat{b}_{\mathbf{i}\sigma}$ by $\hat{A}_{\mathbf{k}\sigma}$ and $\hat{b}_{\mathbf{k}\sigma}$, respectively, (2) takes the form $\hat{A}^{\dagger}_{\mathbf{k}\sigma} = \sum_{b=d,f} a^{*}_{\mathbf{k}b} \hat{b}^{\dagger}_{\mathbf{k}\sigma}$; the expressions for the coefficients $a^{*}_{\mathbf{k}b}$ will not be reproduced here. We can now define new canonical Fermi operators $\hat{C}_{\delta,\mathbf{k}\sigma}$, $\delta = 1, 2$, where $\hat{C}_{1,\mathbf{k}\sigma} = R^{1/2}_{\mathbf{k}} \hat{A}_{\mathbf{k}\sigma}$, with $R^{-1}_{\mathbf{k}} = \sum_b |a_{\mathbf{k}b}|^2$, and $\hat{C}_{2,\mathbf{k}\sigma}$ is determined by the anticommutation rules between $\hat{C}_{1,\mathbf{k}\sigma}$ and $\hat{C}^{\dagger}_{2,\mathbf{k}\sigma}$. It follows that $-\sum_{\mathbf{i},\sigma} \hat{A}^{\dagger}_{I_{\mathbf{i}}\sigma} \hat{A}_{I_{\mathbf{i}}\sigma} + K_d \hat{N} = \sum_{\mathbf{k},\sigma} [(K_d - R^{-1}_{\mathbf{k}}) \times \hat{C}^{\dagger}_{1,\mathbf{k}\sigma} \hat{C}_{1,\mathbf{k}\sigma} + K_d \hat{C}^{\dagger}_{2,\mathbf{k}\sigma} \hat{C}_{2,\mathbf{k}\sigma}] \equiv \hat{H}_g$, such that (3) can be written as $\hat{H} = \hat{H}_g + U\hat{P} + N_{\Lambda}[U - 2(K_d - E_f)]$. In the ground state, using $\hat{P}|\Psi_g\rangle = 0$, the Hamiltonian $\hat{H}$ therefore reduces to $\hat{H}_g$. Thus we succeeded in diagonalizing $\hat{H}$ for the ground state. There are two bands, the lower one having a dispersion $K_d - R^{-1}_{\mathbf{k}}$, while the upper one is dispersionless ("flat"); the Fermi energy is $E_F = K_d$. Such a band structure around E_F has been observed in experiment [25].

The momentum distribution of the d, f electrons becomes $n^b_{\mathbf{k}} = \langle \sum_{\sigma} \hat{b}^{\dagger}_{\mathbf{k}\sigma} \hat{b}_{\mathbf{k}\sigma} \rangle = (2|a_{\mathbf{k}b}|^2 + |a_{\mathbf{k},b' \neq b}|^2) R_{\mathbf{k}}$, with $n_{\mathbf{k}} = \sum_{b=d,f} n^b_{\mathbf{k}} = 3$. Since the coefficients $a_{\mathbf{k}b}$ are regular functions of $\mathbf{k}$ this also holds for $n^d_{\mathbf{k}}$, $n^f_{\mathbf{k}}$, and $n_{\mathbf{k}}$. Consequently, the momentum distributions of the electrons in the interacting ground state have no discontinuities. Since the ground state is paramagnetic and metallic, the system is a *non-Fermi liquid*. This is a consequence of the degeneracy of electrons in the upper band. In terms of the $\hat{C}_{\delta,\mathbf{k}\sigma}$ fermions one finds $\langle \hat{C}^{\dagger}_{1,\mathbf{k}\sigma} \hat{C}_{1,\mathbf{k}\sigma} \rangle = 1$ and $\langle \hat{C}^{\dagger}_{2,\mathbf{k}\sigma} \hat{C}_{2,\mathbf{k}\sigma} \rangle = 1/2$ (upper band half filled).

In summary, we derived the first exact ground state solution of a *three*-dimensional periodic Anderson model with finite hopping and hybridization of d and f electrons in the unit cell. This was achieved by (i) casting the Hamiltonian into a positive semidefinite form using composite operators in combination with 55 coupled, nonlinear matching conditions for the input parameters and (ii) constructing a product wave function of these composite operators in position space. For real hybridization amplitudes we obtained an *insulating* ground state whose compressibility diverges at the boundary of the stability region. By contrast, for imaginary hybridization amplitudes we identified a *conducting non-Fermi liquid* state consisting of one dispersing band and one (upper) flat band. The stability regions of the two ground states extend through an unexpectedly large region of parameter space, e.g., from weak to strong interactions U.

By modifying the structure of the composite operators it is possible to vary the stability regions of these ground states [26], and also to describe magnetically ordered phases.

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[16] In $D = 3$ the vector $\mathbf{r}$ can take 13 different values: $\mathbf{x}_{\tau}$ ($\tau = 1, 2, 3$), $\mathbf{x}_{\tau'} \pm \mathbf{x}_{\tau}$ ($\tau' > \tau$), and $\mathbf{x}_3 \pm \mathbf{x}_2 \pm \mathbf{x}_1$.
[17] The relations read, for example, $\sum_{n=1}^{8} |a_{n,f}|^2 = K_d - E_f - U$, $\sum_{\beta_1,\beta_2=0,1} a^{*}_{n(0,\beta_1,\beta_2),b} a_{n(1,\beta_1,\beta_2),b} = -t^b_{\mathbf{x}_1}$, $\sum_{\beta_1=0,1} a^{*}_{n(0,0,\beta_1),b} a_{n(1,1,\beta_1),b} = -t^b_{\mathbf{x}_1+\mathbf{x}_2}$, etc.
[18] Here $D_{\beta,\alpha} = (1 - \delta_{\beta,-1})\delta_{\alpha,0} + \delta_{\alpha,\beta}(1 - \delta_{\alpha,0})$, $n^{\pm} = n[g^{\pm}(\beta_1, \alpha_1), g^{\pm}(\beta_2, \alpha_2), g^{\pm}(\beta_3, \alpha_3)]$, with $g^{\pm}(\beta, \alpha) = \beta\delta_{\alpha,0} + (1 \mp \alpha)(1 - \delta_{\alpha,0})/2$. The microscopic parameters are contained in $T^{b,b'}_{\bar{\mathbf{r}},\nu} = -(1 - \delta_{\nu,0})[\delta_{b,b'} t^b_{\bar{\mathbf{r}}} + (1 - \delta_{b,b'}) V_{\bar{\mathbf{r}}}] - \delta_{\nu,0}\{\delta_{b,b'}[\delta_{b,f}(E_f + U - K_d) - \delta_{b,d} K_d] + (1 - \delta_{b,b'})\delta_{b,d} V_0\}$, where $\bar{\mathbf{r}} = \sum_{i=1}^{3} \alpha_i \mathbf{x}_i$ is a vector in the unit cell I (which thus determines the values of α_i according to Ref. [16]), or $\bar{\mathbf{r}} = 0$ (i.e., $\alpha_i = 0$), and $\nu = \sum_{i=1}^{3} |\alpha_i|^2$.
[19] Ground states with different total spin have been discussed, e.g., by R. Arita and H. Aoki, Phys. Rev. B **61**, 12 261 (2000).
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[26] In particular, for a simple cubic lattice $|\Psi_g\rangle$ is found to be an exact ground state even for $t^f_{\mathbf{r}} = 0$, i.e., for the conventional PAM, if $\hat{A}_{I_{\mathbf{i}}\sigma}$ is defined on an octahedron centered at $\mathbf{i}$, with $a_{n,f} \neq 0$ only on this central site.