Phase transition arising from the underscreened Anderson lattice model: A candidate concept for explaining hidden order in URu_2Si_2

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We analyze a type of phase transition that appears in the spin-rotationally invariant form of the underscreened Anderson lattice model and we obtain, with decreasing temperature, a continuous transition with the opening of a gap. We suggest that this model might describe the "hidden-order" transition in URu_2Si_2. We also examine the gaps that appear in the electronic dispersion relations of the bands of different orbital character and compare our results with those found through photoelectron spectroscopy.

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I. INTRODUCTION

In 1985 it was found[1] that URu_2Si_2 became superconducting below 0.8 K, and also that there was a large jump in the specific heat at 17.5 K. In 1986, transport, thermal, and magnetic measurements[2] on URu_2Si_2 produced compelling evidence that the transition at 17.5 K produced a gap $\sim$10 meV which spread across about 40% of the Fermi surface. Far-infrared reflectance measurements[3] provided direct evidence for a gap with a magnitude between 5.6 and 7.5 meV which formed below 17.5 K. Recent ultrafast spectroscopy measurements[4] provided corroborating evidence for the existence of gaps of 5 and 10 meV, and scanning tunneling microscopy (STM) measurements[5] have shown the existence of 5-meV gaps. Initially the transition was assumed to be of magnetic origin. Inelastic neutron-scattering measurements[6] showed evidence for the existence of tiny ordered magnetic moments (of the order $10^{-2}\ \mu_B$). However, subsequent pressure measurements[7] showed that a transition to an antiferromagnetic state with well-defined ordered moments (of the order 0.4 μ_B) occurs above $P = 0.5$ GPa. The application of pressure was found to have only a minimal effect on the transition temperature. NMR measurements[8] indicated that at zero pressure the system was inhomogeneous, containing both paramagnetic regions and regions of antiferromagnetism. It was confirmed that the patches of antiferromagnetism can be created either by impurity doping,[9] or by stress fields in pure URu_2Si_2.[10] Hence, it is now thought that the origin of the transition at 17.5 K is not due to the appearance of small moment antiferromagnetism, although there is significant evidence that the transition is produced by Fermi-surface nesting which is similar to that found in the high-pressure Néel state.[11–14] Since experiments were unable to identify the nature of the order parameter, the transition has come to be known as a "hidden-order" transition. Over the 27 years that have elapsed since its first discovery, there have been many theoretical[15–18] and experimental attempts to uncover the nature of the transition. Some recent theories include descriptions of states with rotational spin currents that break spin-rotational invariance but not time-reversal invariance,[15] modulated-spin liquid states that break the C_4 rotational invariance,[16] states with incommensurate hybridization density waves promoted by the spin-independent coulomb interaction between the $5f$ and conduction electrons,[17] or unconventional spin-density wave states where the order parameter has d-wave symmetry.[18] The present status of the field has been comprehensively reviewed in Ref. 19.

In this paper, we shall examine the underscreened Anderson lattice model which describes two itinerant $5f$ bands which resonantly couple to a single conduction band. Like the Anderson lattice model,[20,21] which is a generalization of a single-impurity model introduced to describe a magnetic impurity in a metal,[22] the underscreened Anderson lattice model[23,24] is a generalization of a model introduced to describe the single-impurity underscreened Kondo effect.[25,26] The model is generic and is not specifically tailored to the electronic structure of URu_2Si_2.[27,28]

The underscreened Kondo or Anderson lattice model were recently studied to describe the competition between ferromagnetism and the Kondo effect, which has been observed in uranium and neptunium compounds.[23,24,29] But in the URu_2Si_2 compound, the Kondo effect is not involved in the transition occurring at 17.5 K and we can use a simplified mean-field treatment of the Anderson Hamiltonian at the Hartree-Fock level. Moreover, as it will be explained later, we can simplify the problem by taking a zero value for one of the two d-f hybridization terms, without changing the physical results. Thus in the present model, the f electrons interact via local (spin-rotationally-invariant) Coulomb and exchange interactions. We find that the system exhibits a competition between magnetic ordering and a novel type of ordering. The novel state corresponds to an inhomogeneous state with wave vector $\underline{Q}$ and in which the $5f$ bands are mixed, in contrast the normal state where the $5f$ bands have pure orbital characters. However, the admixture is spin-dependent and, in certain circumstances, corresponds to a broken gauge invariance of the Hamiltonian. The type of correlation is best illustrated in the limit of zero hybridization, where the correlation can be described simply in terms of the $5f$ electron creation operators corresponding to the two bands (labeled by α and β). The correlation can be seen in the even-parity, broken-time-reversal symmetry state constructed from products of operators

of the type

$$\left(\alpha_{\underline{k}} f^{\dagger,\alpha}_{\underline{k}+\underline{Q},\uparrow} + \beta_{\underline{k}} f^{\dagger,\beta}_{\underline{k},\uparrow}\right)\left(\alpha_{\underline{k}} f^{\dagger,\alpha}_{-\underline{k}-\underline{Q},\downarrow} - \beta_{\underline{k}} f^{\dagger,\beta}_{-\underline{k},\downarrow}\right) \tag{1}$$

acting on a vacuum state $|0>$, where the coefficients of the operators are normalized to unity:

$$|\alpha_{\underline{k}}|^2 + |\beta_{\underline{k}}|^2 = 1. \tag{2}$$

It is seen that the mixed two-particle states and the corresponding unmixed two-particle states ($\alpha_{\underline{k}} = 1$, $\beta_{\underline{k}} = 0$) have precisely the same type of expectation values for spin-conserving $5f$ orbital single-particle operators, and likewise for the $5f$ spin operators. The interference terms can only be measured by a combined spin and orbital-sensitive measurement.

II. THE MODEL

The model describes two degenerate localized $5f$ bands (labeled by $\chi = \alpha,\beta$), which acquire itinerant character by direct hopping between neighboring $5f$ shells and the mixing with one itinerant conduction band. The Hamiltonian is written as

$$\hat{H} = \hat{H}_f + \hat{H}_d + \hat{H}_{fd}, \tag{3}$$

where $\hat{H}_f$ describes the f electrons, $\hat{H}_d$ describes the itinerant conduction band, and $\hat{H}_{fd}$ describes the hybridization. The Hamiltonian $\hat{H}_f$ is given by

$$\begin{aligned}\hat{H}_f = &\sum_{\underline{k},\sigma,\chi} E^{\chi}_f(\underline{k}) n^{\chi}_{f,\underline{k},\sigma} \\ &+ \left(\frac{U}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\sigma',\chi,\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\dagger,\chi'}_{\underline{k}'-\underline{q},\sigma'} f^{\chi'}_{\underline{k},\sigma'} f^{\chi}_{\underline{k}',\sigma} \\ &+ \left(\frac{J}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\sigma',\chi,\chi',} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\dagger,\chi'}_{\underline{k}'-\underline{q},\sigma'} f^{\chi}_{\underline{k}',\sigma'} f^{\chi'}_{\underline{k},\sigma},\end{aligned} \tag{4}$$

in which the first term, proportional to $E^{\chi}_f(\underline{k})$, describes the dispersion relation for the χth $5f$ band while the second and third terms describe the screened Coulomb interaction between the $5f$ electrons in the same $5f$ shell. The third term contains an interorbital exchange interaction which is required to make the model spin rotationally invariant.[30] Since we have selected only two $5f$ bands, the model is not invariant under spatial rotations.[31] The conduction electron Hamiltonian $\hat{H}_d$ can be expressed as

$$\hat{H}_d = \sum_{\underline{k},\sigma} \epsilon(\underline{k}) d^{\dagger}_{\underline{k},\sigma} d_{\underline{k},\sigma}, \tag{5}$$

where $\epsilon(\underline{k})$ describes the dispersion relation of conduction electrons labeled by the Bloch wave vector $\underline{k}$. The Hamiltonian describing the on-site hybridization process is given, as usual, by

$$\hat{H}_{fd} = \sum_{\underline{k},\sigma,\chi} \left(V_{\chi}(\underline{k}) f^{\dagger,\chi}_{\underline{k},\sigma} d_{\underline{k},\sigma} + V^{*}_{\chi}(\underline{k}) d^{\dagger}_{k,\sigma} f^{\chi}_{\underline{k},\sigma}\right). \tag{6}$$

The Coulomb interaction can be rewritten in the form

$$\begin{aligned}\hat{H}_{\rm int} = &\left(\frac{U-J}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\chi}_{\underline{k},\sigma} f^{\dagger,\chi'}_{\underline{k}'-\underline{q},\sigma} f^{\chi'}_{\underline{k}',\sigma} \\ &+ \left(\frac{U}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi,\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\chi}_{\underline{k},\sigma} f^{\dagger,\chi'}_{\underline{k}'-\underline{q},-\sigma} f^{\chi'}_{\underline{k}',-\sigma} \\ &+ \left(\frac{J}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\chi'}_{\underline{k},\sigma} f^{\dagger,\chi'}_{\underline{k}'-\underline{q},-\sigma} f^{\chi}_{\underline{k}',-\sigma}.\end{aligned} \tag{7}$$

To aid the analysis,we introduce the normalized non-Hermitian operator $\hat{z}_{\underline{q},\sigma}$:

$$\hat{z}_{\underline{q},\sigma} = \frac{1}{N} \sum_{\underline{k}} f^{\dagger,\beta}_{\underline{k}+\underline{q},\sigma} f^{\alpha}_{\underline{k},\sigma}. \tag{8}$$

This product of operators provides a measure of the coupling between the two types of f bands. The last line in the interaction of Eq. (7) originates from the spin-flip term which was required from considerations of spin-rotational invariance.[30] We also introduce the $5f$ orbital charge-density operator via

$$\hat{\rho}^{\chi}_{\underline{q},\sigma} = \frac{1}{N} \sum_{\underline{k}} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} f^{\chi}_{\underline{k},\sigma}. \tag{9}$$

It should be noted that the first term in the interaction Eq. (7) can be expressed in terms of products of either $\hat{z}_{\underline{q},\sigma}$ or of the orbital density operators $\hat{\rho}^{\chi}_{\underline{q},\sigma}$.

We shall assume that the α and β bands are degenerate and that $V_{\beta}(\underline{k}) = 0$. In this case, one can see that the Hamiltonian is invariant under a gauge transformation of the β electrons, which is independent of the gauge invariance of the α and conduction electrons. This gauge symmetry is analogous to the chiral gauge symmetry present in the massless limit of the Dirac equation. It is important to note that taking $V_{\beta}(\underline{k}) = 0$ does not change the physical results but only simplifies the calculations.

III. THE MEAN-FIELD APPROXIMATION

In the mean-field approximation, the interaction term in the Hamiltonian is expanded in powers of the fluctuations of bilinear products of operators:

$$\begin{aligned}\Delta\hat{n}^{\chi}_{f,\sigma} &= \left(\hat{n}^{\chi}_{f,\sigma} - n^{\chi}_{f,\sigma}\right), \\ \Delta\hat{z}_{\underline{q},\sigma} &= \left(\hat{z}_{\underline{q},\sigma} - z_{\underline{q},\sigma}\right),\end{aligned} \tag{10}$$

where the hats have been dropped for the averaged quantities. We have assumed that the average f electron occupation numbers are translationally invariant (i.e., $n^{\chi}_{f,i,\sigma} = n^{\chi}_{f,\sigma}$), but we have retained the momentum dependence of the expectation values of the non-Hermitian operators. The terms in the Hamiltonian quadratic in the fluctuations are neglected. This approximation reduces the Hamiltonian to an expression quadratic in fermionic operators that can be diagonalized. We shall assume that the average $z_{\underline{q},\sigma}$ is a nonzero complex number for commensurate momentum transfers $\underline{Q}$, where $\underline{Q}$ could be any vector that is both on and normal to the Brillouin

zone boundary. The assumption of a finite momentum transfer corresponds to having an inhomogeneous state. However, the inhomogeneous nature of this state is masked in either purely spin-sensitive or purely orbital-sensitive measurements.

In the Hartree-Fock approximation, the temporal and spatial Fourier transform of the single-electron f-f Green's function satisfies the equations of motion:

$$\begin{aligned}
&\big(\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big)G^{\alpha,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega) \\
&\quad = \delta^{\alpha,\chi'}\delta_{\underline{k},\underline{k}'} + V_{\alpha}(\underline{k})G^{\chi'}_{df,\sigma}(\underline{k},\underline{k}',\omega) \\
&\qquad + \kappa_{-\underline{Q},\sigma}G^{\beta,\chi'}_{ff,\sigma}(\underline{k}+\underline{Q},\underline{k}',\omega), \\
&\big(\omega - E^{\beta}_{f,\sigma}(\underline{k})\big)G^{\beta,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega) \\
&\quad = \delta^{\beta,\chi'}\delta_{\underline{k},\underline{k}'} + V_{\beta}(\underline{k})G^{\chi'}_{df,\sigma}(\underline{k},\underline{k}',\omega) \\
&\qquad + \kappa^{*}_{\underline{Q},\sigma}G^{\alpha,\chi'}_{ff,\sigma}(\underline{k}-\underline{Q},\underline{k}',\omega),
\end{aligned} \tag{11}$$

where the Hartree-Fock f-band dispersion relation $E^{\chi}_{f,\sigma}(\underline{k})$ is given by

$$E^{\chi}_{f,\sigma}(\underline{k}) = E^{\chi}_{f}(\underline{k}) + \sum_{\chi'}\big[(U-J)n^{\chi'}_{f,\sigma}(1-\delta^{\chi,\chi'}) + Un^{\chi'}_{f,-\sigma}\big], \tag{12}$$

and the gap parameter $\kappa_{\underline{Q},\sigma}$ is defined as the complex number

$$\kappa_{\underline{Q},\sigma} = Jz_{-\underline{Q},-\sigma} - (U-J)z_{-\underline{Q},\sigma}. \tag{13}$$

The mixed f-d Green's function is found to satisfy

$$\begin{aligned}
&(\omega - \epsilon(\underline{k}))G^{\chi'}_{df,\sigma}(\underline{k},\underline{k}',\omega) \\
&\quad = V_{\alpha}(\underline{k})^{*}G^{\alpha,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega) + V_{\beta}(\underline{k})^{*}G^{\beta,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega).
\end{aligned} \tag{14}$$

The above equation forms a closed set which is easily solved when $V_{\beta}(\underline{k}) = 0$ and $\underline{Q}$ is commensurate with the lattice. The solutions are given by

$$\begin{aligned}
&G^{\alpha,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega) \\
&\quad = \frac{[\omega - \epsilon(\underline{k})]}{D_{\sigma}(\underline{k},\omega)}\big[\big[\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q})\big]\delta^{\alpha,\chi'}\delta_{\underline{k},\underline{k}'} \\
&\qquad + \kappa_{\underline{Q},\sigma}\delta^{\beta,\chi'}\delta_{\underline{k}+\underline{Q},\underline{k}'}\big], \\
&G^{\beta,\chi'}_{ff,\sigma}(\underline{k},\underline{k}',\omega) \\
&\quad = D_{\sigma}(\underline{k}+\underline{Q},\omega)^{-1}\big[\kappa^{*}_{\underline{Q},\sigma}[\omega - \epsilon(\underline{k}+\underline{Q})]\delta^{\alpha,\chi'}\delta_{\underline{k}+\underline{Q},\underline{k}'} \\
&\qquad + \big(\big[\omega - E^{\alpha}_{f,\sigma}(\underline{k}+\underline{Q})\big][\omega - \epsilon(\underline{k}+\underline{Q})] \\
&\qquad - |V_{\alpha}(\underline{k}+\underline{Q})|^{2}\big)\delta^{\beta,\chi'}\delta_{\underline{k},\underline{k}'}\big],
\end{aligned} \tag{15}$$

where the denominator $D_{\sigma}(\underline{k},\omega)$ is given by

$$\begin{aligned}
D_{\sigma}(\underline{k},\omega) = &\big[\big(\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q})\big)\big(\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big) - |\kappa_{\underline{Q},\sigma}|^{2}\big] \\
&\times(\omega - \epsilon(\underline{k})) - |V_{\alpha}(\underline{k})|^{2}\big(\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q})\big).
\end{aligned} \tag{16}$$

For completeness, we give the d electrons Green's function

$$\begin{aligned}
G_{dd,\sigma}(\underline{k},\underline{k}',\omega) = &\frac{\delta_{\underline{k},\underline{k}'}}{D_{\sigma}(k,\omega)}\big[\big(\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q})\big) \\
&\times\big(\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big) - |\kappa_{\underline{Q},\sigma}|^{2}\big].
\end{aligned} \tag{17}$$

The zeros of the denominator $D_{\sigma}(\underline{k},\omega)$ yield the Hartree-Fock quasiparticle dispersion relations for electrons of spin σ.

The quantity $z_{\underline{Q},\sigma}$ is determined from the expectation value of the product of operators which are off-diagonal in the band indices

$$z^{*}_{\underline{Q},\sigma} = \frac{1}{N}\sum_{k}\big\langle f^{\dagger,\alpha}_{\underline{k},\sigma}f^{\beta}_{\underline{k}+\underline{Q},\sigma}\big\rangle, \tag{18}$$

which can be related to the definition of the real-time Green's function for small negative times $t = -\eta$, where $\eta \to 0$. Upon expressing the real-time Green's function in terms of its Fourier transform and closing the contour in the upper-half complex ω plane, as well as noting the pole structure of the Green's function, one finally arrives at the result

$$z^{*}_{\underline{Q},\sigma} = -\frac{1}{N}\sum_{\underline{k}}\bigg[\int_{C}\frac{d\omega}{2\pi i}f(\omega)G^{\beta,\alpha}_{ff,\sigma}(\underline{k}+\underline{Q},\underline{k},\omega)\bigg], \tag{19}$$

where $f(\omega)$ is the Fermi function and where the contour C encloses the real axis. Since the f-f Green's functions involve $z_{\underline{Q},-\sigma}$, the $z_{\underline{Q}}$'s must be determined self-consistently. Furthermore, since the Green's functions for $5f$ electrons of spin σ with mixed band indices are odd functions of $z_{\underline{Q},-\sigma}$, the self-consistency equations have the trivial solution $z_{\underline{Q},\sigma} = 0\ \forall\ \sigma$, which corresponds to the conservation of the number of electrons in the β band. We shall first consider the trivial solution with $z_{\underline{Q},\sigma} = 0$.

A. The normal state

The normal state is defined as that for which $z_{\underline{Q},\sigma} = 0\,\forall\,\sigma$. The single-electron Green's functions for the $5f$ bands reduce to

$$\begin{aligned}
G^{\beta}_{ff,\sigma}(\underline{k},\underline{k}',\omega) &= \frac{\delta_{\underline{k},\underline{k}'}}{\omega - E^{\beta}_{f,\sigma}(\underline{k})}, \\
G^{\alpha}_{ff,\sigma}(\underline{k},\underline{k}',\omega) &= \frac{[\omega - \epsilon(\underline{k})]\delta_{\underline{k},\underline{k}'}}{\big[\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big][\omega - \epsilon(\underline{k})] - |V_{\alpha}(\underline{k})|^{2}},
\end{aligned} \tag{20}$$

in which the dispersion relation for the β $5f$ Hartree-Fock quasiparticles is simply given by $E^{\beta}_{f,\sigma}(\underline{k})$. The conduction electron states are admixed with $5f$ states of α character and their Green's functions reduce to

$$G_{dd,\sigma}(\underline{k},\underline{k}',\omega) = \frac{\big[\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big]\delta_{\underline{k},\underline{k}'}}{\big[\omega - E^{\alpha}_{f,\sigma}(\underline{k})\big][\omega - \epsilon(\underline{k})] - |V_{\alpha}(\underline{k})|^{2}}. \tag{21}$$

The Green's functions for the αth band can be recast in the form

$$\begin{aligned}
G^{\alpha}_{ff,\sigma}(\underline{k},\underline{k},\omega) &= \frac{|A^{+}_{\sigma}(\underline{k})|^{2}}{\omega - E^{+}_{\sigma}(\underline{k})} + \frac{|A^{-}_{\sigma}(\underline{k})|^{2}}{\omega - E^{-}_{\sigma}(\underline{k})}, \\
G_{dd,\sigma}(\underline{k},\underline{k},\omega) &= \frac{|B^{+}_{\sigma}(\underline{k})|^{2}}{\omega - E^{+}_{\sigma}(\underline{k})} + \frac{|B^{-}_{\sigma}(\underline{k})|^{2}}{\omega - E^{-}_{\sigma}(\underline{k})},
\end{aligned} \tag{22}$$

where the dispersion relations of the hybridized Hartree-Fock quasiparticle bands $E_\sigma^\pm(\underline{k})$ are given by

$$E_\sigma^\pm(\underline{k}) = \left(\frac{E_{f\sigma}^\alpha(\underline{k}) + \epsilon(\underline{k})}{2}\right) \pm \sqrt{\left(\frac{E_{f\sigma}^\alpha(\underline{k}) - \epsilon(\underline{k})}{2}\right)^2 + |V_\alpha(\underline{k})|^2}. \quad (23)$$

The f and d characters of the bands have weights given by $|A_\sigma^\pm(\underline{k})|^2$ and $|B_\sigma^\pm(\underline{k})|^2$, respectively, where

$$|A_\sigma^\pm(\underline{k})|^2 = \frac{1}{2}\left[1 \pm \frac{\left[E_{f\sigma}^\alpha(\underline{k}) - \epsilon(\underline{k})\right]}{\sqrt{\left[E_{f\sigma}^\alpha(\underline{k}) - \epsilon(\underline{k})\right]^2 + 4|V_\alpha(\underline{k})|^2}}\right],$$
$$|B_\sigma^\pm(\underline{k})|^2 = \frac{1}{2}\left[1 \mp \frac{\left[E_{f\sigma}^\alpha(\underline{k}) - \epsilon(\underline{k})\right]}{\sqrt{\left[E_{f\sigma}^\alpha(\underline{k}) - \epsilon(\underline{k})\right]^2 + 4|V_\alpha(\underline{k})|^2}}\right]. \quad (24)$$

The k dependence of the quasiparticle dispersion relations and the form factors are sketched in Fig. 1. In the figure, the energies are given in units of half the conduction bandwidth. The $5f$ densities of states are shown in Fig. 2. Due to the relatively small value of the hybridization ($V = 1/10$) and the large value of the $5f$ bandwidth ($W_f = 6/10$) caused by f-f hopping, the α and β $5f$ densities of states have quite similar shapes at energies removed from the hybridization gap. The hybridization gap is centered on $E_f/(1 + W_f/2)$. It should be noted that near the band edges, the shape of the band is similar to that of the unhybridized bands, except for small energy shifts of the order of $|V|^2$.

Magnetic instabilities

In the Hartree-Fock approximation, the paramagnetic phase is generally expected to retain its stability relative to magnetic states for small values of the Coulomb U and the exchange J interactions. The dynamic spin susceptibility for the Hartree-Fock state can be found from the equations of motion in the random-phase approximation (RPA).[32] The static susceptibility found by setting $\omega = 0$ shows a pole when

$$\left[1 - U\chi_f^{\alpha,\alpha(0)}(\underline{q},0)\right]\left[1 - U\chi_f^{\beta,\beta(0)}(\underline{q},0)\right] - J^2\chi_f^{\alpha,\alpha(0)}(\underline{q},0)\chi_f^{\beta,\beta(0)}(\underline{q},0) = 0, \quad (25)$$

which signals the instability to a spin-density wave with wave vector q. In the above equation, the quantity $\chi_f^{\beta,\beta(0)}(\underline{q},0)$ represents the response of the β band to a Weiss field and is given by

$$\chi_f^{\beta,\beta(0)}(\underline{q},0) = \frac{1}{N}\sum_{\underline{k}}\left(\frac{f\left[E_f^\beta(\underline{k}+\underline{q})\right] - f\left[E_f^\beta(\underline{k})\right]}{E_f^\beta(\underline{k}) - E_f^\beta(\underline{k}+\underline{q})}\right), \quad (26)$$

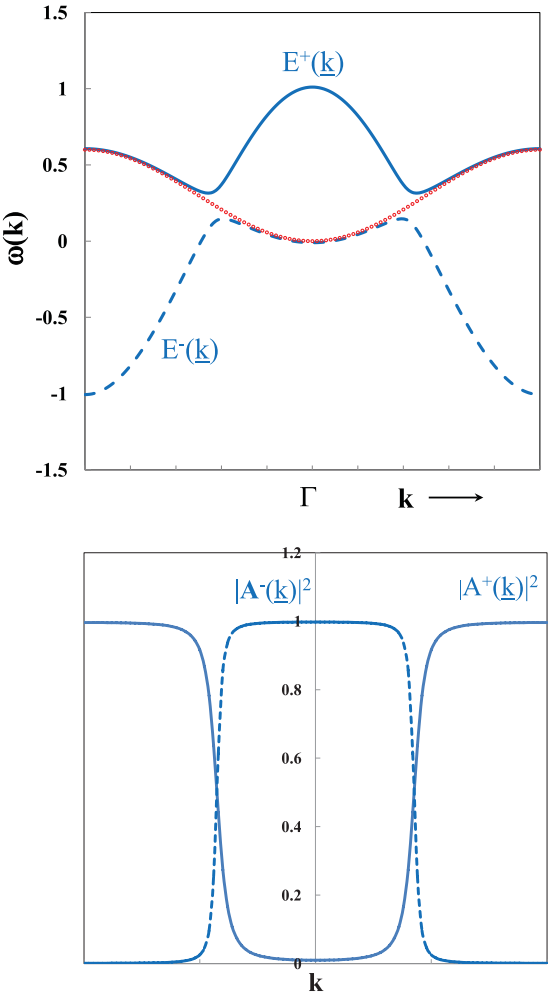

FIG. 1. (Color online) (Upper panel) The three dispersion relations for the bands of the underscreened Anderson lattice model in the normal state (schematic). The momentum $\underline{k}$ is taken to be along the (1,1,1) direction. The upper $[E^+(\underline{k})]$ and lower $[E^-(\underline{k})]$ bands are comprised of α $5f$ states hybridized with the conduction band. The band in the center marked by the red curve (open circles) is the unhybridized β band. (Lower panel) The $5f$ weights of the upper and lower hybridized bands ($|A_\sigma^\pm(\underline{k})|^2$) are plotted as functions of $\underline{k}$. The β band has pure $5f$ character.

and $\chi_f^{\alpha,\alpha(0)}(\underline{q},0)$ is the reduced Hartree-Fock $5f$ spin susceptibility for the α band which is given by

$$\chi_f^{\alpha,\alpha(0)}(\underline{q},0) = \frac{1}{N}\sum_{\underline{k},\pm,\mp}|A^\pm(\underline{k}+\underline{q})|^2|A^\mp(\underline{k})|^2 \times\left(\frac{f[E^\pm(\underline{k}+\underline{q})] - f[E^\pm(\underline{k})]}{E^\mp(\underline{k}) - E^\pm(\underline{k}+\underline{q})}\right). \quad (27)$$

The quantity $\chi_f^{\alpha,\alpha(0)}(\underline{q},0)$ has the same form as the reduced $5f$ susceptibility found from an RPA study of the Anderson lattice.[21] Due to the E_f dependence of the form factors in the α-band $5f$ electron density of states, the susceptibility $\chi_f^{\alpha,\alpha(0)}(\underline{q},0)$ has a band Van-Vleck component in addition to a modified Pauli paramagnetic term. Both Hartree-Fock susceptibilities are always positive. It is expected that if the β band is described in a tight-binding approximation, the

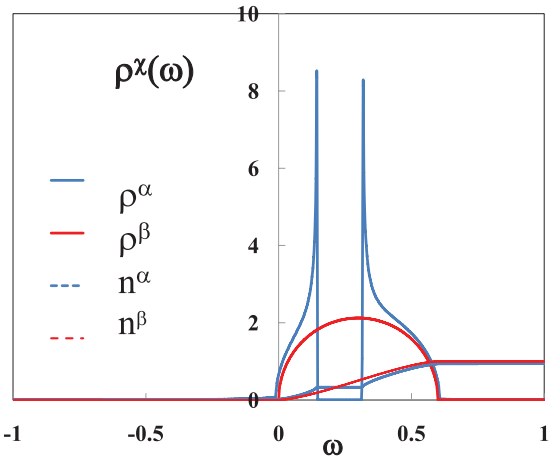

FIG. 2. (Color online) The α and β components of the $5f$ density of states per spin versus ω (solid lines), and n_f^α and n_f^β electrons per spin (dashed lines) as functions of μ, in which the Hartree-Fock energies of the $5f$ orbitals have been kept constant. The simple cubic tight-binding density of states has been approximated by a semielliptical form.

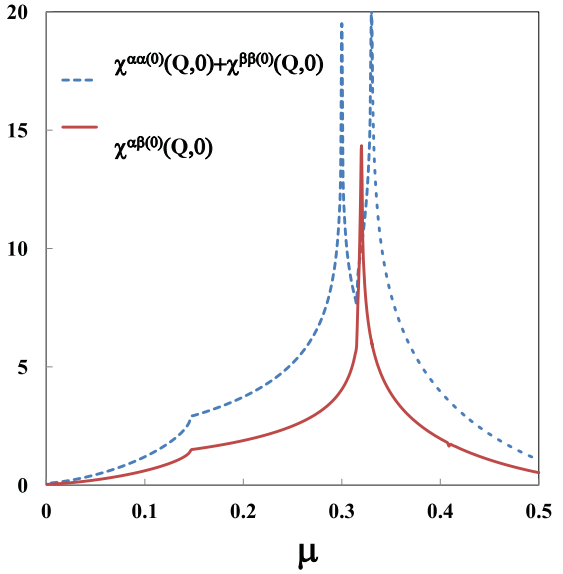

FIG. 3. (Color online) The interband susceptibility $\chi_f^{\alpha,\beta(0)}(\underline{Q})$ (solid line) and the sum of the intraband susceptibilities $\chi_f^{\alpha,\alpha(0)}(\underline{Q}) + \chi_f^{\beta,\beta(0)}(\underline{Q})$ (dashed line) as functions of μ, with fixed Hartree-Fock f electron bands $E_{f,\sigma}^{\chi}(\underline{k})$. The unhybridized f and conduction-band dispersion relations have been described within a simple cubic tight-binding model.

reduced susceptibility $\chi_f^{\beta,\beta(0)}(\underline{q},0)$ may show a divergence at the β-band nesting vector $\underline{Q} = (1,1,1)$ when μ approaches the center of the band. In any case, it should be noted that the magnetic instability is promoted by nesting the Fermi-surface sheets that have the same $5f$ orbital characters.

B. The instability to a novel state

We will now introduce a novel state which is based on a nonzero value of $z_{\underline{Q},\sigma}^*$ given by Eq. (18). This new parameter links the two f electrons of different orbitals α and β and exists in the situation of the underscreened Anderson lattice model, but not in the classical Anderson lattice model. This model is used here since we are now discussing the case of the uranium compound URu_2Si_2.[23]

The self-consistency condition for $z_{\underline{Q},\sigma}$ can be expressed as

$$z_{\underline{Q},\sigma}^* = -\kappa_{\underline{Q},\sigma}^* \frac{1}{N}\sum_{\underline{k}} \int_C \frac{d\omega}{2\pi i} \frac{[\omega - \epsilon(\underline{k})] f(\omega)}{D_\sigma(\underline{k},\omega)}. \tag{28}$$

If the novel transition is second order, then at the transition we expect that $\overline{F}_\sigma \sim 0$, so the above set of equations can be linearized to yield

$$\begin{aligned} \left[1-(U-J)\chi_{f,\sigma}^{\alpha,\beta,(0)}(\underline{Q},0)\right] z_{\underline{Q},\sigma}^* &= -z_{\underline{Q},-\sigma}^* J \chi_{f,\sigma}^{\alpha,\beta}(\underline{Q},0), \\ \left[1-(U-J)\chi_{f,-\sigma}^{\alpha,\beta,(0)}(\underline{Q},0)\right] z_{\underline{Q},-\sigma}^* &= -z_{\underline{Q},\sigma}^* J \chi_{f,-\sigma}^{\alpha,\beta}(\underline{Q},0), \end{aligned} \tag{29}$$

where

$$\chi_{f,\sigma}^{\alpha,\beta,(0)}(\underline{Q},0) = \frac{1}{N}\sum_{\underline{k},\pm} |A_\sigma^\pm(\underline{k})|^2 \left(\frac{f[E_\sigma^\pm(\underline{k})] - f\left[E_{f,\sigma}^\beta(\underline{k}+\underline{Q})\right]}{E_{f,\sigma}^\beta(\underline{k}+\underline{Q}) - E_\sigma^\pm(\underline{k})} \right). \tag{30}$$

The summand in $\chi_{f,\sigma}^{\alpha,\beta,(0)}$ is manifestly positive. Hence, for positive J we may have a state for which the z component of the spin magnetization for each $5f$ band vanishes (i.e., $\overline{n}_{f,\sigma}^{\chi} = \overline{n}_{f,-\sigma}^{\chi}$) and the spin-up with the spin-down dispersion relations are identical, but for which $z_{\underline{Q},\sigma} = -z_{\underline{Q},-\sigma}$. For negative values of J, one may have a paramagnetic solution for which $z_{\underline{Q},\sigma} = z_{\underline{Q},-\sigma}$. If $|z_{\underline{Q},\sigma}| \neq |z_{\underline{Q},-\sigma}|$, the system may have a nonzero value of the z component of the magnetization. We shall, henceforth, restrict our attention to positive J. The critical value of J, J_c, at which this new phase may occur is given by the expression

$$\begin{aligned} &\left[1-(U-J_c)\chi_{f,\sigma}^{\alpha,\beta,(0)}(\underline{Q},0)\right]\left[1-(U-J_c)\chi_{f,-\sigma}^{\alpha,\beta,(0)}(\underline{Q},0)\right] \\ &\quad = J_c^2 \chi_{f,-\sigma}^{\alpha,\beta,(0)}(\underline{Q},0)\chi_{f,\sigma}^{\alpha,\beta,(0)}(\underline{Q},0). \end{aligned} \tag{31}$$

It is seen that the novel transition is promoted by the Fermi-surface nesting between the two bands with different $5f$ orbital characters. In this aspect our theory bares a resemblance to that of Dubi and Balatsky.[17] However, in their case the hybridization wave is driven by a spin-independent interaction, whereas in our theory the transition is driven by the spin-flip part of the Hund's rule exchange and thus breaks spin-rotational invariance. The interband susceptibility $\chi_f^{\alpha,\beta,(0)}(\underline{Q},0)$ is shown as a function of μ in Fig. 3. The graph determines the μ dependence of the critical value of J_c^{-1} at which the novel state first becomes stable, when $U = J$. The figure also shows $\chi_f^{\alpha,\alpha(0)}(\underline{Q},0) + \chi_f^{\beta,\beta(0)}(\underline{Q},0)$ which, when $U = J$, determines the critical value of J^{-1} required for the antiferromagnetic instability. The magnetic susceptibility of the β band diverges logarithmically when the Fermi surface approaches the perfect nesting condition $\mu = E_{f,\sigma}^\beta(\underline{k}) = E_{f,\sigma}^\beta(\underline{k}+\underline{Q})$ at $\mu = 0.3$. The second peak originates from the α-band susceptibility. This is expected since the hybridized α band follows a similar dispersion relation to the β band, except it is split and shifted by an energy of the order of $|V|^2$ by the hybridization and, therefore, should exhibit a similar structure at a shifted value

of the chemical potential. The interband susceptibility shows a similar nesting peak at an intermediate value of μ. The graph indicates that the commensurate novel state may have a narrow region of phase space where it is stable against paramagnetism and Néel antiferromagnetism. The instability criterion can be extended to incommensurate wave vectors $\underline{q}$ by using the RPA. For an incommensurate transition, where the band folding is not appropriate, one should see clear signs of gapping in angle-resolved photoemission, at wave vectors corresponding to the nesting of sheets of the Fermi surface with different orbital characters. However, the gapping is expected to produce a new branch that only has appreciable intensity in the nested region of the Fermi surface. Since the Néel antiferromagnetic state is expected to be produced by intraband nesting, and since this model is characterized by a close proximity of the intra- and interband nesting vectors, it is expected that these two phases are competing for the same regions of the Fermi surface. It should be noted the role of nesting in the electronic structure of URu_2Si_2 has been investigated within the local density approximation (LDA).[27,28] The LDA studies[27,28] have identified a commensurate nesting vector associated with the antiferromagnetic phase and have also discovered the pure character of the $5f$ bands in the normal state. The underscreened Anderson lattice model, although generic, captures these features. Our description is also consistent with the interpretation of inelastic neutron-scattering measurements.[11,12] Hence, it seems highly unlikely that this novel state will coexist homogeneously with antiferromagnetism. This is consistent with the experimental observations[9] on URu_2Si_2. For $U = J$ and a general value of J away from the quantum critical value J_c, the temperature dependence of the gap $|\kappa_{\underline{Q},\sigma}(T)|$ has the usual mean-field variation shown in Fig. 4. The calculated ratio of the gap parameter to T_c of $\sim$2.25 should be compared with the experimentally determined value[5] of 2.9 ± 0.15. The result shown in Fig. 4 is important for the comparison with the compound URu_2Si_2. It supports our hypothesis that the change occurring at 17.5 K is due to an opening of a gap resulting from the underscreened band structure with a twofold degenerate $5f$ level, as expected in uranium compounds.

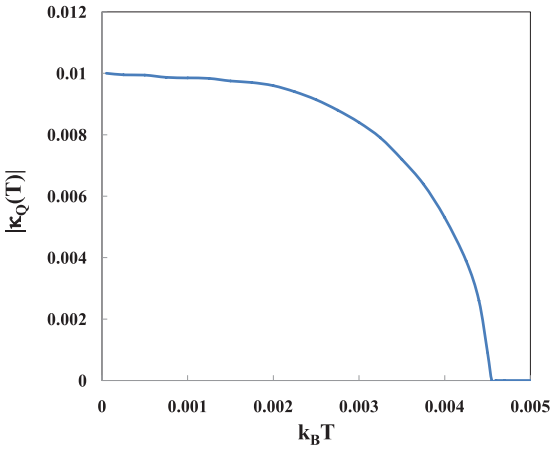

FIG. 4. (Color online) The temperature dependence of the gap parameter $|\kappa_{\underline{Q},\sigma}(T)|$ for a value of $J = 0.128$ and $U = J$. This value of J is comparable to the assumed value of 0.6 for the $5f$ bandwidth due to direct f-f hopping.

IV. RESULTS AND DISCUSSION

The novel state is described by a nonzero value of the complex order parameter $Z_{\underline{Q}}$, defined as the trace over spins of a spin-dependent expectation value

$$Z_{\underline{Q}} = \frac{1}{2N} \sum_{\underline{k},\sigma} \sigma \langle f^{\dagger,\beta}_{\underline{k}+\underline{Q},\sigma} f^{\alpha}_{\underline{k},\sigma} \rangle, \tag{32}$$

which characterizes a type of spin inter-$5f$ orbital-density wave. Since this appears to be a second-order instability which breaks a continuous gauge symmetry through short-ranged interactions,[33] there should be a branch of collective Goldstone modes associated with it.[34] However, unlike the case of ordinary magnetic instabilities,[32] the Goldstone modes are not expected to be easily accessed via inelastic neutron-scattering spectroscopy. Therefore, we shall outline the signatures of the novel state that may be accessed in orbitally sensitive, angle-resolved photoemission measurements.

In the novel state, the $5f$ quasiparticle dispersion relations are modified and the orbital characters of the bands are mixed. The dispersion relations and the $5f$ orbital characters of the bands are shown in Fig. 5 for wave vectors along the nesting direction. The weights for each character when summed over the bands yield unity. It can be seen that the set of bands containing the α character contains a pair of adjacent band segments with disjoint dispersion relations which are quite similar to those of the upper and lower hybridized bands of the normal state. The $5f$ α intensities of this pair of band segments grossly follow the same pattern as the intensities of the pair of hybridized bands in the normal state. However, the individual α weights of the segments do show sharp jumps in the regions where gaps, either at the Fermi-surface gaps or above, are found. It is the gapping of the Fermi surface that stabilizes the novel state. A Fermi-surface gap occurs for $|k| \sim 0.48$, and a smaller gap above the Fermi-surface gap can be seen for $|k| \sim 0.37$. It should be noted that Fermi-surface gaps at $k \sim \pm 0.56$ have been inferred from the experimental measurements of Dakovski *et al.*[36] In the momentum intervals enclosed by these gaps, the dispersion relation marked by solid red triangles has a gradual variation in intensity caused by the hybridization of the $5f$ α band with the conduction band. The set of bands with β character contain two adjacent segments that, when combined, resemble the pure β band of the normal state. The β weights of these two adjacent segments form a (disjoint) curve that remains almost constant over almost the entire Brillouin zone, similar to the normal state. However, there are rapid changes in the intensity for the $\underline{k}$ values where the energy gaps occur between the consecutive segments. It is seen that the Fermi-surface gaps for the β-character bands occur at $k \sim \pm 0.52$, which slightly differ from the k values for which the Fermi-surface gaps occur in the bands with α character. This leads to a double-gap structure seen in Fig. 6. It should be noted that despite the gapping of the Fermi surface for the normal-state derived bands, the occurrence of new bands that cross the Fermi energy, albeit with reduced intensities, allows the novel (mean-field) phase to be classified as metallic. This can be seen

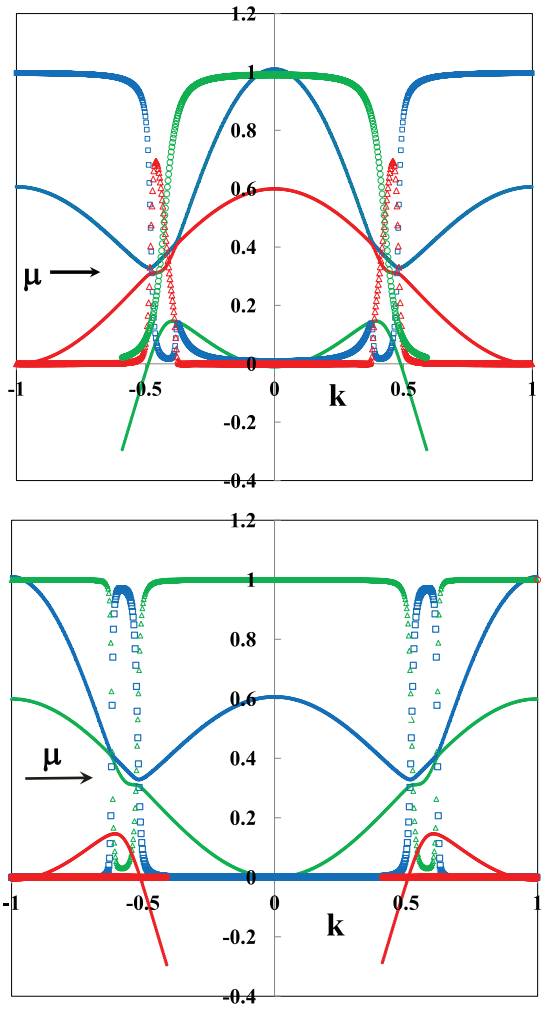

FIG. 5. (Color online) (Upper panel) A schematic close-up view of the dispersion relations (filled markers) for the bands with α character in the novel state and their $5f$ α weights (unfilled markers). The wave vector $\underline{k}$ is directed along the $(1,1,1)$ direction. The position of the Fermi energy μ is marked by the arrow. The α intensities for the various branches of dispersion relations are indicated by symbols of the same type. (Lower panel) The dispersion relations for the bands with β character and their $5f$ β weights are plotted as functions of $\underline{k}$.

in the density of states shown in Fig. 7. For the commensurate case considered here, the picture greatly simplifies if one folds the Brillouin zone. Indeed, evidence of a modified periodicity (such as from simple tetragonal to body-centered tetragonal) in the "hidden-order" state of URu_2Si_2 has been inferred from angle-resolved photoemission experiments.[35]

In summary, we propose that this concept of a spin-interorbital density wave may describe the "hidden-order" state of URu_2Si_2. The order parameter is complex, indicating that the transition breaks a continuous gauge symmetry of the Hamiltonian. The correlations in this state are not readily accessible by purely spin or purely orbital measurements. However, the novel state is produced by the nesting between sheets of the Fermi surface with different (unmixed) orbital characters. Furthermore, below the transition temperature, the Fermi surface will gap at these points, leading to the formation of small patches of dispersion relations that describe electrons

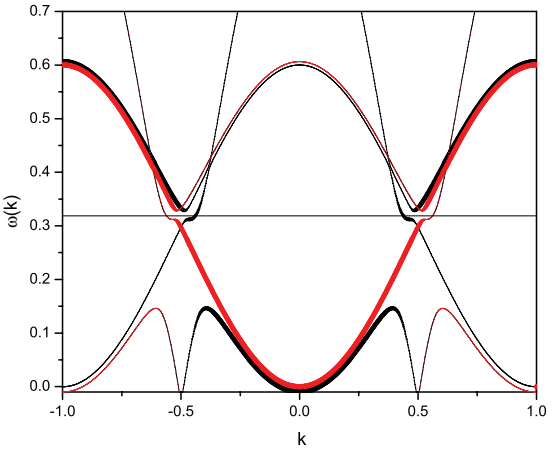

FIG. 6. (Color online) The dispersion relations for the $5f$ α (black line) and $5f$ β (red line) electrons along the (k,k,k) direction. The widths of the lines are proportional to their intensities. The Fermi energy μ is set at about 0.32 and is indicated by the horizontal line. The α-dispersion relations shows the existence of a direct gap of the order of $2|V| \sim 0.2$ between the two branches. For other wave vectors, the α and β branches follow similar dispersion relations; however, their degeneracy is lifted by a small energy of the order of $|V|^2$. Gaps at the Fermi energy are seen to occur at points which are connected by the commensurate nesting vector $\underline{Q} = (1,1,1)$. (Figure courtesy of T. Durakiewicz.)

with mixed orbital characters. The existence of two distinct gaps with mixed characters of $5f$ states may be identifiable through orbitally sensitive angle-resolved photoemission measurements. Indeed, such gaps shifting states away from the Fermi level at specific locations in the Brillouin zone have been seen[36] to evolve in the hidden-order phase of URu_2Si_2. Since antiferromagnetism is favored by nesting between sheets with the same (unmixed) orbital characters, and since the

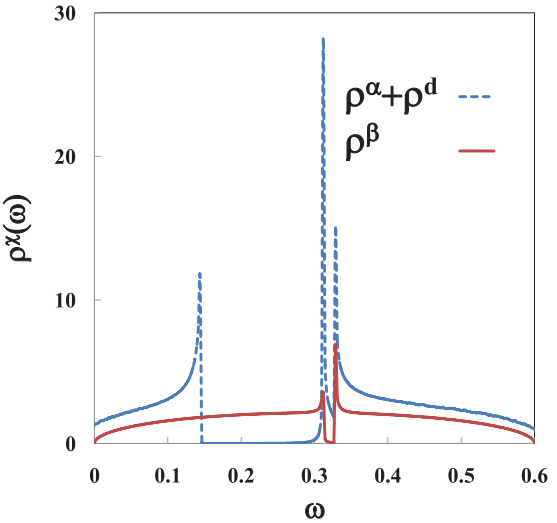

FIG. 7. (Color online) The combined α $5f$ $\rho^{\alpha}(\omega)$ and conduction-band density of states for the ordered state as a function of ω. The β $5f$ density of states $\rho^{\beta}(\omega)$ is also shown as a function of ω. It seen that the gap structure associated with the novel ordering is highly asymmetric.

interband and intraband nesting points are close, the novel ordering is expected to compete with antiferromagnetism, as has been found to be the case for URu_2Si_2. Thus, we have presented a new model starting from two $5f$-localized bands hybridized with a conduction band within the underscreened Anderson lattice model. We have obtained an electronic structure with gaps which increase with decreasing temperature. Our model can account for the opening of a gap observed in a number of different experiments (including recent photoemission measurements) in the hidden-order phase of URu_2Si_2.

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