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Gap-anisotropic model for the narrow-gap Kondo insulators

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A theory is presented which accounts for the dynamical generation of a hybridization gap with nodes in the Kondo insulating materials CeNiSn and CeRhSb. We show that Hund’s interactions acting on virtual 4f$^2$ configurations of the cerium ion can act to dynamically select the shape of the cerium ion by generating a Weiss field which couples to the shape of the ion. In low symmetry crystals where the external crystal fields are negligible, this process selects a nodal Kondo semimetal state as the lowest energy configuration.

Pacs numbers:
creates a conduction electron in a \( l = 3, j \equiv 5/2 \) Wannier state at site \( j \) with shape-spin quantum numbers \((a, \sigma)\), \( N \) is the number of sites and
\[
\gamma_{a\sigma}^{m_j}(\mathbf{k}) = Y_3^{m_j, -\sigma}(\mathbf{k}) \left( \frac{1}{2}, 3 \right) m_j + \sigma \left( \frac{3}{2} \right) m_j
\] (7)
defines the form-factors, in terms of spherical harmonics and the Clebsch-Gordan coefficients of the \( j = 5/2 \) \( f^1 \)-state, where \( m_j \equiv m_j(a, \sigma) \) maps the spin-shape quantum numbers to the original azimuthal quantum number of the \( f \)-scattering channel. Following previous authors, \( H \) is a low energy Hamiltonian, so that hybridization strength \( V \) is a renormalized quantity, that takes into account the high energy valence and spin fluctuations.

The term
\[
H_f = \sum_j \left[ E_f n_f(j) + \frac{U}{2} (n_f(j) - 1)^2 - \frac{g}{2} \Gamma^2 \right]
\] (8)
describes the residual low-energy interactions amongst the \( f \)-electrons: the second term is a Coulomb interaction term. The third term is a Hund's interaction which favors \( f^2 \) states with maximal total angular momentum. In an isotropic environment, this interaction would take the form \( -\frac{g}{2} \Gamma^2 \), where \( J \) is the total angular momentum operator, but in a crystalline environment, it takes on a reduced symmetry which we model in simplified form by \( -\frac{g}{2} \Gamma^2 \). In general the Hund's interaction is only invariant under discrete rotations so that fluctuations into the \( f^2 \) state enable the system to sample the crystal symmetry even when the conventional crystal field splittings are absent.

Suppose the crystal electric field term were unquenched, so that \( H \rightarrow H - \sum \alpha \cdot \Gamma_j \). The shape of the Erbium ion \( (\Gamma_j) = \Gamma \) is determined by the condition that the energy is stationary with respect to variations in \( \Gamma \),
\[
N^{-1}_s \delta(H_o) / \delta \Gamma = \alpha + g \Gamma.
\] (9)
The second term is a feedback or “Weiss” contribution to the crystalline electric field, created by fluctuations into the \( f^2 \) state. Generally, the induced field \( \Gamma \) will follow the crystalline electric fields \( \alpha \), but in situations where the valence and spin fluctuations are rapid enough to quench the external crystal electric field, then \( \alpha = 0 \), and the Weiss field becomes free to explore phase space to minimize the total energy. In such a situation, the shape of the Erbium ion is determined by the interactions, rather than the local conditions around each ion.

To explore this process, we carry out a Hubbard-Stratonovich decoupling of the interactions,
\[
H_f(j) \rightarrow f_j^\dagger \left[ (E_f + \lambda_j) \mathbf{1} + \Delta_j \cdot \mathbf{A} \right] f_j + E_o[\lambda_j, \Delta_j]
\] (10)
where
\[
E_o[\lambda_j, \Delta_j] = \frac{\Delta^2}{2g} - \frac{\lambda_j^2}{2U} - \lambda_j
\] (11)
Here \( \Delta^a(j) \sim -g \Gamma^o(j) \) is a dynamical Weiss field, \( f_j \) denotes the spinor \( f_j \equiv f_{\sigma}(j) \). Note that in the path integral, the fluctuating part of \( \lambda_j \), associated with the suppression of charge fluctuations, is imaginary. We now seek a mean-field solution where the Weiss field \( \lambda_j = \lambda \) and \( \Delta_j = \Delta \), and \( E(\lambda, \Delta_j) = E_o \). Such an expectation value does not break the crystal symmetry. However, the selected crystal field matrix \( \Delta \Delta \) must adjust to minimize the total energy. Supposing we diagonalize this matrix, writing \( \Delta \Delta = U \Delta^o U^\dagger \), where \( \Delta^o = \text{diag}(\Delta_1, \Delta_2, \Delta_3) \), and \( \Delta_1 > \Delta_2 > \Delta_3 \). In the basis, \( f_{\sigma}(j) = U_{\sigma\alpha}^o f_j^o(\sigma, j) \), the crystal field is diagonal. In practice, the strengths of the Hund’s interaction \( g \) is so large that the excitation energies \( \Delta_{1,2} - \Delta_3 \) substantially exceed the Kondo temperature. In this case, the mean-field Hamiltonian must be projected into the subspace of the lowest eigenvalue.

In the hybridization, we therefore replace
\[
c_j^\dagger f_j = c_j^\dagger U \hat{f}_j \rightarrow b_{\alpha}[c_{\alpha\sigma}(j) \hat{f}_\sigma(j)]
\] (12)
where \( \hat{f}_\sigma(j) \equiv \hat{f}_{3\sigma} \) (dropping the superfluous index “3”) describes the lowest Kramers doublet and \( b_\alpha \equiv U_{\alpha3} \). To satisfy the constraint \( (n_f(j)) = 1 \), the energy of the lowest Kramers doublet must be zero, i.e. \( E_f + \lambda + \Delta_3 = 0 \). We then arrive at the mean-field Hamiltonian
\[
H^* = H_o + V \sum_k [\phi_{\alpha\sigma}(k) c_k^\dagger f_{\alpha k} + H.c] + N_s E_o
\] (13)
where \( \phi_{\alpha\sigma}(k) = \sum \alpha b_\alpha Y_{\alpha\sigma}(k) \) is the dynamically generated form-factor of the hybridization. The transformed hybridization is no longer rotationally invariant: all information about the anisotropic wavefunction of the Cerium ion is now encoded in the vector \( \mathbf{b} \). The quasiparticle energies associated with this Hamiltonian are
\[
E_{k}^\pm = \epsilon_k/2 \pm \sqrt{(\epsilon_k/2)^2 + V_k^2}
\] (14)
Here, the hybridization can be written in the convenient form \( V_k = V^2 \phi_{\hat{k}}(k) \), where \( \phi_{\hat{k}}(k) = (1/2) \sum_{\alpha, \sigma} b_{\alpha} Y_{\alpha\sigma}(k) \) contains all the details of the gap anisotropy. The ground-state energy is then the sum of the energies of the filled lower band
\[
E_g = -2 \sum_k \sqrt{(\epsilon_k/2)^2 + V_k^2} + N_s E_o
\] (15)
Now both \( \lambda \) and \( \Delta_3 \) are fixed independently of the direction of \( \mathbf{b} \), so that \( E_o \) does not depend on \( \mathbf{b} \). To see this, write the eigenvalues of the traceless crystal field matrix as \( \Delta_{1,2} = \frac{1}{\sqrt{3}} \Delta \pm \delta \), \( \Delta_3 = -\frac{1}{\sqrt{3}} \Delta \). Since the two upper two crystal field states are empty, stationarity w.r.t to \( \delta \) requires \( \delta = 0 \). Since \( \Delta_3 \) couples directly to the \( f \)-charge, we obtain \( \partial E_g / \partial \Delta = -\sqrt{2/3} (n_f(j) + \Delta/j) = 0 \), so that
\[
\Delta = \sqrt{\frac{3}{2}} g. \text{ Thus both } \lambda = -\Delta_3 - E_f \text{ and } \Delta_3 \text{ are fixed.}
\]
where the hybridization is.

**FIG. 1.** Contour plot of the ground-state energy in mean-field theory as a function of the two first components of the unit vector \( \hat{b} \) (the third one is taken as positive). The darkest regions correspond to lowest values of the free-energy. Arrows point to the three global and three local minima.

The relative stability of the IM and the octahedral state will, in general, be dependent on details of our model, such as the detailed conduction electron band-structure. For this reason, both possibilities should be considered as candidates for the nodal semi-metallic states of CeNiSn and CeRhSb. The inset in Fig (2) shows the density of states predicted by these two possibilities. Although both are gapless, the v-shaped pseudogap of the quasi-octahedral state is far more pronounced than in the axial state, and is closer in character to the observed tunneling density of states. A more direct probes of the anisotropy is provided by the thermal conductivity which, unlike the resistivity, does not show a strong sample dependence in these compounds.

To compute and compare the theoretical thermal conductivity with experiments, we compute the thermal current correlator

\[
\kappa^{ij} = \frac{1}{2T} \int_{-\infty}^{\infty} d\omega \omega^2 \left(-\frac{\partial f}{\partial \omega}\right) \frac{N(\omega)}{\Gamma(\omega)} \langle \hat{V}^i \hat{V}^j \rangle_{\omega},
\]

where \( f \) is the Fermi function, \( \Gamma(\omega) \) is the quasiparticle scattering rate and

\[
N(\omega) \langle \hat{V}^i \hat{V}^j \rangle_{\omega} = \sum_k \hat{V}^i_k \hat{V}^j_k \delta(\omega - \hat{E}_k)
\]

describes the quasiparticle velocity distribution where \( \hat{V}_k = \hat{\nabla}_k E_k \) and \( E_k \) is given by equation (14). For our calculation, we have considered quasiparticle scattering off a small, but finite density of unitarily scattering impurities or “Kondo holes”. We use a self-consistent T-matrix approximation, following the lines of earlier calculations except for one key difference. In these calculations, which depend critically on the anisotropy, it is essential to include the momentum dependence of the hybridization potential in the evaluation of the quasiparticle current. Previous calculations underestimated the anisotropy by neglecting these contributions.

The single node in the IM state leads to a pronounced enhancement of the low-temperature thermal conductivity along the \( \hat{z} \) axis. By contrast, in the quasi-octahedral state the distribution of minima in the gap give rise to a modest enhancement of the thermal conductivity in the basal plane. Experimental measurements tend to favor the latter scenario, showing an enhancement in thermal conductivity that is much more pronounced in \( \kappa_\parallel \) than in \( \kappa_\perp \) or \( \kappa_\perp \).

Three aspects of our theory deserve more extensive examination. Nodal gap formation is apparently unique to CeNiSn and CeRhSb; the other Kondo insulators SmB\(_6\), CeB\(_6\)Pt\(_3\) and YbB\(_6\) display a well-formed gap. Curiously, these materials are cubic, leading us to speculate that their higher symmetry prevents the dynamically generated contribution to the crystal field from exploring...
FIG. 2. Normalized thermal conductivity versus temperature along the z-axis (solid line) and in the basal plane (dashed line). Top: for the Ikeda-Miyake state. Bottom: for the quasi-octahedral scenario. Insets show density of states as a function of the energy. The adjustable parameters have been chosen as \( V/D = 0.08 \) and an impurity scattering phase-shift of \( \pi/2 \).

the region of parameter space where a node can develop. At present, we have not included the effect of a magnetic field, which is known to suppress the gap nodes. There appears to be the interesting possibility that an applied field will actually modify the dynamically generated crystal field to eliminate the nodes. Finally, we note that since the spin-fluctuation spectrum will reflect the nodal structure, future neutron scattering experiments should in principle be able to resolve the axial or octahedral symmetry of the low energy excitations.

To conclude, we have proposed a mechanism for the dynamical generation of a hybridization gap with nodes in the Kondo insulating materials \( \text{CeNiSn} \) and \( \text{CeRhSb} \). We have found that Hunds interactions acting on the virtual \( 4f^2 \) configurations of the Cerium ions generate a Weiss field which acts to co-operatively select a semi-metal with nodal anisotropy. Our theory predicts two stable states, one axial, the other quasi-octahedral in symmetry. The quasi octahedral solution appears to be the most promising candidate explanation of the various transport and thermal properties of the narrow-gap Kondo insulators.

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