Insulator-to-metal phase transition in Yb-based Kondo insulators

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Abstract – The periodic Anderson lattice model for the crystalline electric field (CEF) split 4f quartet states is used to describe the Yb-based Kondo insulators. In the slave-boson mean-field approximation, we derive the hybridized quasiparticle bands, and surprisingly find that decreasing the hybridization difference of the two CEF quartets may induce a continuous insulator-to-metal phase transition. The resulting metallic phase has a hole and an electron Fermi pocket. Such a phase transition may be realized experimentally by applying pressure, reducing the difference in hybridization of the two CEF quartets in real materials.

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It is well known that Kondo insulators or semiconductors also belong to strongly correlated electron systems [1, 2], in which the conduction electrons hybridize with the localized 4f-electrons and the strong Coulomb repulsion results in highly renormalized quasiparticle bands with a small indirect energy gap [3–6]. To study these materials at low temperatures, some experiments attempted to make the energy gap vanish by applying an external magnetic field [7,8] or pressure [9], leading to an insulator-to-metal phase transition. The phase transition under the magnetic field has been studied intensively [10–14], however, the microscopic mechanism for the pressure-induced insulator-to-metal transition remains far from being fully understood.

For the Yb-based Kondo insulators, such as YbB12, an external pressure can affect the hybridization between 5d band electrons and the more atomic-like 4f-electrons. The Yb valence is directly related to the number of 4f-holes $n_h$ by $v = 2 + n_h$. At the ambient pressure, $n_h$ spans a range between 0 and 1, and the intermediate valence reflects the hybridization of the energetically close configurations of Yb$^{2+}$($4f^{14}$) and Yb$^{3+}$($4f^{13}$). The Yb$^{3+}$ electronic configuration can be regarded as a single hole in the 4f-shell, while the Yb$^{2+}$ configuration corresponds to the closed 4f-shell. Taking into account the presence of a larger spin-orbit coupling (1.3 eV) in the Yb-based compounds [15], a $j = 7/2$ f-hole state is split into a quartet and two doublet states by the crystalline electric field (CEF) under the cubic symmetry, which is the lattice structure of the typical material YbB12. These two doublets are almost degenerate and may be treated as a quasi-quartet. Thus, a periodic Anderson lattice model with $U \rightarrow \infty$ for the CEF split 4f states can be used to describe the Yb-based Kondo semiconductors or insulators [16].

It has been recently pointed out that the anisotropic hybridizations of the two CEF quartets play an important role in the formation of the two dispersive spin resonances at the continuum threshold [16], the most salient features observed by inelastic neutron scattering experiments in YbB12 (refs. [5,6]). Motivated by this analysis, in this paper we carefully study the periodic Anderson lattice model with $U \rightarrow \infty$ for the CEF split 4f quartet states. Using the slave-boson mean-field approximation, we will derive four quasiparticle bands resulting from the hybridization between the conduction electrons and localized 4f-hole states. Apart from the insulating state at the large anisotropic hybridizations of the two CEF quartets, we surprisingly find that there exists a threshold of the CEF splitting, above which decreasing the difference in the hybridization of the two CEF quartets may induce an overlap between the lower and upper hybridized quasiparticle bands, leading to an insulator-to-metal phase transition. Experimentally, this
phase transition can be realized by applying pressure, which reduces the difference in the hybridization of the two CEF quasi-quartets in real materials. Actually, the pressure-induced insulator-to-metal transition has been observed in the Kondo insulator SmB$_6$ (ref. [9]).

To describe the Yb-based Kondo insulators or semiconductors, the periodic Anderson lattice model with $U \to \infty$ for the CEF split 4$f$ states has been introduced [16]

$$
\mathcal{H} = \sum_{k, \gamma} \epsilon_k d_{k\gamma}^\dagger d_{k\gamma} + \sum_{k, \gamma} (\epsilon_f + \Delta_\gamma) f_{k\gamma}^\dagger f_{k\gamma} + \frac{1}{\sqrt{N}} \sum_{i, k, \gamma} (V_{k\gamma} e^{i k \cdot R_i} f_{i, k\gamma}^\dagger d_{k\gamma} b_i + \text{h.c.}),
$$

where the first term denotes the conduction electron band, the second term stands for the binding energy of the 4$f$-hole, $\gamma = 1, 2$ denote the two quasi-quartets, and $\Delta_\gamma$ ($\Delta_1 = 0$, $\Delta_2 = \Delta$) is the CEF splitting energy for the two quasi-quartets, where each quartet has a fourfold orbital degeneracy. Due to the exclusion of the double occupancy, a projection has been implemented by using the slave-boson representation [17]. Then the Yb occupation, a projection has been implemented by using orbital degeneracy. Due to the exclusion of the double occupancy, a projection has been implemented by using the slave-boson representation [17]. Then the Yb configuration with a $4f^{14}$ configuration without a $4f^{15}$ configuration with a $4f$-hole state is represented by a fermion state $f_{k\gamma}^\dagger$. The conduction electrons hybridize with the $f$-hole at each lattice site in both quartets with different strengths. At each lattice site the constraint $Q_i = b_i = \sum_{k} f_{k\gamma}^\dagger f_{k\gamma} = 1$ has to be enforced, and the total Hamiltonian is $\mathcal{H} + \sum_i \lambda_i(Q_i - 1)$, where $\lambda_i$ is the Lagrangian multiplier.

Now, the slave-boson mean-field approximation is performed by neglecting the fluctuation of the Bose field $(b_i^\dagger) = (b_i) = b$ and the site dependence of the local field $\lambda_i = \lambda$. Within these approximations, the mean-field model Hamiltonian can be written as

$$
\mathcal{H}_{MF} = \sum_{k, \gamma} [\epsilon_k d_{k\gamma}^\dagger d_{k\gamma} + \tilde{\epsilon}_f f_{k\gamma}^\dagger f_{k\gamma} + \tilde{V}_f (d_{k\gamma}^\dagger f_{k\gamma} + \text{h.c.})] + N \epsilon_0,
$$

where $\tilde{\epsilon}_f = \epsilon_f + \Delta_\gamma + \lambda$ is the renormalized energy level of the localized states, $\tilde{V}_f = b N \epsilon_f$, and $\epsilon_0 = \lambda (b^2 - 1)$. It should be noticed that the dependence of the hybridization strengths on $k$ has been neglected, i.e., $V_{k\gamma} = V \gamma$. By performing the Bogoliubov transformation

$$
\alpha_{k\gamma} = \mu_{k\gamma} d_{k\gamma} + \nu_{k\gamma} f_{k\gamma}, \quad \beta_{k\gamma} = -\nu_{k\gamma} d_{k\gamma} + \mu_{k\gamma} f_{k\gamma},
$$

we can diagonalize the quadratic Hamiltonian and obtain

$$
\mathcal{H}_{MF} = \sum_{k, \gamma} \left( E_{k\gamma}^+ \alpha_{k\gamma}^\dagger \alpha_{k\gamma} + E_{k\gamma}^- \beta_{k\gamma}^\dagger \beta_{k\gamma} \right),
$$

where the four hybridized quasiparticle bands are derived

$$
E_{k\gamma}^\pm = \frac{1}{2} \left[ \epsilon_k + \tilde{\epsilon}_\gamma \pm \sqrt{(\epsilon_k - \tilde{\epsilon}_\gamma)^2 + 4 \tilde{V}_f^2} \right],
$$

and the Bogoliubov parameters $\mu_{k\gamma}$ and $\nu_{k\gamma}$ are given by

$$
\begin{align*}
(\mu_{k\gamma}, \nu_{k\gamma}) &= \frac{1}{\sqrt{2}} \sqrt{\frac{\epsilon_k - \tilde{\epsilon}_\gamma}{\sqrt{(\epsilon_k - \tilde{\epsilon}_\gamma)^2 + 4 \tilde{V}_f^2}}}
\end{align*}.
$$

These two parameters describe the contributions of the conduction electrons and localized $f$-hole states to the hybridized quasiparticles, respectively.

Moreover, the ground-state energy per site can be calculated as

$$
E_g = \frac{1}{N} \sum_{k, \gamma} \left[ E_{k\gamma}^+ \theta(E_{k\gamma}^+) + E_{k\gamma}^- \theta(E_{k\gamma}^-) \right] + \epsilon_0,
$$

where $\theta(E_{k\gamma}^\pm)$ is the step function. The chemical potential $\mu$ and the Lagrangian multiplier $\lambda$ have to be determined self-consistently according to the conservation of the total number of particle per lattice site $n_+ + n_- = 2$. Depending on the parameter values $\tilde{\epsilon}_f$, $\Delta$, and $\tilde{V}_f$, the variational parameters $b$ and $\lambda$ have to be self-consistently determined. From the hybridized quasiparticle band structure, the ground state of the system can be an insulating state, where the lower two bands are filled completely, leaving an indirect energy gap. As the $k$-dependence in $E_g$ appears through the conduction electron energy $\epsilon_k$, summations over $k$ can be transformed into an integral over energy $\epsilon$ in the interval $[-D, D]$. By assuming a constant density of states, the ground-state energy is thus evaluated as

$$
E_g = \frac{1}{8D} \sum_{\gamma} \left\{ 4D \tilde{\epsilon}_\gamma - 4 \tilde{V}_f^2 \ln \Lambda_\gamma^2(D) + D - \tilde{\epsilon}_\gamma 
\right. 
- \left[ (D - \tilde{\epsilon}_\gamma) \Lambda_\gamma^2(D) + (D + \tilde{\epsilon}_\gamma) \Lambda_\gamma^2(D) \right] \right\} + \epsilon_0,
$$

where

$$
\Lambda_\gamma^\pm(D) = \sqrt{D \pm \tilde{\epsilon}_\gamma} + \tilde{V}_f, \quad \tilde{\epsilon}_\gamma = \tilde{\epsilon}_f + \Delta_\gamma, \text{and} \quad \tilde{V}_f = b (V_1 + \delta V).
$$

Minimizing the ground-state energy density with respect to $b$ and $\lambda$, respectively, we obtain the following self-consistent equations:

$$
\begin{align*}
&b^2 = \frac{1}{4D} \sum_{\gamma} \left[ \Lambda_\gamma^+(D) - \Lambda_\gamma^-(D) \right], \\
&\lambda = \frac{1}{2D} \sum_{\gamma} V_f^2 \ln \Lambda_\gamma^2(D) + D - \tilde{\epsilon}_\gamma.
\end{align*}
$$

However, apart from the insulating case, we notice that there exists another possible structure of the quasiparticle bands, where the chemical potential $\mu$ cuts through the two middle hybridized quasiparticle bands $E_{k1}^+$ and $E_{k2}^+$ at $\xi_1$ and $\xi_2$, respectively. Both these energy parameters are determined by the equation $E_{k1}^+ = E_{k2}^+ = \mu$. From the condition of the total number of particles per lattice site, we can derive the result of $\xi_1 = -\xi_2 \equiv -\xi$, leading to

$$
2 \xi + \Delta = \Lambda_\gamma^+(\xi) + \Lambda_\gamma^-(\xi).
$$
Here $\xi$ can be used to characterize the insulator-to-metal phase transition. When $0 < \xi < D$, the ground state should be metallic, while for $\xi = D$ the ground state corresponds to a critical point. The corresponding ground-state energy density in the metallic phase is thus expressed as

$$E_g = \frac{1}{4D} [(3D - \xi)\tilde{\varepsilon}_1 + (D + \xi)\tilde{\varepsilon}_2 + \xi^2 - D^2]$$

$$+ \frac{\tilde{V}_1^2}{2D} \ln \frac{\Lambda_1^+(\xi) - \xi - \tilde{\varepsilon}_1}{\Lambda_1^+(\xi) + \xi - \tilde{\varepsilon}_1} - \frac{\tilde{V}_2^2}{2D} \ln \frac{\Lambda_2^-(\xi) + \xi - \tilde{\varepsilon}_2}{\Lambda_2^-(\xi) - \xi - \tilde{\varepsilon}_2}$$

$$- \frac{1}{8D} \left[ (\xi + \tilde{\varepsilon}_1)\Lambda_1^+(\xi) + (D - \tilde{\varepsilon}_1)\Lambda_1^-(\xi) \right]$$

$$- \frac{1}{8D} \left[ (\xi - \tilde{\varepsilon}_2)\Lambda_2^+(\xi) + (D + \tilde{\varepsilon}_2)\Lambda_2^+(\xi) \right] + \epsilon_0.$$  \hfill (12)

By minimizing $E_g$ with respect to $b$ and $\lambda$, the corresponding self-consistent equations can be deduced to

$$b^2 = \frac{1}{4D} [\Lambda_1^+(\xi) + \xi - \tilde{\varepsilon}_1]$$

$$\lambda = \frac{\tilde{V}_1^2}{2D} \ln \frac{\Lambda_1^+(\xi) - \xi - \tilde{\varepsilon}_1}{\Lambda_1^+(\xi) + \xi - \tilde{\varepsilon}_1} + \frac{\tilde{V}_2^2}{2D} \ln \frac{\Lambda_2^-(\xi) + \xi - \tilde{\varepsilon}_2}{\Lambda_2^-(\xi) - \xi - \tilde{\varepsilon}_2}.$$  \hfill (13)

In order to deduce the ground-state phase diagram, we should first numerically solve eq. (10) for the insulating phase and eqs. (11), (13) for the metallic phase, respectively. Our numerical calculations have been performed with $V_1 = 0.4D$, $\epsilon_f = -0.5D$, and $\Delta = 0.1D$, which are chosen as the same as the previous investigation [16]. The obtained hybridized quasiparticle band energy vs. the momentum along the diagonal direction are plotted in fig. 1 for three different values of $\delta V$. As shown in fig. 1(a) for $\delta V = 0.18D$, there opens an indirect gap between the middle upper and lower bands, corresponding to an insulating phase. In fig. 1(b) for $\delta V = 0.126D$, the middle upper and lower bands just meet at the chemical potential, corresponding the critical point of the transition. Since we have $\xi = D$ at the critical point, the ground-state energies of the metallic and insulating phases are equal. Finally, in fig. 1(c) for $\delta V = 0.01D$, the middle lower and upper bands overlap, and the chemical potential cuts through these two bands, which corresponds to the metallic phase.

The critical condition under which the insulator-metal phase transition occurs can be determined from eq. (11) and eq. (13) by setting $\xi = D$. For $V_1 = 0.4D$, $\epsilon_f = -0.5D$ and $\Delta = 0.1D$, the ground-state energy density $E_g$ is continuous at the transition point $\delta V/D = 0.126$ and is plotted as a function of $\delta V$ in fig. 2(a). Its first-order derivative $\partial E_g/\partial (\delta V)$ can also be calculated and is displayed in fig. 2(b) as a function of $\delta V$, which has a cusp at the transition point. These results indicate that this insulator-to-metal phase transition is a continuous second-order transition. The nature of this transition differs from the conventional Mott metal-insulator transition driven by the Coulomb interactions and should belong to the Lifshitz transition.

Next the ground-state phase diagram is constructed for $V_1 = 0.4D$ and $\epsilon_f = -0.5D$ and is shown in fig. 3(a). Clearly there exists a threshold of the CEF splitting energy $\Delta_0$, and only when $\Delta > \Delta_0$, the insulator-to-metal phase transition occurs by turning the difference in hybridization of the two CEF quasi-quartets. The change of the indirect gap is another evidence to characterize the insulator-to-metal phase transition, and can be also calculated and displayed in fig. 3(b) for $\Delta = 0.1D$. It shows that the indirect quasiparticle gap decreases almost linearly with decreasing the hybridization difference of the two CEF quartets, and this energy gap finally vanishes at $\delta V_c$. There is another critical value $\delta V^*$, where the top energy levels of the two lower quasiparticle bands interchange with each other around the Brillouin zone boundary. Thus the indirect energy gap has a cusp.

Actually, such an insulator-to-metal phase transition can be realized experimentally in Yb-based Kondo insulators (hole-type materials). Here we would like to emphasize that applying pressure usually decreases the hybridization strength between the conduction electrons and the localized $f$-electrons, which is just opposite to the pressure effect on the electron-type Ce compounds. We thus believe that the hybridization difference between upper and lower bands just meet at the chemical potential, corresponding the critical point of the transition.
two split crystalline electric field quartet states will also be reduced by applying pressure. For instance, in YbB\(_{12}\), if the CEF splitting is strong enough \(\Delta > \Delta_c\), applying pressure can continuously reduce the difference in hybridization of the two CEF quasi-quartets but almost no change of the CEF splitting. So below the critical value \(\delta V\), YbB\(_{12}\) is the usual insulator with an indirect gap as observed in experiments [3–6], while above this critical value \(\delta V\), this material can be transformed into a heavy electron metal with an enhanced effective mass due to the presence of heavy charge carriers. Such a phase transition in YbB\(_{12}\) should be confirmed in the future experiments.

Since a constant density of states for the conduction electron band was assumed in the above slave-boson mean-field calculation, the obtained results are independent of the spatial dimensionality of the model. In order to see the special Fermi surface structure of the metallic phase, the model Hamiltonian eq. (1) can be defined on a twodimensional square lattice system with the conduction electron band

\[
\epsilon_k = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y,
\]

where \(t\) denotes the nearest-neighbor hopping and \(t'\) denotes the next-nearest-neighbor hopping. Then the above slave-boson mean-field calculation can still be performed numerically, and for a set of parameters \(V_1 = 0.4D, \epsilon_f = -0.5D, t = 0.25D,\) and \(t' = 0.3t\), the insulator-to-metal phase transition also takes place when decreasing the parameter \(\delta V\). In the metallic phase, we have calculated the corresponding Fermi surface structure shown in fig. 4. There exist two Fermi pockets: one electron-like in the center of the Brillouin zone and one hole-like in the corners of the Brillouin zone. These two Fermi pockets have exactly the same size in the first Brillouin zone. So such a heavy electron metal corresponds to a semi-metal. Decreasing the hybridization difference \(\delta V\) below the critical value, the sizes of the electron and hole Fermi pockets become larger and larger, as displayed in fig. 4.

According to the quasiparticle band structure derived above, it has been seen that the Fermi surface of the resulting metallic phase should consist of a hole and an electron pockets. As the temperature is lowered enough, such a semi-metal state will not be stable. Considering the strong mixed valence characteristics in such systems, the additional on-site Coulomb interaction between the conduction electrons and localized \(f\)-electrons should be taken into account. In the slave-boson representation, such an interaction is given by

\[
H_I = U_f c_\beta^\dagger c_\beta c_\alpha^\dagger c_\alpha + \sum_{\gamma, \gamma'} f_{\gamma, \gamma'}^\dagger f_{\gamma, \gamma'}.
\]

When the coupling strength \(U_f\) is assumed to be small, we can rewrite this additional interaction in terms of the hybridized quasiparticles \(\alpha_{k,1}\) and \(\beta_{k,2}\) as

\[
H_I = \frac{U_f}{N} \sum_{k_1, k_2, k_3, k_4} \left( \nu_{k_1,1} \mu_{k_2,2} \nu_{k_3,2} \mu_{k_4,1} \alpha_{k_1,1}^\dagger \alpha_{k_2,1}^\dagger \alpha_{k_3,1} \alpha_{k_4,1} \alpha_{k_1,1}^\dagger \alpha_{k_2,1}^\dagger \alpha_{k_3,1} \alpha_{k_4,1} \right) + \nu_{k_1,1} \mu_{k_2,2} \nu_{k_3,2} \mu_{k_4,1} \alpha_{k_1,1}^\dagger \alpha_{k_2,1}^\dagger \alpha_{k_3,1} \alpha_{k_4,1}^\dagger \beta_{k_1,2} \beta_{k_2,2} \beta_{k_3,2} \beta_{k_4,2} + \nu_{k_1,1} \mu_{k_2,2} \nu_{k_3,2} \mu_{k_4,1} \alpha_{k_1,1}^\dagger \alpha_{k_2,1}^\dagger \alpha_{k_3,1} \alpha_{k_4,1}^\dagger \beta_{k_1,2} \beta_{k_2,2} \beta_{k_3,2} \beta_{k_4,2}
\]

where \(k_1 + k_2 = k_3 + k_4\) should be satisfied and we have only considered the two quasiparticle bands crossing the Fermi energy: \(\alpha_{k,1}\) and \(\alpha_{k,1}^\dagger\) are defined on the electron Fermi pocket, while \(\beta_{k,2}\) and \(\beta_{k,2}^\dagger\) are defined on the hole Fermi pocket. Among these residual quasiparticle interactions, the first two terms represent the intra-pocket scatterings with a small momentum transfer, while the last two terms correspond to the inter-pocket scatterings with a large momentum transfer. Since no quasiparticle pair hoppings exist between the two Fermi pockets, there will be no superconductivity instability with the \(s_\pm\)-wave pairings.

Fortunately, a recent renormalization group analysis for the two-band interacting electron model with electron and hole Fermi pockets has been performed and demonstrated that the inter-pocket quasiparticle scatterings plays an important role in determining the final ground state at low temperatures [18]. Therefore, the inter-pocket quasiparticle scatterings should be focused. When we set \(\bf q\) as a small momentum and \(\bf Q\) as a large momentum which is the distance between the centers of two Fermi pockets, then inter-pocket quasiparticle interactions can

![Fig. 3: (a) Ground-state phase diagram for \(V_1 = 0.4D\) and \(\epsilon_f = -0.5D\); (b) Indirect energy gap vs. the hybridization difference of the two CEF quartets \(\delta V\) for \(\Delta = 0.1D\).](image)

![Fig. 4: Fermi surface structure of the two-dimensional model Hamiltonian on a square lattice with \(V_1 = 0.4D\), \(\Delta = 0.1D\), and \(\epsilon_f = -0.5D\). (a) \(\delta V = 0.08D\) (b) \(\delta V = 0.05D\) and (c) \(\delta V = 0.01D\).](image)
be approximated as

\[
\frac{-U_{fc}}{N} \sum_{q q'} (\mu_{q,1} \mu_{q',1} + \mu_{q,2} \mu_{q',2} + \nu_{q,1} \nu_{q',1} + \nu_{q,2} \nu_{q',2}) \\
\times \alpha_{q,1}^\dagger \beta_{q+q',2} \beta_{q,2}^\dagger \alpha_{q',1}.
\]

(17)

When a strong nesting effect is present between the hole and electron Fermi pockets, this inter-pocket interaction can induce a particle-hole pairing between the quasiparticles, yielding to a charge-density wave ordering. The corresponding order parameter can be defined by \( \langle \alpha_{q,1}^\dagger \beta_{q+q',2} \rangle \) or \( \langle \beta_{q+q',2}^\dagger \alpha_{q',1} \rangle \), and an energy gap will open up in the charge excitations. This is a further prediction of our present theory, which is certainly needed to be investigated in future studies.

In conclusion, by using the slave-boson mean-field approximation, we have investigated the Yb-based Kondo insulators with a strong CEF splitting in the framework of the periodic Anderson lattice model. The obtained ground-state phase diagram and the indirect gap have demonstrated that there exists a continuous insulator-to-metal phase transition via reducing the hybridization difference of the two CEF quasi-quartets. Our theory provides a generic microscopic mechanism of the pressure induced insulator-to-metal transition, as increasing pressure can effectively reduce the anisotropy of the hybridization strengths of the two CEF quartets experimentally. The resulting metallic phase has a hole and an electron Fermi pockets, which may exhibit an instability of a charge-density wave ordering at low temperatures. The predicted phase transition is certainly needed to be confirmed experimentally in the future.

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