Mechanism for Opening of Energy Gap in Kondo Insulators with Orbital Degeneracies

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Abstract

We have performed a new LDA+U band calculation on the prototypical Kondo insulator material YbB_{12}, and constructed a simple tight-binding model with 5dε and 4f Γ_8 orbitals on Yb atoms with effective (ddσ) and(dfσ) integrals. A formation mechanism of the energy gap in Kondo insulators is clarified for the first time in a *realistic* model with orbital degeneracies in both conduction bands and 4f states.

Key words: Kondo insulator, energy gap, LDA+U band calculation, YbB_{12}
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The simplest theoretical model to describe the Kondo insulators is the periodic Anderson model (PAM). However, it has already been criticized that such a too simple model does not work in realistic systems with orbital degeneracy.[1] Consider the case shown in Fig.1(a) where the conduction band has two-fold orbital degeneracy. (The spin degeneracy is not explicitly shown here.) It is clear from Fig.1(b) that no gap appears after the hybridization.[2] We need a more sophisticated model and an explanation of the formation of a gap in real materials based on reliable band calculations. YbB_{12} is the best material for such purpose because it is one of the most intensively investigated materials, and has the simple crystal structure (NaCl type), where Yb ions and B_{12} clusters are located at the interpenetrating fcc sites.

Previous LDA band calculation[3] resulted in a semimetal because of a small overlap of the conduction and valence bands. Here, we have performed a new FLAPW band calculation for YbB_{12} using the LDA+U method[4] with slight extension.[5] "+U" term makes the occupied states lower in energy, so that a gap tends to open. The position of the 4f states is slightly shifted down to remedy a deficiency of LDA. We thus obtained an energy gap of about 0.0013

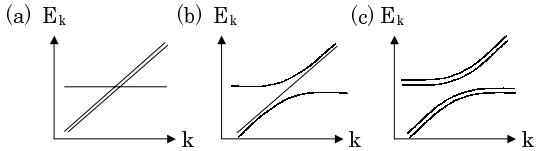

Fig. 1. The case that the hybridization gap does not open because of the degeneracy in the conduction band: (a) without the mixing, (b) after the mixing and (c) the case that both conduction and f bands are doubly degenerate.

Ryd as shown in Fig.2. The 4f levels are split into Γ_6, Γ_7 and Γ_8 under the cubic symmetry with the energies $E_{\Gamma_6} < E_{\Gamma_7} < E_{\Gamma_8}$. Under the hole picture, this is consistent with the crystal field levels $E_{\Gamma_6} > E_{\Gamma_7} > E_{\Gamma_8}$ suggested by the neutron scattering experiment.[6]

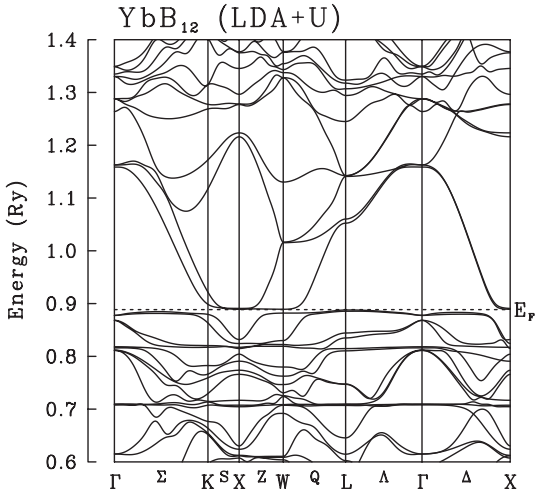

Fig. 2. LDA+U band calculation for YbB_{12}. The three flat bands correspond to the 4f Γ_8, Γ_7 and Γ_6 states, respectively.

We found that the energy bands obtained by the LDA+U calculation can be fitted well by a simple tight-binding model with only the (ddσ) overlapping integral among the 5dε (xy, yz and zx) orbitals on Yb ions, and (dfσ) between the 5d and 4f ($J = 7/2$, Γ_8) states. This (ddσ) should be regarded as being produced by the effective hopping through the B_{12} clusters. The energy dispersions of the d-bands are given by the following simple expressions $E_{\mathbf{k}}^{\alpha\beta} = E_{d\varepsilon} + 3(\mathrm{dd}\sigma)\cos(\mathrm{k}_\alpha/2)\cos(\mathrm{k}_\beta/2)$ for $(\alpha, \beta) = (x, y), (y, z)$ and (z, x) with $E_{\mathrm{d}\varepsilon}$=1.0 Ryd and (dd$\sigma$)= 0.06 Ryd. The bands running down from Γ to X(110) through K and from Γ to X(100) are doubly degenerate. Therefore, a simple hybridization with the f state does not yield an energy gap, as was mentioned above (Fig.1(b)).

Mixing matrix elements between the d (xy, yz and zx) and the f states (Γ_8) are calculated as, e.g. $\langle xy\uparrow|H|\Gamma_8^{(1)}+\rangle = 5it_1(c_x s_y - is_x c_y)$, where $|\Gamma_8^{(1)}+\rangle = \sqrt{7/12}|J_z = 7/2\rangle - \sqrt{5/12}|J_z = -1/2\rangle$, $c_x = \cos(k_x/2)$, $s_y = \sin(k_y/2)$ and $t_1 = \sqrt{5/56}(\mathrm{df}\sigma)$. Details will be given elsewhere.[7] Diagonalizing the Hamil-

tonian matrix for $E_{\Gamma_8} = 0.88$ Ryd and (dfσ)=0.01 Ryd, and shifting down the occupied bands by $\Delta E = -0.005$ Ryd based on the same spirit as the LDA+U treatment, we found that a small gap can open as shown in Fig.3 which is an indirect gap of about 0.003 Ryd between X and L points. The integrals (dfπ) $= -0.005$ Ryd and (ffσ) $= -0.002$ Ryd are also included here to improve the agreement with the band calculation.

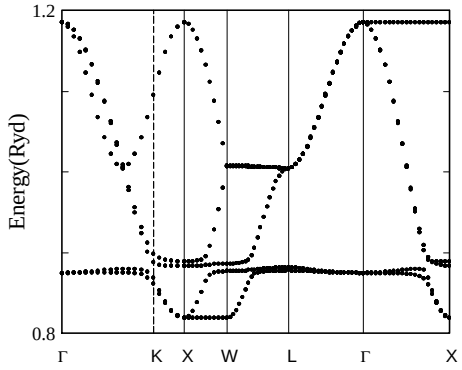

Fig. 3. Energy dispersion of the tight-binding model for the YbB_{12}. The 4f Γ_8 states are placed at 0.88 Ryd.

We finally point out that the gap opens only when the ground state of the 4f is Γ_8, which has two-fold orbital degeneracy (in addition to the Kramers one) as shown in Fig.1(c). Otherwise, if the ground state has only the Kramers degeneracy (e.g. Γ_7), Fig.1(b) applies and no gap opens.

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