A Simple Tight-Binding Model Description of the Conduction Band of the Kondo Insulator YbB_{12}

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Abstract

It is shown that the conduction band of typical Kondo insulator YbB_{12} can be expressed rather well by a simple tight-binding model of 5dϵ orbitals on Yb. The $(dd\sigma)$ overlapping integral is considered to be produced by the hopping through B_{12} clusters.The density of states is also calculated. If the mixing with the f-states is properly taken into account, this model can be a useful starting point for incorporating the strong correlation effect, and can consistently explain all the thermal, thermoelectric, transport and magnetic properties of YbB_{12}.

Key words: Tight-binding model; YbB_{12}; Kondo insulator;

1. Introduction

The Kondo insulator is considered to be a band insulator with a strong correlation.[1,2] Many examples are known among the rare earth compounds, e.g. SmB_6, YbB_{12}, C_3Bi_4Pt, CeRhSb, etc., and FeSi as an example among the transition metal compoumds.[3] Recently, some of these compounds are attracting renewed interests because of a potential candidate for an efficient themoelectric device.[4] However, quantitative analysis on these materials have been hindered because of the lack of a simple description of the basic electronic structures. LDA Band calculations on the Kondo insulators including the f-electrons as itenerant ones are carried out, giving rising to an energy gap around the Fermi energy,[5] or at least a tendency towords the opening of the gap.[6] However, the obtained band structures look rather complicated, so that a simpler tight-binding model description is necessary to explore the effect of the strong correlation starting from the band structure calculations.

2. Tight-binding model for YbB_{12}

YbB_{12} is the best material for such a purpose because it is one of the most intensively investigated materials.[7,8] In addition, the crystal structure is the simple NaCl type, where Yb ions and B_{12} clusters are located at the interpenetrating fcc sites. Previous LDA band calculation[6] resulted in a semimetal with small overlap of the conduction and valence bands, but the recent calculation with the LDA+U method[9] does exhibit a small gap of about 0.01eV, which is due to the mixing of the 4f Γ_8 state and the conduction band of the t_{2g}character. Whole of the electronic band seems very complicated, but if one looks at the energy dispersion curves near the Fermi level, one finds that it is not so much complicated.

Therefore, I tried to express the energy bands near the Fermi level E_F by the simple tight-binding model[11] with only the $(dd\sigma)$ overlapping integral between $5d\epsilon$ and $5d\gamma$ orbitals on Yb ions. This $(dd\sigma)$ should be regarded as being produced by the effective hopping through the B_{12} clusters. We take the energy levels of $5d\epsilon$ and $5d\gamma$ orbitals as $E_{d\epsilon}$=0.3 Ryd and $E_{d\gamma}$ =0.7 Ryd, respectively, and $(dd\sigma) = 0.07$ Ryd[10].

The resulting bands, shown in Fig. 1, consist of the

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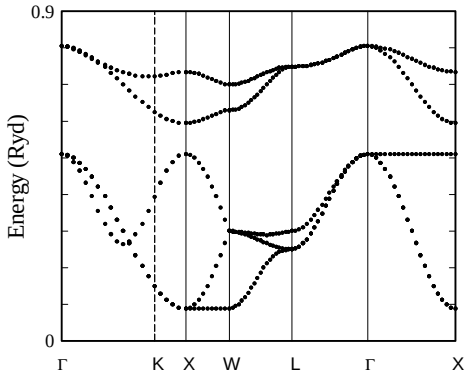

Fig. 1. Energy dispersion of the tight-binding model for the YbB_{12} conduction band.

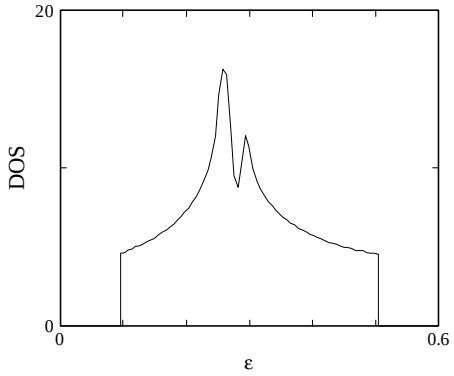

Fig. 2. Density of states of the tight-binding model for the YbB_{12} conduction band.

lower $5d\epsilon$ and the higher $5d\gamma$ bands, and look very similar to the dispersions of the conduction bands of t_{2g} character near E_F in the LDA and LDA+U calculations, if the f states are removed. The density of states for the lower band is shown in Fig. 2. The shapr band edges at 0.1 and 0.5 Ryd are due to the two dimensional character of the top and bottom of this simple model band.

It is expected that the inclusion of the f states at 0.15 Ryd and the mixing with the conduction bands in Fig. 1 will yield the bands with the energy gap as obtained by the LDA+U calculation[9]. However, the lowest branch in Fig.1 along Γ-X line is doubly degenerate, so that a simple mixing band model cannot yield an energy gap. One has to take account of the symmetry of the 4f states with spin-orbit interaction (Γ_8) and the conduction band (t_{2g}) properly.[6] The band calculation does include these features and yield the energy gap. Therefore, our tight-binding band will also yield an energy gap if these features are taken into account properly. The mixing matrix elements should be given by the extended Slater-Koster integrals between d and f states.[12] Such analysis is now in progress.

3. Conclusions

I have constructed a simple tight-binding band model of the conduction band of the most typical Kondo insulator YbB_{12}. It consists of the $5d\epsilon$ orbitals on Yb and the effective overlap integral ($dd\sigma$) is regarded as being produced by the hopping through the B_{12} clusters. This model can describe the t_{2g} conduction band very well, so that the inclusion of the mixing with the f states with proper account of the crystalline field and the spin-orbit interaction should describe the gap structure of this material correctly. This simple model will be very useful in constructing a theory with correlation effect, which can consistently explain all the thermal, thermoelectric, transport and magnetic properties of YbB_{12}.[13] Such a calculation is now in progress. Finally, I note that it is impossible to express the conduction band of YbB_{12} by a free-electron model with an anisotropic mixing with f-electrons.[14,15]

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