Calculation of Optical Conductivity for Kondo insulator YbB_{12} and Ce-skutterudites using Realistic Tight-binding Model

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Abstract

In order to understand the electronic structures of the typical Kondo insulator YbB_{12} and some Ce-based skutterudite compounds with an energy gap or a pseudo-gap, e.g. $CeOs_4Sb_{12}$ or $CeRu_4Sb_{12}$, simple tight-binding band models are constructed. Based on these models, the optical conductivity spectra are calculated to confirm our models and to understand the many-body effect therein. The resultant spectra can explain the shape and the temperature-dependence of the experiments rather well. Especially, the mid-infrared peak due to the f-d transitions and its red-shift at lowering temperature are well reproduced.

Key words: YbB_{12}, Ce-skutterudites, optical conductivity
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Measurement of the optical conductivity is a superior tool to investiate the electronic structures of materials, especially the strongly correlated systems, since the far infra-red spectra can probe the low energy scales of these materials.[1–3] It, however, needs theoretical models and careful calculations to analyze and utilize the experimental results.

We previously found that the electronic structures of the typical Kondo insulator YbB_{12} and some of the Ce-based skutterudite compounds with an energy gap or a pseudo-gap, e.g. $CeOs_4Sb_{12}$ or $CeRu_4Sb_{12}$ can be described by the simple tight-binding band models.[4,5] Schematic figures are shown in Fig.1 and the tight-binding band for $CeRu_4Sb_{12}$ is displayed in Fig.2.[5]

Based on these models, we have calculated the optical conductivity spectra to confirm our models and to understand the many-body effect therein. The latter was taken into account by the self-consistent second-order perturbation theory. In the present paper, we will furnish an improved model and a calculation, and further comparison with experiments. We also discuss some problems which are still to be solved. Because of the limited space, we focus on $CeRu_4Sb_{12}$ in the present paper, while the result for YbB_{12} will be found in the previous paper.[4]

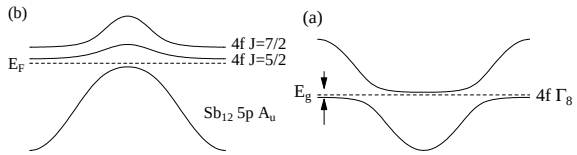

Fig. 1. Schematic energy-band models for (a)$CeRu_4Sb_{12}$ and (b)YbB_{12}.

As in the previous calculations, we use the joint-DOS type formula,

$$\sigma_{\rm indir}(\omega) \equiv \sum_{\alpha,\alpha'} \int {\rm d}\varepsilon \frac{f(\varepsilon) - f(\varepsilon+\omega)}{\omega} \rho_\alpha(\varepsilon)\rho_{\alpha'}(\varepsilon+\omega)$$

for the calculation of the optical conductivity. Here $\rho_\alpha(\varepsilon)$ is the quasi-particle density of states of the α's band. This formula simulates the possible existence of the indirect transitions, which seems necessary to explain the low energy tail below 0.1eV. Without the in-

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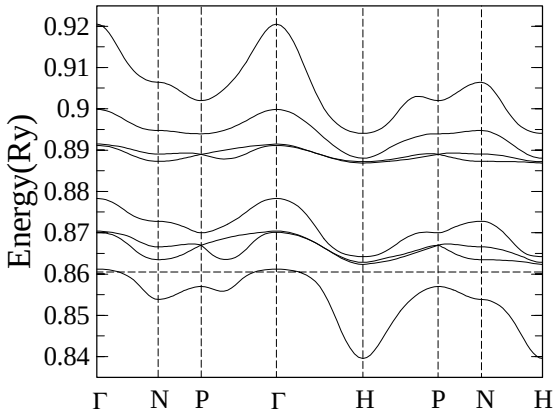

Fig. 2. Tight-binding model for $CeRu_4Sb_{12}$.

direct transitions, the spectra show sharp threshold at the direct gap energy ∼0.1 eV and cannot explain the experiments.[2] The resultant spectra can explain the gross shape and the temperature-dependence of the experiments[1–3] rather well.[5] Especially, the gap-filling feature with raising temperature and the mid-infrared peak due to the f-d transitions and its red-shift at lowering temperature are well reproduced because of the inclusion of the many-body effect.

However, since we assumed an indirect energy gap of about 0.02 eV in our tight-binding model, the sharp Drude part in experiments at low ω and low T was not reproduced. In addition, the resistivity measurement shows the apparent metallic behavior at low temperatures.[2]

In order to improve these points, we present here a calculation corresponding to the slightly metallic case due to a possible non-stoichiometry with the Fermi energy below the top of the valence band by 0.01eV. Other parameters are the same as before.[5] The result is displayed in Fig.3, which shows Drude part at low temperature and the f-d transition peak observed in experiments. However, the tail below this peak does not extend to low enough energy compared to the experiment, and the shape of the Drude part is not completely reproduced. It seems necessary to take account of the effect of indirect transitions more correctly including the many-body effect to fully explain the experiments. A proposal is made in such direction by e.g. [6].

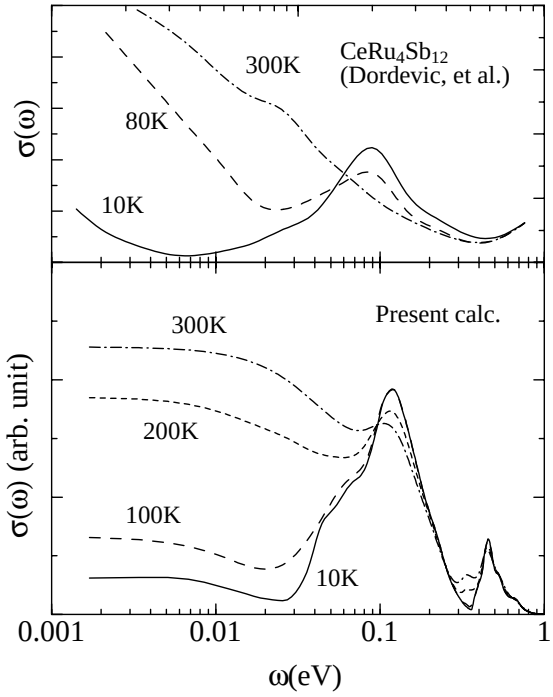

Fig. 3. Optical conductivity (a) by experiment, and (b) calculated with the tight-binding band in Fig.2.

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References

[1] H. Okamura, S. Kimura, H. Shinozaki, T. Nanba, F. Iga, N. Shimizu and T. Takabatake: Phys. Rev. B **58** (1998) R7496.

[2] S. V. Dordevic, D. N. Basov, N. R. Dilley, E. D. Bauer and M. B. Maple, Phys. Rev. Lett. **86** (2001) 684.

[3] M. Matsunami, H. Okamura, T. Nanba, H. Sugawara and H. Sato: J. Phys. Soc. Jpn. **72** (2003) 2722.

[4] T. Saso and H. Harima: J. Phys. Soc. Jpn. **72** (2003) 1131; T. Saso: J. Phys. Soc. Jpn. **73** (2004) 2894.

[5] T. Mutou and T. Saso: J. Phys. Soc. Jpn. **73** (2004) 2900.

[6] N. S. Vidhyadhiraja, V. E. Smith, D. E. Logan and H. R. Krishnamurthy, J. Phys.: Condens. Matter. **15** (2003) 4045.