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Optical Conductivity of Ce-Skutterudite Kondo Insulators

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A simple tight-binding model is constructed for the description of the electronic structure of some Ce-based filled skutterudite compounds showing an energy gap or pseudogap behavior. Assuming band-diagonal electron interactions on this tight-binding model, the Hamiltonian is expressed as

$$\begin{aligned}\mathcal{H} &= \sum_{\gamma}\sum_{\mathbf{k},\sigma} E^{\gamma}_{\mathbf{k}} c^{\dagger}_{\gamma\mathbf{k}\sigma} c_{\gamma\mathbf{k}\sigma} + U\sum_{\gamma}\sum_{i} n_{\gamma i\uparrow} n_{\gamma i\downarrow} \\ &\quad + U_2 \sum_{\gamma<\gamma'}\sum_{i,\sigma} n_{\gamma i\sigma} n_{\gamma' i\bar{\sigma}} + U_3 \sum_{\gamma<\gamma'}\sum_{i,\sigma} n_{\gamma i\sigma} n_{\gamma' i\sigma} - J\sum_{\gamma<\gamma'}\sum_{i,\sigma} c^{\dagger}_{\gamma i\sigma} c_{\gamma i\bar{\sigma}} c^{\dagger}_{\gamma' i\bar{\sigma}} c_{\gamma' i\sigma}, \qquad (1)\end{aligned}$$

the optical conductivity spectrum is calculated by the joint-DOS-type formula,

$$\sigma(\omega) \equiv \sum_{\gamma,\gamma'} \int \mathrm{d}\varepsilon \rho^{\gamma}(\varepsilon)\rho^{\gamma'}(\varepsilon+\omega)\frac{f(\varepsilon)-f(\varepsilon+\omega)}{\omega}. \qquad (2)$$

and by applying the second-order self-consistent perturbation theory to treat the electron correlation. The correlation effect is found to be of great importance on the description of the temperature dependence of the optical conductivity. The rapid disappearance of an optical gap with increasing temperature is obtained as observed in the optical experiment for Ce-based filled-skutterudite compounds.[1, 2] The present method is successfully applied also to the typical Kondo insulator YbB_{12}.[3]

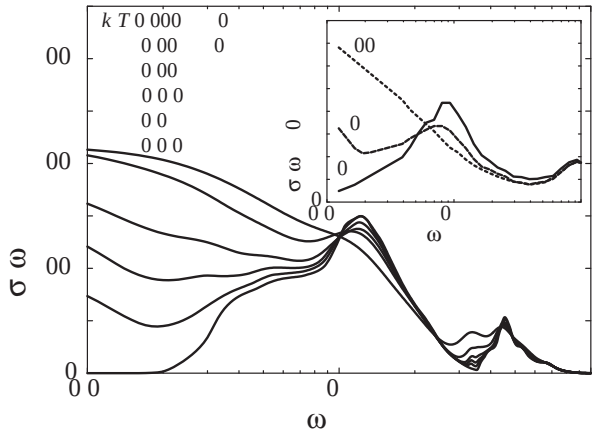

Figure 1: The temperature and frequency dependences of the optical conductivity are shown. Inset shows the experimental data of $CeRu_4Sb_{12}$ [2].

References

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