Band calculation using the FLEX approximation on the basis of LAPW

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Abstract

There are some problems in the density functional theory using the local density approximation (LDA). We pick up two problems among them. One is that it is difficult to describe the physical phenomena at finite temperatures. The other is that the strong Coulomb interaction is not sufficiently treated in strongly correlated electron systems such as high-T_c superconductors. What should we do to solve these two problems?

In the density functional theory, the motion of the electron is treated within the mean field approximation, and the electron does not interact with the low-energy collective excitations. An important correction at finite temperatures is an inclusion of the spin-fluctuation effect in d-electron systems. We adopt the fluctuation exchange approximation (FLEX approximation) for this purpose.

First, we perform a band structure calculation within the LDA by using the full-potential linearized augmented-plane-wave (LAPW) method. Second, we introduce an empirical Coulomb interaction for the d electrons, which is treated within the FLEX approximation. The single-electron Matsubara Green-function is evaluated by using the wave-function obtained by the LDA calculation. Then, the generalized spin susceptibility is calculated, and the electron self-energy is evaluated by the FLEX approximation. In the process of the self-consistent calculation, the spin susceptibility is enhanced by the effective d-electron Coulomb interaction.

The band structure, the Fermi surface, the susceptibility and the nuclear magnetic relaxation rate have been calculated for Sr_2RuO_4 and $La_{2-x}Ba_xCuO_4$.