(P2-26)

Extension of the NCA for the Orbital Degenerate Anderson Model with Finite Coulomb Repulsion

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The non-crossing approximation (NCA) is a theory which can take into account strong correlations between local electrons with reasonable computational effort. In the case of large degeneracy n of the local states, the NCA derives proper dynamics of the Anderson model with infinite Coulomb repulsion U. For the Anderson model with finite-U, however, an accurate energy scale of the Kondo effect is not reproduced by the simple application of the NCA even though n is large. We generalize the NCA so as to yield proper energy scales in finite-U.

Sakai *et al.* have developed an approximation which incorporates leading contributions in large-n limit of the finite-U Anderson model, and have called it NCAf^2v [1]. Resolvents, which are propagators of the $4f$ states, of the NCAf^2v scheme yield the proper Kondo temperature $T_{\rm K}$. However, the resummation procedure for the single-particle excitation spectrum does not give a conserving approximation. With use of the resolvents of NCAf^2v, we have derived a formula for the single-particle Green function which includes all leading contributions [2].

Figure 1(a) shows density of states of $4f$ electron around the Fermi level for several values of U at temperatures much lower than $T_{\rm K}$ ($n = 6$). $\rho_f^{(\rm S)}$ are results computed with the formula in ref. [1]. It turns out that the present scheme reproduces the scaling behavior of the Kondo resonance while $\rho_f^{(\rm S)}$ fails to do. The specific heat are properly scaled by the characteristic energy as well (Fig. 1(b)). Furthermore, the Kondo temperature $T_{\rm K}$ obtained in the present theory is consistent with an analytic estimate by the scaling theory.

The present theory has the advantage that physical quantities are computed with almost the same computational effort as in the original NCA. Consequently, the theory is easily applicable to the dynamical mean field theory, and to models with complex $4f$ levels and realistic band structures.

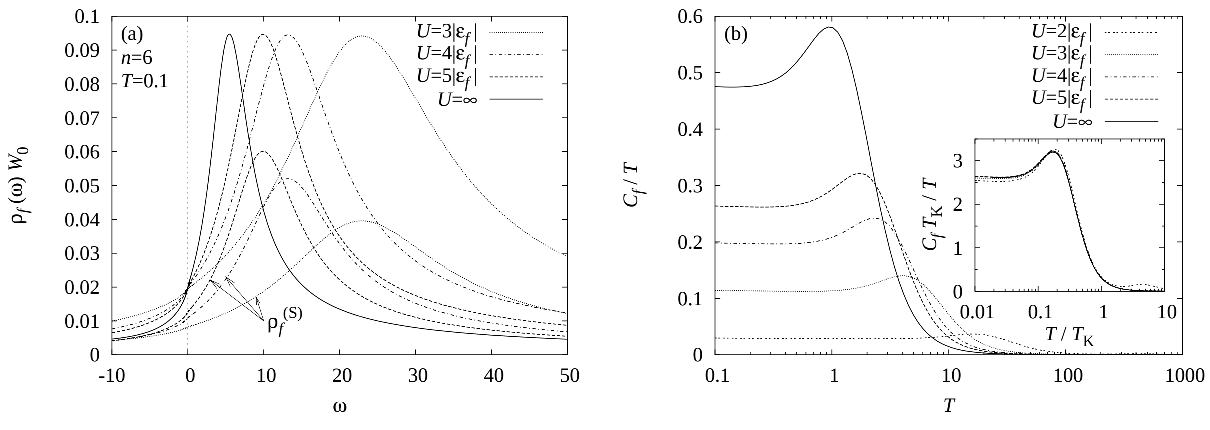

Figure 1: (a) Density of states $\rho_f(\omega)$ for several values of U. (b) Temperature dependence of the specific heat C_f of $4f$ electrons. Parameters are $D = 10^4$, $\epsilon_f/D = -0.12$ and $W_0 = V^2\rho_c = 30$.

[1] O. Sakai, M. Motizuki and T. Kasuya: in *Core-Level Spectroscopy in Condensed Systems Theory*, ed. J. Kanamori and A. Kotani (Springer-Verlag, Berlin, 1988) p. 45.
[2] J. Otsuki and Y. Kuramoto: cond-mat/0602584, to appear in J. Phys. Soc. Jpn. **75** (2006) No. 6.