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Projection operator method CPA to single-particle excitation spectra YOSHIRO KAKEHASHI, PETER FULDE, Max-Planck-Institute for PKS — Single-site theories for electron correlations such as the many-body CPA, the dynamical CPA, and the dynamical-mean field theory are useful as a starting point to describe strongly correlated electron systems. Nevertheless, simple and useful treatments of correlations being applicable to the realistic system has not yet been well developed. We propose here the projection operator technique combined with the many-body CPA which allows us to calculate the excitation spectrum directly from the retarded Green function. The basic idea is to introduce an energy dependent Liouville operator for the description of the dynamics of correlated electrons. The self-energy obtained by a renormalized perturbation scheme describes the overall features of excitation spectra. The quasiparticle weight for a half-filled band in infinite dimensions show a simple analytic form $Z = [1 - (U/U_{c2})^2]/[1 + (U/U_2)^2]$ with $U_{c2} = 3.705$ and $U_2 = 2.522$ (hypercubic lattice) which reproduces well the result of the numerical renormalization group calculations. The critical Coulomb interaction U_{c1} for a gap formation is 3.69 when the Hartree-Fock wave function is used for the evaluation of the static average, and 3.24 when the correlated wave function is used. The latter agrees with the result of the NRG within 1% error.

Yoshiro Kakehashi
Max-Planck-Institute for PKS

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