

CMT P19 A DIAGRAM APPROACH TO THE STRONG COUPLING IN THE TWOFOLD-DEGENERATE ANDERSON IMPURITY MODEL

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It is well known that orbital degeneracy plays an essential role in the Mott metal-insulator transition. Here, we study the role of the Hund-rule coupling in an orbitally degenerate model using a diagram approach and taking the intra-atomic Coulomb interactions of two electrons with opposite spins occupying the same or different orbitals into account on an equal footing with the intra-atomic exchange.

The investigations are based on our diagram theory for strongly correlated electron systems previously developed for the nondegenerate [1-8] and twofold degenerate [9] models.

Our approximation includes only local self-energy terms. It is well known that such an approximation is well justified for a large coordination number. The nonlocal terms [10] corresponding to a higher-order approximation in the inverse coordination number are neglected here.

We first determined all the energy eigenfunctions and eigenvalues of the localized d -electron part of the Hamiltonian. We obtained their dependence on the intra- and inter-orbital Coulomb interactions and on the Hund-rule coupling constant. We developed the perturbation theory around the atomic limit and determine the Matsubara Green's functions in the normal state.

We obtained a Dyson-type equation for these functions and discussed its analytical solutions in detail.

Because the main elements of our diagram technique are the irreducible Green's functions, we calculated the simplest two-particle irreducible Green's function and determined its dependence on the spin and orbital quantum numbers. This quantity, found only in the low-temperature limit, was approximated by taking contributions of statistical weight $e^{-\beta E_0}$ into account assuming that the ground state of our system is the two-particle triplet state E_0 . Knowing this quantity and summing a specific class of diagrams, we obtained the correlation function.

We found two solutions for the renormalized Green's functions of the d electrons and determined their spectral weight.

We proved that orbital degeneracy gives an additional contribution to the "metallization" of the impurity states, i.e. enhances the transfer of spectral weight to the Fermi level.

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