Gutzwiller variational approach to the two-impurity Anderson model for a metallic host at particle-hole symmetry

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Abstract:

We study Gutzwiller-correlated wave functions as variational ground states for the two-impurity Anderson model (TIAM) at particle-hole symmetry as a function of the impurity separation R. Our variational state is obtained by applying the Gutzwiller many-particle correlator to a single-particle product state. We determine the optimal single-particle product state fully variationally from an effective non-interacting TIAM that contains a direct electron transfer between the impurities as variational degree of freedom. For a large Hubbard interaction U between the electrons on the impurities, the impurity spins experience a Heisenberg coupling proportional to $V^2/U$ where V parameterizes the strength of the on-site hybridization. For small Hubbard interactions we observe weakly coupled impurities. In general, for a three-dimensional simple cubic lattice we find discontinuous quantum phase transitions that separate weakly interacting impurities for small interactions from singlet pairs for large interactions.

Keywords:

impurity scattering, RKKY interaction, Gutzwiller wave function

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