Kondo effect vs RKKY in real lattices: A DMRG and ECA study

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Magnetic interactions between strongly correlated impurities coupled to a sea of conduction electrons is a subject of great interest from both, experimental and theoretical studies. When many magnetic impurities are attached to the same conduction band a rich phase diagram can arise. By one hand the magnetic impurities can be strongly coupled to the spin of the electrons of the conduction band forming a singlet. This is the well known Kondo effect. By the other, through electron of the conduction band, a spin-spin interaction between the impurities can appears as a consequence the Rutherman-Kittel-Kasuda-Yosida interaction. In this later case a singlet state between the impurities will appears. This new singlet will compete with the singlet formed by the Kondo effect. In this two effects is important the well description of the electrons with energy close to the Fermi level. Systems like the square lattice, with a van-Hove singularity at the middle of the band, or Graphene, with Dirac electrons, or Carbon nanotubes with multiple bands and multiples van Hove singularities need a proper description of the electrons in the lattice Hamiltonian.

In this work we present a numerical method to study problems with several magnetic impurities coupled to arbitrary lattices. First we separate the Hamiltonian in two parts. One part that contains the impurities and the coupling with the band and the other that have just the lattice Hamiltonian. Using the lattice sites that couples to the impurities as seed in a Lanczos-type procedure we manage to map the real-space lattice Hamiltonian into a ladder type Hamiltonian. This canonical transformation, known as block Lanczos tri-diagonalization, can be now solved using different numerical techniques as DMRG or ECA. This method is not restricted to analyze barvais lattice Hamiltonians but a wide variety of systems as a Bethe lattice or even systems with disorder can be also studied.

To introduce this method we will present a study of the competition between the Kondo effect and the RKKY interaction in a square and a rectangular lattices.