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Electronic Structure of Transition Metal Compounds by Variational Cluster Approximation

Abstract:

A famous theorem by Luttinger and Ward states that the grand canonicalpotential of an interacting Fermion system can be represented as a functionalof its self-energy and that this functional is stationary at the exact self energy. The variational cluster approximation is an application of this theorem, whereby trial self-energies are generated by exact diagonalization of small clusters. In applying this method to transition metal compounds it is important to treat the Coulomb interaction between electrons in the d-shell by means of multiplet theory. Applications of the method to 3d transition metal oxides and the spin-state transition in LaCoO3 will be discussed.