SPIN- ROTATIONAL- INVARIANT FLUCTUATION THEORY OF FINITE-TEMPERATURE MAGNETISM: APPLICATION TO A SINGLE- SITE MODEL

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In this talk we will review recent developments in the theory of the magnetic properties of transition-metal clusters at finite-temperatures. After a brief introductory overview of the experimental situation, we present the theoretical framework, which is based on a Hubbard-Stratonovich functional-integral formulation of the corresponding canonical and grand-canonical equilibrium partition functions. Previous applications to Fe, Co and Ni clusters and monolayers are discussed. An interpretation of our electronic results in terms of Ising or Heisenberg models of localized magnetism implies a strong dependence of the effective interatomic exchange couplings $J_{\text{ik}}$ on size and local coordination number, which defies straightforward transferability and easy generalizations. The main drawbacks and limitations of this approximation are analyzed. Finally, A spin-rotational invariant approach to the spin-fuctuation theory of itinerant-electron magnetism is proposed and evaluated in the framework of a d-band model Hamiltonian including the coupling to a local magnetic field $B$. Using a vector-field Hubbard-Stratonovich transformation, we obtain a static approximation to the density-matrix operator from which the equilibrium properties are directly derived. The method is applied to a single-site model taking Fe as representative example. The quantum-mechanical origin of some important drawbacks found in previous vector-field static approaches is identified.

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