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Generalized mean-field theory for metals and semiconductors with magnetic impurities

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Abstract

Random systems of magnetic moments positioned in cites of a crystal lattice and interacting via RKKY- or Bloembergen–Rowland-type interaction are considered in the framework of *generalized* mean-field theory (GMFT) based on calculating and analyzing *distribution functions* $F(H)$ of random *local* magnetic fields H. For *concentrated* systems (where the random local field is produced by a number of interacting magnetic moments), the function $F(H)$ turns out to be Gaussian one and all information about the system is contained in two parameters of that distribution only—it's width and maximum position. For *rarefied* systems (where the average distance between interacting moments is comparable with or larger than the interaction length), distribution functions are essentially non-Gaussian. GMFT has been applied for calculating the magnetic state of metals and semiconductors diluted with magnetic impurities.

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1. Introduction

It is well known that diluting non-magnetic materials by magnetic impurities changes the composite properties (magnetic susceptibility, specific heat, etc.). Such systems might be classified by the matrix type: (i) diamagnetic metal, (ii) semiconductor, and (iii) insulator. Examples of the first-type systems are the long-studied metal alloys $Cu_{1-x}(Mn, Fe)_x$, $Au_{1-x}Fe_x$ [1] where impurity magnetic moments μ interact indirectly via intrinsic charge carriers of the metal matrix whose concentration is not practically changed during the dilution. The second-type systems are, for instance, diluted magnetic semiconductors $Ga_{1-x}Mn_xAs$ [2] or $Cd_{1-x}Mn_xTe$ [3] having been extensively investigated in the context of their perspectives for the new electron devices and,

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especially, spintronic ones. In these systems, magnetic impurities provide those charge carriers which lead to the inter-impurity interaction. The third-type systems remain to be insulating after diluting, and magnetic interaction in those systems is of dipole–dipole type. The example of such a system is $LiY_{1-x}Ho_xF_4$. Its properties are studied in Ref. [4] and are not considered in the paper.

The common feature of all those systems is a *random* arrangement of the impurities in the sites of the parent lattice. It is known that the mean field theory describes non-adequately properties of such a *disordered* (random) system of magnetic moments. The aim of the paper is to generalize the mean field theory for the systems with the indirect interaction of the magnetic impurities taking into account the random character of their spatial arrangement. We restrict ourselves by the Ising approximation and assume that the indirect interaction of impurity magnetic moments is either RKKY-interaction via the polarization of free charge carriers [2,3,5–7] (in a diamagnetic metal with paramagnetic impurities) or Bloembergen–Rowland interaction [8] (in a non-magnetic semiconductor diluted by magnetic impurities).

2. Generalized mean field theory for Ising system

Ising model is the lattice-like system of magnetic moments of two possible (opposite) directions that interact with their neighbors only. There is the exact solution [9,10] of that model for two-dimensional rectangular lattice (L. Onsager, 1944) and approximate, but quite accurate, solution of Wakefield for three-dimensional simple cubic lattice [10]:

$$kT_C = 2.27J \quad \text{(square lattice)},$$
$$kT_C \approx 4.5J \quad \text{(simple cubic lattice)}, \tag{1}$$

where T_C is Curie temperature, J is the energy of neighbor interaction.

Generalizing those results for cases where the interaction is extended beyond the first coordination sphere, and for more complex lattices, is inconvenient. In those cases the mean field theory is commonly used which determines Curie temperature as $kT_C = zJ$ (z is the number of the neighbors), that is

$$kT_C = 4J \quad \text{(square lattice)},$$
$$kT_C = 6J \quad \text{(simple cubic lattice)}. \tag{2}$$

We notice that mean-field results differ significantly from the exact ones. In addition to the known defect of the mean-field theory that does not take into account the correlation of the moments, one further error of the model is that it assumes the *equivalence* of all lattice sites. This is reflected in the fact that the mean field supposed to be the same in all sites though, in fact, it varies from one site to another. In this connection it is natural to account for this randomness and to appreciate whether the accuracy of the solution obtained with the *generalized* mean-field theory is higher. That approach was first used in Ref. [6] on considering the system of randomly arranged magnetic dipoles. Later it was analyzed extensively in the series of papers [11] where the starting point was the distribution function of pair interaction energies being defined ad hoc. The essence of such a model is replacing the standard mean-field equation

$$j = \tanh\left(\frac{\lambda j}{kT}\right), \tag{3}$$

where j is the reduced magnetization of the system, λ is the mean-field constant, with its generalized analog

$$j = \int_{-\infty}^{\infty} \tanh\left(\frac{\mu H_3}{kT}\right) F(j; H_3)\, dH_3, \tag{4}$$

where $F(j; H_3)$ is the distribution function of local magnetic fields H_3. Those fields are generated in the random system of magnetic moments with magnetization j at the position of one of them by all other moments (equal to μ). Obviously, in calculating the distribution function it would be more proper to proceed from spatial dependence of the pair interaction energy $W(r)$ but not from the distribution function of those energies defined "by hands" (as was done in Ref. [11]). Notice that the mean-field equation (3) is equivalent to the