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Nonextensive quantum method for itinerant-electron ferromagnetism: Factorization approach

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ABSTRACT

Magnetic and thermodynamical properties of itinerant-electron (metallic) ferromagnets described by the Hubbard model have been discussed with the use of the generalized Fermi–Dirac (GFD) distribution for nonextensive quantum systems. We have derived the GFD distribution within the superstatistics, which is equivalent to that obtained by the maximum-entropy method to the Tsallis entropy with the factorization approximation. By using the Hartree–Fock approximation to the electron–electron interaction in the Hubbard model, we have calculated magnetic moment, energy, specific heat and Curie–Weiss-type spin susceptibility, as functions of the temperature and entropic index q expressing the degree of the nonextensivity: $q = 1.0$ corresponds to the Boltzmann–Gibbs statistics. It has been shown that by increasing the nonextensivity of $|q - 1|$, the temperature dependence of magnetic moment becomes more significant and the low-temperature electronic specific heat is very much increased. This is attributed to enlarged Stoner excitations in the GFD distribution, which is elucidated by an analysis with the use of the generalized Sommerfeld expansion. We discuss the difference and similarity between the effects of the nonextensivity on metallic and insulating ferromagnets.

1. Introduction

Since Tsallis proposed the nonextensive statistics in 1988 [1], considerable work on related topics has been done (for a recent review, see Ref. [2]). It is based on the generalized entropy (called the Tsallis entropy) which is a one-parameter generalization of the Boltzmann–Gibbs entropy with the entropic index q: the Tsallis entropy in the limit of $q = 1.0$ reduces to the Boltzmann–Gibbs entropy. The nonextensive statistics has been successfully applied to a wide class of subjects including physics, chemistry, information science, biology and economics [3]. Despite elegant formalism of the Tsallis nonextensive statistics, there are four possible methods in an evaluation of expectation values with the maximum-entropy method (MEM): (i) original method [1], (ii) unnormalized method [4], (iii) normalized method [5] and (iv) the optimal Lagrange multiplier method [6]. However the four methods are equivalent in the sense that distributions derived in them are easily transformed into each other [7]. A comparison among the four methods is made in Ref. [2].

An alternative approach to nonextensive systems is superstatistics [8,9]. Complex nonextensive systems are expected to undergo temporary and spatial fluctuation. It is assumed that locally the equilibrium state is described by the Boltzmann–Gibbs statistics, and that their global properties may be expressed by a superposition of them over some intensive physical quantity, *e.g.* the inverse temperature [8–11]. Many applications of the concept of superstatistics have been pointed out (for a recent review, see Ref. [11]). It is however not clear, how to obtain the mixing probability distribution of a fluctuating parameter from first principles. This problem is currently controversial and some attempts in this direction have been proposed [12–16].

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The nonextensive statistics has been applied not only to classical systems but also to quantum ones [17–42]. For fermion systems, the generalized Fermi–Dirac (GFD) distribution was derived by the asymptotic approach for $|q-1|/k_BT \to 0$ [17] and by the MEM (ii) with the factorization approximation [18]. With the use of the MEM (ii) and MEM (iii), Refs. [21,22] have derived the formally exact expression for the grand canonical partition function of nonextensive systems, which is expressed as a contour integral in terms of the Boltzmann–Gibbs counterpart. Although the exact formulation is very valuable, the actual calculation of the contour integral is difficult and it may be performed only in the limited cases at the moment [26]. Quite recently, the nonextensive quantum extension has been proposed by using the MEM (iv) [29]. Among the three approaches of the asymptotic [17], factorization [18] and exact methods [21,22] in nonextensive quantum statistics, the factorization approach is the easiest way for handling physical systems [20,24]. The nonextensive quantum statistics has been applied to various subjects including black-body radiation [17,30], Bose–Einstein condensation [24,25,31,32], metallic [33] and superconducting materials [34,35], spin systems [36–40] and nano-magnetism [41,42].

Now we pay our attention to magnetic systems. Although there are many magnetic materials, they are classified into two categories: insulating and metallic magnets. The latter are often referred to also as itinerant-electron, collective-electron or band magnets (*metallic* and *itinerant-electron* are interchangeably used hereafter). In insulating magnets, for example, of rare-earth elements such as Gd and La, f electrons form the localized spin at each atomic site which yields integer magnetic moment in units of μ_B (Bohr magneton). On the contrary, in itinerant-electron magnets of transition metals such as Fe, Co and Ni, d electrons not only form magnetic moment at each atomic site but also itinerate in crystals, by which materials become metallic. The magnetic moment of itinerant-electron magnets is not integer in units of μ_B. A modern theory of magnetism has a long history over the last half century since the advent of quantum mechanics. Insulating magnets are well described by the Heisenberg model. With the Weiss molecular-field theory and more advanced theories for the Heisenberg model, our understanding of magnetic properties such as magnetic structures and phase transition has been much deepen. On the other hand, a study of itinerant-electron magnets was initiated by Stoner [43] and Slater [44]. Later Hubbard proposed the so-called Hubbard model [45], which has been widely adopted for a study of itinerant-electron magnetism. Studies with the Hartree–Fock (mean-field) approximation to the electron–electron interaction in the Hubbard model account for the non-integral magnetic moment and the large T-linear coefficient of the specific heat at low temperatures, which are experimentally observed.

Nonextensive statistics has been applied to insulating ferromagnets, by using the MEM (ii) [36,37] and the MEM (iii) [38–41]. Peculiar magnetic properties observed in manganites are reported to be well accounted for by the nonextensive statistics [36–40]. The purpose of the present paper is to apply the nonextensive quantum statistics to itinerant-electron ferromagnets with the use of the GFD distribution derived within the superstatistics. The resultant GFD distribution is equivalent to that obtained by the MEM (ii) with the factorization approximation [18], which is valid for dilute fermion gas [19,20,24]. The factorized GFD distribution [18] has been applied to various quantum subjects [25,31–35] because it is expected to be a good, practical approximation [20,24]. We have calculated the magnetic moment, energy, specific heat and Curie–Weiss-type susceptibility of itinerant-electron ferromagnets described by the Hubbard model with the Hartree–Fock approximation. Such a calculation is worthwhile, clarifying the effect of the nonextensivity on metallic ferromagnets which is different from that on insulating counterparts. Our study is the first application of the nonextensive quantum method to itinerant-electron ferromagnets, as far as we are aware of.

The paper is organized as follows. In Section 2, we discuss the adopted Hubbard model and the GFD distribution derived by the superstatistics. Analytical expressions for magnetic moments, energy, specific heat and susceptibility are presented with some model calculations. In Section 3, qualitative discussions on magnetic and thermodynamical properties are made with the use of the generalized Sommerfeld low-temperature expansion for physical quantities. Relevance of our calculation to heterogeneous magnets such as metallic spin glass and amorphous metals is discussed. Section 4 is devoted to our conclusion.

2. Formulation

2.1. Adopted model

We have considered itinerant-electron ferromagnets described by the Hubbard model given by [45]

$$\hat{H} = \sum_{\sigma}\sum_{i} \epsilon_0 n_{i\sigma} + \sum_{\sigma}\sum_{i,j} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu_B B \sum_{i} (n_{i\uparrow} - n_{i\downarrow}), \tag{1}$$

where $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$, $a_{i\sigma}$ ($a^{\dagger}_{i\sigma}$) denotes an annihilation (creation) operator of a σ-spin electron ($\sigma = \uparrow, \downarrow$) at the lattice site i, ϵ_0 the intrinsic energy of atom, t_{ij} the electron hopping, U the intra-atomic electron–electron interaction and B an applied magnetic field. We have adopted the Hartree–Fock approximation to the electron–electron interaction of the third term in Eq. (1), as given by

$$U n_{i\uparrow} n_{i\downarrow} \simeq U\langle n_{\uparrow}\rangle n_{i\downarrow} + U\langle n_{\downarrow}\rangle n_{i\uparrow} - U\langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle, \tag{2}$$

where $\langle n_{\sigma}\rangle$ denotes the average of number of electrons with spin σ to be evaluated shortly [see Eqs. (27) and (28)]. With the Hartree–Fock approximation, Eq. (1) becomes the effective one-electron Hamiltonian given by

$$\hat{H} \simeq \hat{H}_{\uparrow} + \hat{H}_{\downarrow} - U\langle n_{\uparrow}\rangle\langle n_{\downarrow}\rangle, \tag{3}$$