Nonextensive quantum method for itinerant-electron ferromagnetism: Factorization approach

Hideo Hasegawa

Department of Physics, Tokyo Gakugei University, Koganei, Tokyo 184-8501, Japan

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 spinsusceptibility, 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].
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 \(|q-1|/k_B T \to 0\) [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 \(\mu_B\) (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 \(\mu_B\). 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 deepened. 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 manganesites 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]

\[
\hat{H} = \sum_\sigma \sum_i \varepsilon_\sigma n_{i\sigma} + \sum_\sigma \sum_{ij} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu_B B \sum_i (n_{i\uparrow} - n_{i\downarrow}),
\]

(1)

where \(n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}\), \(a_{i\sigma}(a_{i\sigma}^\dagger)\) denotes an annihilation (creation) operator of a \(\sigma\)-spin electron \((\sigma = \uparrow, \downarrow)\) at the lattice site \(i\), \(\varepsilon_0\) 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

\[
U n_{i\uparrow} n_{i\downarrow} \simeq U \langle n_{i\uparrow}\rangle n_{i\downarrow} + U \langle n_{i\downarrow}\rangle n_{i\uparrow} - U \langle n_{i\uparrow}\rangle \langle n_{i\downarrow}\rangle,
\]

(2)

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

\[
\hat{H} \simeq \hat{H}_1 + \hat{H}_1 - U \langle n_{i\uparrow}\rangle \langle n_{i\downarrow}\rangle,
\]

(3)
where
\[ \hat{H}_0 = \sum_i \epsilon_{\sigma} n_{i\sigma} + \sum_{i,j} t_{ij} a_i^\dagger a_j^\sigma \quad (\sigma = \uparrow \text{ and } \downarrow), \] (4)

with
\[ \epsilon_{\uparrow,\downarrow} = \epsilon_0 + U n_i \mp \mu B, \] (5)

the minus (plus) sign in Eq. (5) being applied to \( \uparrow \)-spin (\( \downarrow \)-spin) electrons.

2.2. GFD distribution within the superstatistics

We have considered the nonextensive fermion system consisting of many clusters, each of which includes \( N \) particles with total energy \( E \). Non-equilibrium or quasi-equilibrium states of the system are expected to temporary and spatially fluctuate. However, locally the equilibrium state of a given cluster is assumed to be described by the Boltzmann–Gibbs statistics in the superstatistics [8–10]. The probability distribution for \( \{ n_k \} \) in a given cluster with the local temperature \( \tilde{T} \) is given by

\[ p_{BG}(\tilde{\beta}, \{ n_k \}) = \frac{1}{\Xi(\tilde{\beta})} \prod_k e^{-\beta(\epsilon_k - \mu)n_k}, \] (6)

where the grand-partition function \( \Xi(\tilde{\beta}) \) is given by

\[ \Xi(\tilde{\beta}) = \prod_k [1 + e^{-\tilde{\beta}(\epsilon_k - \mu)}]. \] (7)

Here \( \tilde{\beta} = 1/k_B \tilde{T} \), \( k_B \) is the Boltzmann constant, and \( n_k \) and \( \epsilon_k \) denote the number of states and energy, respectively, of the state \( k \).

After the concept of the superstatistics [8–10], we have assumed that the inverse of the temperature \( \tilde{\beta} \) fluctuates and its distribution is given by the \( \chi^2 \)-distribution with rank \( n \) given by

\[ g(\tilde{\beta}) = \frac{1}{\Gamma(\frac{n}{2})} \left( \frac{n}{2\tilde{\beta}} \right)^{\frac{n}{2}} \tilde{\beta}^{-\frac{n}{2}} e^{-\frac{n}{2\tilde{\beta}}}, \] (8)

where \( \Gamma(x) \) denotes the gamma function. The average and variance of \( \tilde{\beta} \) are given by \( \langle \tilde{\beta} \rangle_\beta = \beta \) and \( \langle (\tilde{\beta}^2) - \beta^2 \rangle/\beta^2 = 2/n \), respectively. The distribution averaged over the system with the temperature \( T (= 1/k_B \beta) \) is assumed to be given by

\[ p(\beta, \{ n_k \}) = \int_0^\infty p_{BG}(\tilde{\beta}, \{ n_k \}) g(\tilde{\beta}) \, d\tilde{\beta}. \] (9)

When we adopt the type-A superstatistics in which the \( \tilde{\beta} \) dependence of \( \Xi(\tilde{\beta}) \) is neglected [11], Eqs. (8) and (9) yield

\[ p(\beta, \{ n_k \}) = \frac{1}{Z_q} \prod_k \exp[-\beta(\epsilon_k - \mu)n_k], \] (10)

with

\[ Z_q = \prod_k [1 + \exp[-\beta(\epsilon_k - \mu)]], \] (11)

\[ q = \frac{2}{n} + 1, \] (12)

where \( \exp_q(x) \) stands for the \( q \)-exponential function defined by

\[ \exp_q(x) = [1 + (1 - q)x]^{\frac{x}{q}} \quad \text{for } 1 + (1 - q)x \geq 0, \] (13)

\[ = 0 \quad \text{for } 1 + (1 - q)x < 0. \] (14)

Eq. (14) expresses the cut-off properties of the \( q \)-exponential function.

The probability of occupation of the state \( k \) by \( n_k \) particles is given by

\[ P(n_k) = \frac{[1 - (1 - q)\beta(\epsilon - \mu)n_k]^{\frac{1}{1-q}}}{Z_q} \times \prod_{j \neq k} [1 + [1 - (1 - q)\beta(\epsilon_j - \mu)]^{\frac{1}{1-q}}] \] (15)

\[ = \frac{[1 - (1 - q)\beta(\epsilon - \mu)n_k]^{\frac{1}{1-q}}}{1 + [1 - (1 - q)\beta(\epsilon_k - \mu)]^{\frac{1}{1-q}}}. \] (16)
where the factorization approximation is employed [18]. The probability of occupation of the quantum state with the energy \( \epsilon_k \), \( f_q(\epsilon_k) \), is given by

\[
f_q(\epsilon_k) = \sum_{n_k} P(n_k) n_k, \tag{17}
\]

\[
= \frac{1}{1 + (\exp_q[-\beta(\epsilon_k - \mu)])^{-1}}. \tag{18}
\]

Averages of the number of electrons and energy per cluster are expressed in terms of \( f_q(\epsilon_k) \) by

\[
N = \sum_k f_q(\epsilon_k), \tag{19}
\]

\[
E = \sum_k f_q(\epsilon_k) \epsilon_k. \tag{20}
\]

The GFD distribution given in Eq. (18) is equivalent to that obtained by the MEM (ii) with the factorization approximation for \( 0 < q < 2 \) [18]. In the present paper, we will adopt the GFD distribution given by Eq. (18) not only for \( q \geq 1.0 \) but also \( q < 1.0 \), although it is valid for \( q \geq 1.0 \) within the superstatistics [Eq. (12)]. One of the advantages of the superstatistics is that the entropic index \( q \) is expressed in terms of model parameters as given by Eq. (12) (related discussion being given in Section 3).

In the limit of \( n \to \infty \) where \( g(\tilde{\beta}) = \delta(\tilde{\beta} - \beta) \) [Eq. (8)] and \( q = 1.0 \) [Eq. (12)], Eq. (18) reduces to the conventional Fermi–Dirac distribution obtained in the Boltzmann–Gibbs statistics,

\[
f_1(\epsilon_k) = f_{BG}(\epsilon_k) = \frac{1}{1 + \exp[-\beta(\epsilon_k - \mu)]}. \tag{21}
\]

In the zero-temperature limit of \( \beta \to \infty \), both Eqs. (18) and (21) reduce to

\[
f_q(\epsilon_k) = f_1(\epsilon_k) = \theta(\mu - \epsilon_k) \quad \text{for} \quad \beta \to \infty, \tag{22}
\]

where \( \theta(x) \) denotes the Heaviside function: \( \theta(x) = 1 \) for \( x > 0 \) and zero otherwise. Eq. (22) shows that the quantum state at \( T = 0 \) is not modified by the nonextensivity [24]. The derivative of \( f_q(\epsilon) \) with respect to \( \epsilon \) is given by

\[
\frac{\partial f_q(\epsilon)}{\partial \epsilon} = -\frac{\beta(\exp_q[-\beta(\epsilon - \mu)])^{q-2}}{[1 + (\exp_q[-\beta(\epsilon - \mu)])^{-1}]^2}, \tag{23}
\]

\[
\to -\frac{\beta e^{\beta(\epsilon - \mu)}}{[1 + e^{\beta(\epsilon - \mu)}]^2} \quad \text{for} \quad q \to 1.0. \tag{24}
\]

In the high-temperature limit of \( \beta \to 0 \), Eq. (18) becomes

\[
f_q(\epsilon_k) \simeq \exp_q(-\beta \epsilon_k) \quad \text{for} \quad \beta \to 0, \tag{25}
\]

with \( \mu = 0 \). Fig. 1(a) and (b) show the \( \epsilon \) dependence of \( f_q(\epsilon) \) and \( -\partial f_q(\epsilon)/\partial \epsilon \), respectively, for various \( q \) values with \( \beta = 1.0 \). When \( q \) is increased (decreased) from \( q = 1.0 \), the distribution at \( \epsilon < \mu \) and \( \epsilon > \mu \) is increased (decreased). The effect of \( q \) on the GFD distribution is more clearly seen in its derivative of \( \partial f_q(\epsilon)/\partial \epsilon \), which has a power-law tail at \( |\epsilon - \mu| \gg 1 \) for \( q \neq 1.0 \).

Because of the cut-off properties of the \( q \)-exponential function given by Eq. (14), we obtain

\[
f_q(\epsilon) = 0.0, \quad \frac{\partial f_q(\epsilon)}{\partial \epsilon} = 0 \quad \text{at} \quad (\epsilon - \mu) > \frac{1}{(1-q)\beta} \quad \text{for} \quad q < 1, \tag{26}
\]

\[
f_q(\epsilon) = 1.0, \quad \frac{\partial f_q(\epsilon)}{\partial \epsilon} = 0 \quad \text{at} \quad (\epsilon - \mu) < \frac{1}{(q-1)\beta} \quad \text{for} \quad q > 1,
\]

which is clearly realized in Fig. 1.

2.3. Magnetic moment

By using Eqs. (3), (18) and (19) with \( \epsilon_0 + Un/2 = 0 \), we obtain the self-consistent equations for the magnetic moment \( \langle m \rangle \) and the number of electrons \( \langle n \rangle \) per lattice site, given by

\[
m = n_\uparrow - n_\downarrow = \int [\rho_\uparrow(\epsilon) - \rho_\downarrow(\epsilon)] f_q(\epsilon) \, d\epsilon, \tag{27}
\]

\[
n = n_\uparrow + n_\downarrow = \int [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] f_q(\epsilon) \, d\epsilon, \tag{28}
\]
Fig. 1. (Color online) The energy dependence of (a) the generalized Fermi–Dirac distribution \( f_q(\epsilon) \) in the factorization approximation and (b) its derivative \( -\partial f_q(\epsilon)/\partial \epsilon \) for various \( q \) with \( \beta = 1.0 \).

with

\[
\rho_{\uparrow,\downarrow}(\epsilon) = \rho_0 \left( \epsilon \pm \left[ \frac{U m}{2} + \mu_B B \right] \right),
\]

\[
\rho_0(\epsilon) = \frac{1}{N_a} \sum_k \delta(\epsilon - \epsilon_k),
\]

where \( \rho_0(\epsilon) \) denotes the density of states and \( N_a \) the number of lattice sites: the plus and minus signs in Eq. (29) are applied to \( \uparrow \) - and \( \downarrow \) - spin electrons, respectively. From Eqs. (27)–(30), \( m \) and \( \mu \) are self-consistently determined as a function of \( T \) for given parameters of \( q, n \) and \( U \) and density of state, \( \rho_0(\epsilon) \).

Bearing Fe, a typical transition-metal ferromagnet, in mind, we have performed model calculations with a bell-shape density of states for a single band given by

\[
\rho_0(\epsilon) = \left( \frac{2}{\pi W} \right) \sqrt{1 - \left( \frac{\epsilon}{W} \right)^2} \Theta(W - |\epsilon|),
\]

where \( W \) denotes a half of the total bandwidth. It has been reported that \( U \sim 2W \approx 5 \) eV for Fe [46,47]. Fig. 2 shows the ground-state magnetic moment as a function of \( U/W = 1.75 \) which leads to magnetic moment of \( m = 0.47 \mu_B \) at \( k_B T/W = 0.0 \). Adopted values of \( n = 1.4 \) electrons and \( m = 0.47 \mu_B \) roughly correspond to those of Fe which has seven d electrons and the ground-state magnetic moment of 2.2\( \mu_B \) (i.e., 7.0/5 = 1.40 electron and 2.2/5 = 0.44\( \mu_B \) per orbital). It is noted that the \( U-m \) relation shown in Fig. 2 is valid for \( 0 < q < 2 \) because \( f_q(\epsilon) \) is independent of \( q \) at \( k_B T/W = 0 \) [Eq. (22)]. We have solved self-consistent Eqs. (27)–(30) by changing \( q \) and \( T \) with the use of the Newton–Raphson method, which is indispensable in our calculations, in particular for \( q \leq 0.4 \) and \( q \geq 1.6 \) (see the Appendix).

Fig. 3 (a) and (b) show the temperature dependence of the magnetic moment, \( m \), for \( q \leq 1.0 \) and \( q \geq 1.0 \), respectively. With increasing \( |q - 1| \), the temperature dependence of magnetic moments becomes more significant and the Curie temperature becomes lower. This is more clearly seen in Fig. 4, where \( T_C \) is plotted as a function of \( q \). The \( q-T_C \) plot is almost symmetric with respect to \( q = 1.0 \) where we obtain the maximum value of \( k_B T_C/W = 0.143 \). If we adopt \( W \sim 2.5 \) eV obtained by the band-structure calculation for Fe [47], the calculated Curie temperature at \( q = 1.0 \) is \( T_C \approx 3500 \) K, while the observed \( T_C \) of Fe is 1044 K [48].
Fig. 2. The $U$ dependence of the magnetic moment $m$ for $k_B T/W = 0.0, \mu_B B/W = 0.0$ and $n = 1.4$ electrons, the arrow denoting the $U/W$ value ($=1.75$) adopted in model calculations.

Fig. 3. (Color online) The temperature dependence of the magnetic moment $m$ for (a) $q \leq 1.0$ and (b) $q \geq 1.0$ with $\mu_B B/W = 0.0$.

Fig. 4. The Curie temperature $T_C$ as a function of $q$.

2.4. Energy and specific heat

We calculate the energy per lattice site given by

$$E = \int \epsilon [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] n(\epsilon) d\epsilon - \frac{U}{4} (n^2 - m^2),$$

(32)
from which the specific heat is given by
\[ C = \frac{dE}{dT} = \frac{\partial E}{\partial T} + \frac{\partial E}{\partial m} \frac{dm}{dT} + \frac{\partial E}{\partial \mu} \frac{d\mu}{dT}, \]  
(33)
with
\[ \frac{\partial E}{\partial T} = -\frac{1}{T} \int \epsilon (\epsilon - \mu) [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] f_q(\epsilon) \, d\epsilon, \]  
(34)
\[ \frac{\partial E}{\partial m} = -Um - \frac{U}{2} \int \epsilon [\rho_\uparrow(\epsilon) - \rho_\downarrow(\epsilon)] \frac{\partial f_q(\epsilon)}{\partial \epsilon} \, d\epsilon, \]  
(35)
\[ \frac{\partial E}{\partial \mu} = -\int \epsilon [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] \frac{\partial f_q(\epsilon)}{\partial \epsilon} \, d\epsilon. \]  
(36)
Analytic expressions for \( dm/dT \) and \( d\mu/dT \) in Eq. (33) are expressed by Eqs. (A.9) and (A.10) (for details see the Appendix).

Fig. 5(a) and (b) show the temperature dependence of the specific heat \( C \) for \( q \leq 1.0 \) and \( q \geq 1.0 \), respectively. With increasing \( |q - 1.0| \), the specific heat at low temperatures is increased and its temperature dependence is considerably modified.

2.5. Spin susceptibility

The spin susceptibility is expressed by
\[ \chi = \frac{dm}{dB}, \]  
(37)
from which the paramagnetic spin susceptibility is given by
\[ \chi = \mu_\|^2 \frac{2\chi_0}{1 - U\chi_0}, \]  
(38)
with
\[ \chi_0 = -\int \rho(\epsilon) \frac{\partial f_q(\epsilon)}{\partial \epsilon} \, d\epsilon. \]  
(39)

The temperature dependence of the inverse of calculated susceptibility, \( 1/\chi \), for \( q \leq 1.0 \) and \( q \geq 1.0 \) is shown in Fig. 6(a) and (b), respectively. The Curie temperature \( T_C \), which is realized at \( 1/\chi = 0 \), is decreased with increasing \( |q - 1.0| \), as shown in Fig. 4.

Fig. 7 shows the Curie temperature \( T_C \) as a function of \( U \) for various \( q \), which are determined by the divergence of the susceptibility. The Curie temperature vanishes at \( U/W \leq 1.66 \) independently of \( q \) because the GFD distribution does not depend on \( q \) [Eq. (22)]. The Curie temperature is lowered with increasing \( |q - 1| \) (Fig. 4).
Fig. 6. (Color online) The temperature dependence of the inversesusceptibility $1/\chi$ for (a) $q \leq 1.0$ and (b) $q \geq 1.0$. Insets show the enlarged plots for $0.0 \leq T \leq 0.4$.

Fig. 7. (Color online) The $U$ dependence of the Curie temperature $T_C$ for $q = 1.0$ (the dashed curve), $q = 0.2$ (the chain curve) and $q = 1.8$ (the solid curve).

3. Discussion

It is possible to qualitatively elucidate the magnetic and thermodynamical properties of nonextensive itinerant-electron ferromagnets presented in the preceding section, with the use of the generalized Sommerfeld expression of various quantities. The integral $I$ including an arbitrary function $\phi(\epsilon)$ and the GFD distribution $f_q(\epsilon)$ is given by

$$ I = \int \phi(\epsilon) f_q(\epsilon) \, d\epsilon, $$

$$ = \int^{\mu} \phi(\epsilon) \, d\epsilon + \sum_{n=1}^{\infty} c_n T^n \phi^{(n-1)}(\mu), $$

with

$$ c_n = - \int_{-\infty}^{\infty} \epsilon^n \frac{d}{dx} \left( \frac{1}{1 + \exp_q(-x)} \right) \, dx, $$

which is valid at low temperatures. Expansion coefficients for $q = 1.0$ are given by $c_2 = \pi^2/6 (= 1.645)$, $c_4 = 7\pi^4/360 (= 1.894)$, and $c_n = 0.0$ for odd $n$.

The $q$ dependence of $c_n$ for $n = 1$ to 4 is plotted in Fig. 8, which shows the followings: (1) $c_1$ and $c_3$ are not zero for $q \neq 1.0$ [33] (though a magnitude of $c_1$ is small) in contrast with $c_1 = c_3 = 0$ in the conventional Fermi–Dirac distribution, (2) with increasing $|q - 1|$, $c_2$, $|c_3|$ and $c_4$ are much increased, and (3) the $q$ dependence of $c_2$ and $c_4$ are almost symmetric with
respect to $q = 1.0$ while those of $c_1$ and $c_3$ are nearly anti-symmetric. The obtained $q$ dependence of $c_n$ may be understood as follows.

When we expand $f_q(\epsilon)$ given by Eq. (18) in a series of $(q - 1)^n/2$ [24], we obtain

\begin{equation}
\begin{align*}
f_q(\epsilon) &= f_1(\epsilon) + \frac{(q - 1)}{2} \beta^2 (\epsilon - \mu)^2 e^{\beta(\epsilon - \mu)} f_1(\epsilon)^2 + \cdots, \\
&= f_1(\epsilon) - \frac{(q - 1)}{2} \beta(\epsilon - \mu)^2 \frac{\partial f_1(\epsilon)}{\partial \epsilon} + \cdots.
\end{align*}
\end{equation}

Substituting Eq. (44) to Eq. (41) and using the integral by part, we obtain $I$ given by

\begin{equation}
I = \int \phi(\epsilon) f_1(\epsilon) \, d\epsilon + \frac{(q - 1)}{2T} \int [2(\epsilon - \mu) \phi(\epsilon) + (\epsilon - \mu)^2 \phi'(\epsilon)] f_1(\epsilon) \, d\epsilon.
\end{equation}

By using Eq. (41) for the second term of Eq. (45), we obtain

\begin{equation}
\begin{align*}
c_1(q) &= \frac{(q - 1)\pi^2}{6} + \cdots, \\
c_2(q) &= c_2(1) + O((q - 1)^2), \\
c_3(q) &= \frac{7(q - 1)\pi^4}{60} + \cdots, \\
c_4(q) &= c_4(1) + O((q - 1)^2),
\end{align*}
\end{equation}

where contributions of $O(q - 1)$ to $c_2$ and $c_4$ are vanishing. Thus the $q$ dependence of $c_2$ and $c_4$ is almost symmetric with respect to $q = 1.0$ whereas that of $c_1$ and $c_3$ is nearly anti-symmetric, as Fig. 9 shows.

Setting $\phi(\epsilon) = \rho_1(\epsilon) - \rho_1(\epsilon)$, $\phi(\epsilon) = \rho_1(\epsilon) + \rho_1(\epsilon)$, and $\phi(\epsilon) = \epsilon [\rho_1(\epsilon) + \rho_1(\epsilon)]$ in Eq. (41) with $c_1 = 0$, we obtain (hereafter we adopt the reduced units in which $W = k_B = \mu_B = 1$)

\begin{equation}
m(T) = m(0) + c_2 [\rho_1' - \rho_1']T^2 + \cdots,
\end{equation}

\begin{equation}
n(T) = n(0) + c_2 [\rho_1' + \rho_1']T^2 + \cdots.
\end{equation}
\[ E(T) = E(0) + c_2 [\rho_\uparrow + \rho_\downarrow + \mu (\rho_\uparrow' + \rho_\downarrow')] T^2 + \left( \frac{U}{4} \right) m(T)^2 + \cdots, \]  
(52)

where \( \rho_\sigma = \rho_\sigma (\mu) \) and \( \rho_\sigma' = d\rho(\mu)/de \). Simple calculations using Eqs. (50)–(52) lead to

\[ m(T) = m(0) - \alpha T^2, \]
(53)
\[ C(T) = \gamma T, \]
(54)

with

\[ \alpha = c_2 (\rho_\uparrow' - \rho_\downarrow'), \]
(55)
\[ \gamma = 2 c_2 (\rho_\uparrow + \rho_\downarrow) - \alpha U m(0). \]
(56)

The \( T^2 \)-decrease in \( m(T) \) arises from the Stoner excitations. When we take into account spin-wave excitations, which are neglected in the Hartree–Fock approximation, magnetization decreases following the \( T^3/2 \) power at low temperatures. A rapid decrease in \( m(T) \) and a large specific heat with increasing \( |q - 1| \) shown in Figs. 3 and 5, are attributed to an enlarged \( c_2 \) shown in Fig. 8.

Setting \( \phi(\epsilon) = d\rho(\epsilon)/de \) in Eq. (41), we obtain

\[ \chi_0 = \rho + c_2 \rho^{(2)} T^2 + c_3 \rho^{(3)} T^3 + \cdots, \]
(57)

where \( \rho^{(\ell)} = \rho^{(\ell)} (\mu) (\ell = 2, 3) \). The Curie temperature \( T_C \) is implicitly given by \( U \chi_0 (T_C) - 1 = 0 \), which yields

\[ T_C = \left( \frac{U \rho - 1}{-c_2 \rho^{(2)}} \right)^{1/2}. \]
(58)

A significant decrease in \( T_C \) with increasing \( |q - 1| \) shown in Fig. 4 is again due to an enlarged \( c_2 \).

For a calculation of the susceptibility at \( T > T_C \), contributions from higher terms than \( T^2 \) are necessary. From Eqs. (38) and (57), the inverse of the susceptibility is given by

\[ \frac{1}{\chi} = \frac{U [c_2 \rho^{(2)} (T^2 - T_C^2) + c_3 \rho^{(3)} (T^3 - T_C^3) + \cdots]}{2 [\rho + c_2 \rho^{(2)} T^2 + c_3 \rho^{(3)} T^3 + \cdots]} . \]
(59)

We note in Eq. (59) that if \( c_3 = 0 \), the temperature dependence of \( 1/\chi \) becomes symmetric with respect to \( q = 1.0 \) because of a symmetry of \( c_2 \). It is not the case because of the significant contribution from \( c_3 \), as shown in Fig. 6.

In the present study, we have employed the GFD distribution of \( f_{\epsilon}(\epsilon) \) given by Eq. (18) obtained within the superstatistics [8–10]. It is worthwhile to point out that the resultant GFD distribution depends on a way how the average is performed over the fluctuating field in the superstatistics. Indeed, if taking the average of \( f_{\text{BC}}(\epsilon_k) \) given by Eq. (21) over the \( \chi^2 \)-distribution, we obtain

\[ \tilde{f}_q(\epsilon_k) = \int_0^\infty f_{\text{BC}}(\epsilon_k) g(\hat{\beta}) \ d\hat{\beta}, \]
(60)
\[ = \int_0^\infty \frac{1}{1 + e^{\hat{\beta}(\epsilon_k - \mu)}} g(\hat{\beta}) \ d\hat{\beta}. \]
(61)

The \( \epsilon \) dependence of \( \tilde{f}_q(\epsilon_k) \) calculated by numerical methods is shown in Fig. 9. We note that \( \tilde{f}_q(\epsilon_k) \) is rather different from \( f_{\epsilon}(\epsilon_k) \) given by Eq. (18) except for \( q = 1.0 \). Fig. 9 clearly shows that the average over the fluctuating field in Eq. (61) leads to result different from \( f_{\epsilon}(\epsilon_k) \) given by Eq. (18). The chain curve in Fig. 9 will be explained below.

It is noted that some applications of the nonextensive quantum statistics have employed the GFD distribution given by [33,34]

\[ \tilde{f}_q(\epsilon) = \frac{1}{1 + (\exp_q [-\beta(\epsilon - \mu)])^{-q}}, \]
(62)

in place of \( f_q(\epsilon_k) \) in Eq. (18). A power index \( q \) in the denominator of Eq. (62) arises from the \( q \)-average of \( \langle \hat{O} \rangle_q = \text{Tr} \hat{\rho}^q \hat{O} \) in the MEM (ii), where \( \text{Tr} \) denotes the trace, \( \hat{\rho} \) the density matrix and \( \hat{O} \) a given operator. Such an averaging does not appear in either classical or quantum superstatistics [8–10]. The chain curve in Fig. 9 shows the \( \epsilon \) dependence of \( f_q(\epsilon) \) for \( q = 1.2 \), which is similar to \( \tilde{f}_q(\epsilon) \) shown by the solid curve.

Magnetization of manganites like \( \text{La}_{0.60} \text{Y}_{0.07} \text{Ca}_{0.33} \text{MnO}_3 \) shows a peculiar temperature dependence, which has been shown to arise from the cut-off properties in the generalized Brillouin function for nonextensive localized spin systems [36–40]. In metallic ferromagnets under consideration, the cut-off properties appear in the GFD distribution [Eq. (14)]. Because \( m, E \) and \( C \) are integrated quantities over the GFD distribution, effects of the cut-off properties are hardly realized in their temperature dependence. In both metallic and insulating ferromagnets, the temperature dependence of \( m \) becomes more significant with further increasing the nonextensivity.
When employing Eq. (56) for paramagnetic metals ($\rho_\uparrow = \rho_\downarrow = \rho$), we obtain the $T$-linear coefficient of the specific heat given by $\gamma = 4c_2\rho$, which leads to the enhancement of the linear coefficient of the specific heat by the nonextensivity:

$$\frac{\gamma'(q)}{\gamma'_{\rho}(1)} = \frac{c_2(q)}{c_2(1)}. \quad (63)$$

This ratio is increased with increasing $|q - 1|$: it is 4.28 and 10.46 for $|q - 1| = 0.5$ and 0.9, respectively [Fig. 8]. Within the superstatistics, this phenomenon may be interpreted as due to the effect of fluctuating $\delta$ (for $q > 1$). Similar enhancements in the specific heat are realized in effects of spin fluctuations at low temperatures [49,50] and of critical fluctuations near the transition temperatures. It has been reported that in some heterogeneous magnetic metals such as metallic spin glasses and metallic amorphous ferromagnets, contributions from electronic specific heat are abnormally large compared to that in normal metals. The temperature dependence of the specific heat and susceptibility in nano-magnets has been shown to considerably depend on the nonextensivity [41,42]. It would be interesting to analyze these materials from the viewpoint of the nonextensive statistics.

4. Conclusion

By using the factorization approach to the GFD distribution [18], we have discussed magnetic and thermodynamical properties of nonextensive itinerant-electron ferromagnets described by the Hubbard model with the Hartree–Fock approximation. Our calculation has shown that with increasing the nonextensivity of $|q - 1|$, Stoner excitations is much increased, which induces a significant decrease in the magnetization and a considerable increase in the specific heat at low temperatures. The adopted Hartree–Fock approximation has some disadvantages: it cannot well explain the $T^{3/2}$-power law of magnetization at low temperatures, the large specific-heat anomaly around $T_C$, and the Curie–Weiss susceptibility. Nevertheless, the Hartree–Fock approximation has an advantage that it provides a reasonable overall description for magnetic and thermodynamical properties. For a more accurate description of nonextensive quantum systems, it is necessary to go beyond the factorization approximation to the GFD distribution [51]. Our study may be generalized to various directions: extensions to ferromagnetic (and antiferromagnetic) metals and alloys with more complicated structures, and calculations of various physical quantities such as spin waves and conductivity. We may extend our theory to include effects of spin fluctuations in nonextensive itinerant-electron ferromagnets with the use of the functional–integral method which is useful for (extensive) bulk ferromagnets [46,52].

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Appendix. Calculations of $dm/dT$ and $d\mu/dT$

The terms of $dm/dT$ and $d\mu/dT$ in Eq. (33) may be derived as follows. From Eqs. (27) and (28), we obtain

$$a_{11} \left( \frac{dm}{dT} \right) + a_{12} \left( \frac{d\mu}{dT} \right) = b_1, \quad (A.1)$$

$$a_{21} \left( \frac{dm}{dT} \right) + a_{22} \left( \frac{d\mu}{dT} \right) = b_2, \quad (A.2)$$

with

$$a_{11} = 1 + \left( \frac{U}{2} \right) \int [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] \frac{\partial f_\uparrow(\epsilon)}{\partial \epsilon} \, d\epsilon, \quad (A.3)$$

$$a_{12} = \int [\rho_\uparrow(\epsilon) - \rho_\downarrow(\epsilon)] \frac{\partial f_\uparrow(\epsilon)}{\partial \epsilon} \, d\epsilon, \quad (A.4)$$

$$a_{21} = \left( \frac{U}{2} \right) \int [\rho_\uparrow(\epsilon) - \rho_\downarrow(\epsilon)] \frac{\partial f_\downarrow(\epsilon)}{\partial \epsilon} \, d\epsilon, \quad (A.5)$$

$$a_{22} = \int [\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] \frac{\partial f_\downarrow(\epsilon)}{\partial \epsilon} \, d\epsilon, \quad (A.6)$$

$$b_1 = - \frac{1}{T} \int (\epsilon - \mu)[\rho_\uparrow(\epsilon) - \rho_\downarrow(\epsilon)] \frac{\partial f_\uparrow(\epsilon)}{\partial \epsilon} \, d\epsilon, \quad (A.7)$$

$$b_2 = - \frac{1}{T} \int (\epsilon - \mu)[\rho_\uparrow(\epsilon) + \rho_\downarrow(\epsilon)] \frac{\partial f_\downarrow(\epsilon)}{\partial \epsilon} \, d\epsilon. \quad (A.8)$$
By solving Eqs. (A.1) and (A.2), we obtain
\[
\frac{dm}{d\tau} = \frac{(a_{22} b_1 - a_{12} b_2)}{\Delta},
\]
\[
\frac{d\mu}{d\tau} = \frac{(-a_{21} b_1 + a_{11} b_2)}{\Delta},
\]
where \(\Delta = a_{11} a_{22} - a_{12} a_{21}\).

Coefficients given by Eqs. (A.3)–(A.6) are used also for solving Eqs. (27) and (28) by the Newton–Raphson method. The \(\ell\)th iterative solution of \(m_\ell\) and \(\mu_\ell\) of Eqs. (27) and (28) are given by
\[
m_\ell = m_{\ell-1} + \frac{(a_{22} c_1 - a_{12} c_2)}{\Delta},
\]
\[
\mu_\ell = \mu_{\ell-1} + \frac{(-a_{21} c_1 + a_{11} c_2)}{\Delta},
\]
with
\[
c_1 = \int [\rho_1(\epsilon) - \rho_1(\epsilon)] f_\ell(\epsilon) \, d\epsilon - m_{\ell-1},
\]
\[
c_2 = \int [\rho_2(\epsilon) + \rho_2(\epsilon)] f_\ell(\epsilon) \, d\epsilon - n,
\]
where the first terms in Eqs. (A.13) and (A.14) are expressed in terms of the \((\ell - 1)\)th solutions of \(m_{\ell-1}\) and \(\mu_{\ell-1}\).

References