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Some metallic properties in the framework of Tsallis generalized statistics

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Abstract. Some metallic quantities are calculated on the grounds of Tsallis generalized statistics: the specific heat at constant volume, $c_V(T)$; the chemical potential, $\mu(T)$; the Pauli paramagnetic susceptibility, $\chi(T)$ and the Korringa constant, $C_{\rm K}$. First it is found that for a general value of q, the Sommerfeld expansion series will exhibit both, odd and even terms, contrary to what is obtained if we use the Fermi-Dirac (FD) statistics, where only even terms appear. It follows that: (i) the specific heat coefficient, γ, is q-dependent, but the temperature dependence of c_V remains linear, as in the FD case; (ii) the Fermi energy, $E_{\rm F}$, differs from the chemical potential by a *linear* term in T, and not quadratic, as in FD, the same happening for $\chi(T)$; (iii) the Korringa constant is q-dependent, but *not* T-dependent. In the limit $q \to 1$ the results of FD statistics are recovered. Metallic thin films and multilayers exhibiting fractal surface structures are possible systems where the present results could be tested.

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1 Introduction

Since the turn of this century, starting with the work of Drude, the study of metals have been one of the main branches of research in condensed matter [1]. From the simple but effective model of Sommerfeld, an astonishing number of metallic effects have been predicted and verified experimentally [2]. These are calculated under the assumption of validity of the Fermi-Dirac (FD) statistics for the electron gas in a metal [1]:

$$f(E) = \frac{1}{{\rm e}^{\beta(E-\mu)}+1} \tag{1}$$

where $\beta = 1/k_{\rm B}T$. Using the Sommerfeld expansion, it can be shown [1] that the chemical potential, $\mu(T)$ differ from the Fermi energy, $E_{\rm F}$, by a factor $(k_{\rm B}T/E_{\rm F})^2 \approx 0.000006$ at room temperature in a typical metal, which allows replacing μ by $E_{\rm F}$ in equation (1) in many practical situations.

From the distribution function one can calculate important metallic properties, like the specific heat at constant volume, $c_V(T)$, and the Pauli paramagnetic susceptibility of the electron gas, $\chi(T)$ [1,3]:

$$c_V(T) = \frac{\partial}{\partial T}\int_{-\infty}^{+\infty} Eg(E)f(E){\rm d}E \tag{2}$$

$$\chi(T) = \frac{\mu_{\rm B}}{2}\frac{\partial}{\partial B_0}\left\{\int_{-\mu_{\rm B}B_0}^{+\infty} g(E+\mu_{\rm B}B_0)f(E){\rm d}E - \int_{+\mu_{\rm B}B_0}^{+\infty} g(E-\mu_{\rm B}B_0)f(E){\rm d}E\right\} \tag{3}$$

where $\mu_{\rm B}$ is the Bohr magneton, and B_0 a external static magnetic field. $g(E)$ is the conduction electrons density of states [1].

Another important metallic property, yet less common in solid state textbooks, which also depends on the distribution function is the spin-lattice relaxation rate [4]:

$$\frac{1}{T_1} = \frac{C_{\rm K}}{k_{\rm B}}\int_0^{\infty} f(E)[1-f(E)]{\rm d}E. \tag{4}$$

Upon equation (1), at low temperatures, one can approximate $f(E)[1-f(E)] \approx k_{\rm B}T\delta(E-E_{\rm F})$ to obtain a famous relation known as the Korringa law: $1/T_1 = C_{\rm K}T$ [4]. This expression relates the spin-lattice relaxation rate, $1/T_1$, to the equilibrium temperature of the system, T. The factor $C_{\rm K}$ is called the Korringa constant, and is related to the properties of conduction electrons in a metal. The measurement of $1/T_1$ as a function of T has been a very powerful tool in the investigation of electronic properties in solids (see [5–7] for recent investigations).

The recent proposal of Tsallis [8] for the generalization of Boltzmann-Gibbs statistics has successfully been applied to a variety of situations, where nonextensivity or long-range interactions are present, or still fractal boundary conditions exist. Generalization is based on the entropic form [8]:

$$S_q = k_{\rm B}\frac{1-\sum_i p_i^q}{q-1} \tag{5}$$

where q is the *entropic index*, and p_i are probabilities satisfying $\sum_i p_i = 1$.

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Nonextensivity follows from equation (5). If A and B are two independent physical systems, it can be shown that the generalized entropy of the combined system $A+B$ satisfies [9]:

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B). \quad (6)$$

Superextensivity corresponds to $q < 1$, and *subextensivity* to $q > 1$. Extensivity corresponds to the particular case $q = 1$. The actual value of q is determined by the microscopic dynamics of the system. A comprehensive recent review can be found in [9].

Although by the present date over 340 papers have been reported on the subject of generalized statistics [15], to the best of the author knowledge, none concerns properties of electrons in metals. In usual metallic bulk samples one can obviously expect the traditional Boltzmann-Gibbs statistics to hold. However, in thin films and multilayers, physical properties are by large determined by the surface structure of these materials. Fractal patterns have been recently observed in gold thin films [16], Ag-Co multilayers, and even in simple magnetic metals (Fe, Co, Cr and Ni) [17]. These are examples of possible systems where the predictions of Tsallis statistics can be directly tested. Theoretical developments concerning fractal structures in metals can be also found in [18–20].

Following [21,22], according to Tsallis proposal, one must replace the FD distribution function in equation (1) by its generalized form:

$$f_q(E) = \frac{1}{[1+(q-1)\beta(E-\mu)]^{\frac{q}{q-1}}+1} \quad (7)$$

where q is the same parameter appearing in the definition (5). By applying the generalized expression of exponential function [8,21]:

$$\mathrm{e}^x = \lim_{q\to 1}[1+(1-q)x]^{\frac{1}{1-q}}$$

one sees that equation (7) reduces to equation (1) in the limit $q \to 1$.

On the present paper we investigate the effect of $f_q(E)$ on some well known metallic properties, namely, the specific heat, the chemical potential, the Pauli paramagnetic susceptibility, and the Korringa constant.

2 Generalized Sommerfeld expansion

Figure 1a shows a plot of $f_q(E)$ for $q = 1.2$ and $q = 1.05$ for $T = 4$ K and $E_\mathrm{F} = 5$ eV, a typical value for a common metal [1]. Figure 1b shows the derivative of these functions. There are three important features to be emphasized in these pictures: (i) as much as the FD function, at low temperatures, $f_q(E)$ varies appreciably only in an interval $k_\mathrm{B}T$ within E_F; (ii) although the functions do not differ much from each other for different values of q, their *derivatives* are very sensitive to the value of q, and diverge very quickly as $q \to 1$; (iii) for a general value of q the derivative of $f_q(E)$ will *not* be an even function of $(\mu - E_\mathrm{F})$.

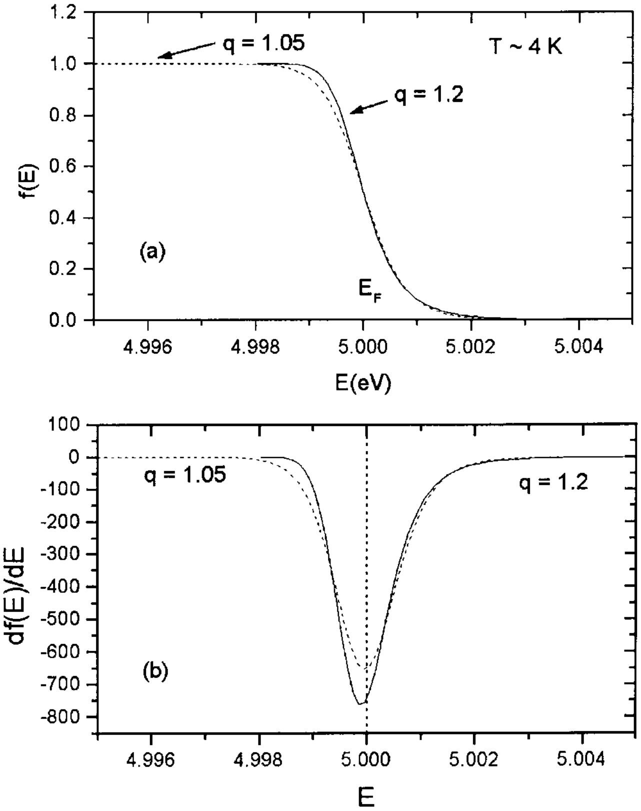

Fig. 1. (a) Generalized distribution function, $f_q(E)$, for $q = 1.05$ and $q = 1.2$; (b) derivatives of $f_q(E)$ from part (a). The variation is strongly dependent on q, and is *not* symmetrical in respect to the Fermi level.

Property (i) warrants that any integral function like

$$\int_{-\infty}^{+\infty} H(E)f_q(E)\mathrm{d}E$$

where $H(E)$ is well behaviored, can be expanded in *Sommerfeld series* [1]. Property (ii) means that the terms of the expansion will be dependent on the value of q and, finally, property (iii) means that for a general value of q there will be both, *even and odd* terms in the series, contrary to what happens if we use the FD statistics, where *only even* terms contribute. Having these features in mind we obtain the *generalized Sommerfeld expansion*:

$$\int_{-\infty}^{+\infty} H(E)f_q(E)\mathrm{d}E = qa(q)\left[\int_0^{E_\mathrm{F}} H(E)\mathrm{d}E + (\mu - E_\mathrm{F})H(E_\mathrm{F})\right] + q\sum_{n=1}^{\infty} b_n(q)(k_\mathrm{B}T)^n \frac{\mathrm{d}^{n-1}}{\mathrm{d}E^{n-1}}H(E)_{E=\mu} \quad (8)$$

where:

$$a(q) = \int_{-\infty}^{+\infty} \frac{[1+(1-q)x]^{\frac{1}{1-q}}}{\{[1+(1-q)x]^{\frac{1}{1-q}}+1\}^2}\mathrm{d}x \quad (9)$$

Table 1. Numerical values for q and $qa(q)$ (see text)

q	$a(q)$	$qa(q)$
1.2	0.828	0.994
1.1	0.905	0.995
1.05	0.949	0.996

and

$$b_n(q) = \int_{-\infty}^{+\infty} \frac{x^n}{n!} \frac{[1+(1-q)x]^{\frac{1}{1-q}}}{\{[1+(1-q)x]^{\frac{1}{1-q}}+1\}^2} \mathrm{d}x. \tag{10}$$

The function $a(q)$ has been numerically integrated for a few values of q. The results are shown in Table 1. One notices that although $a(q)$ varies approximately 14.5% in the interval, the product $qa(q)$ varies only about 0.2%, and remains fairly close to 1. Therefore, one can make the approximation $qa(q) \approx 1$ in equation (8).

The precise way the value of q relates to the dimension of a physical system (and the range of interactions which may be present), remains an open question on Tsallis formalism. In practice, q is used rather as a "fitting parameter" to experimental data, and therefore must be determined to each system in separate. The range of values of q for the present calculation has been chosen in accordance to what has been observed in some other systems [9]. For a general discussion on the q-dependence of specific heat and magnetic susceptibility, see references [10,11]. For the connections with fractality see [12–14].

3 Metallic observables

In this section we apply equation (8) to the calculation of some metallic observables.

3.1 Specific heat and chemical potential

Replacing $H(E) = Eg(E)$ on equation (8) one obtains the internal energy density of the electron gas to second order [1]:

$$\begin{aligned} u(T) = u_0 + \{&(\mu - E_\mathrm{F})g(E_\mathrm{F}) \\ &+ qb_1(q)(k_\mathrm{B}T)g(E_\mathrm{F}) + qb_2(q)(k_\mathrm{B}T)^2 g'(E_\mathrm{F})\}E_\mathrm{F} \\ &+ qb_2(q)(k_\mathrm{B}T)^2 g(E_\mathrm{F}) \end{aligned} \tag{11}$$

where u_0 is the energy density at $T = 0$. But since $qa(q) \approx 1$, the term between brackets vanishes for constant electronic density [1]. Therefore one obtains:

$$u(T) = u_0 + qb_2(q)(k_\mathrm{B}T)^2 g(E_\mathrm{F}) \tag{12}$$

from which we get:

$$c_V = \left(\frac{\partial u}{\partial T}\right)_V = \gamma T; \quad \gamma = 2qb_2(q)k_\mathrm{B}^2 g(E_\mathrm{F}) \tag{13}$$

and

$$\mu(T) = E_\mathrm{F}\left\{1 - qb_1(q)\left(\frac{k_\mathrm{B}T}{E_\mathrm{F}}\right) - qb_2(q)(k_\mathrm{B}T)^2 \frac{g'(E_\mathrm{F})}{E_\mathrm{F}g(E_\mathrm{F})}\right\}. \tag{14}$$

Table 2. Numerical values for q, $qb_1(q)$ and $qb_2(q)$ (see text)

q	$b_1(q)$	$qb_1(q)$	$b_2(q)$	$qb_2(q)$
1.2	0.147	0.177	2.313	2.778
1.1	0.124	0.137	2.630	2.893
1.05	0.073	0.077	2.879	3.023

Table 2 shows numerical results for $qb_1(q)$ and $qb_2(q)$. One sees that, as $q \to 1$, $qb_1(q) \to 0$ and $qb_2(q) \to \pi^2/3$, recovering the results obtained from the usual Sommerfeld expansion [1]. For a free-electron gas, at room temperature, the linear term in equation (14) can be estimated as 10^{-3}, for $q = 1.2$, whereas the quadratic term will be of order 10^{-5}.

3.2 Pauli paramagnetic susceptibility

The Pauli paramagnetic susceptibility, $\chi(T)$, can be obtained applying equation (8) separately to $n_\uparrow$, the number of "spins up" in a static magnetic field, and $n_\downarrow$, the number of "spins down", and having in mind that, since for a metal $\mu_\mathrm{B}B_0 \ll E_\mathrm{F}$, one can expand $g(E_\mathrm{F} \pm \mu_\mathrm{B}B_0) \approx g(E_\mathrm{F}) \pm \mu_\mathrm{B}B_0 g'(E_\mathrm{F})$ [3]. The result is:

$$\begin{aligned} \chi(T) = \chi(0)\Bigg\{&1 + q(q-1)b_1(q)(k_\mathrm{B}T)\frac{g'(E_\mathrm{F}}{g(E_\mathrm{F}} \\ &+ qb_2(q)(k_\mathrm{B}T)^2\left[q\left(\frac{g'(E_\mathrm{F})}{g(E_\mathrm{F}})\right)^2 - \left(\frac{g''(E_\mathrm{F})}{g(E_\mathrm{F})}\right)\right]\Bigg\} \end{aligned} \tag{15}$$

where $\chi(0) = 2\mu_\mathrm{B}^2 g(E_\mathrm{F})$ is the value of χ at $T = 0$. Again one notices that for a general value of q, the first term of temperature correction will be linear in T, and not quadratic, as in the usual Sommerfeld expansion. For $q = 1.2$, in a free-electron gas at room temperature, the linear term will be one order of magnitude larger than the quadratic one. We also see that the FD result is recovered in the limit $q \to 1$.

3.3 Spin-lattice relaxation rate

Replacing equation (7) in equation (4), for the spin-lattice relaxation rate, one obtains the generalized expression:

$$\frac{1}{T_1} = C_\mathrm{K}T\zeta(q,T) \tag{16}$$

where

$$\zeta(q,T) = \int_0^\infty \frac{\mathrm{d}x}{2 + [1+(1-q)(x-\epsilon)]^{\frac{q}{q-1}} + [1+(1-q)(x-\epsilon)]^{\frac{q}{1-q}}} \tag{17}$$

with $\epsilon = E_\mathrm{F}/k_\mathrm{B}T$. Although the temperature explicitly appears in the expression of ζ, the numerical integration

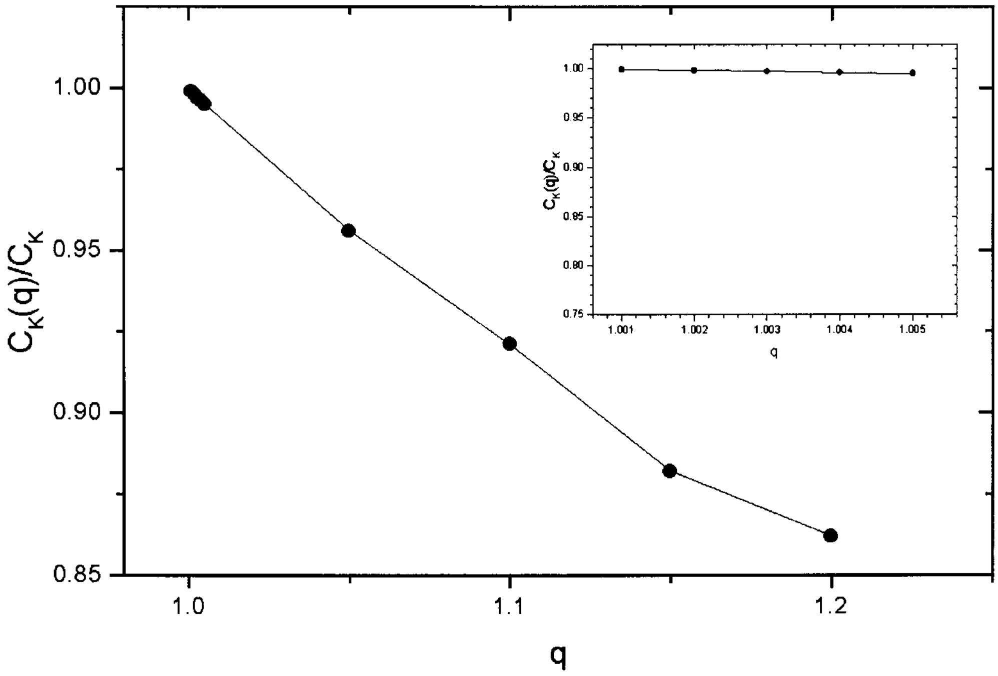

Fig. 2. Ratio of the Korringa constants obtained from the Tsallis statistics, $C_{\mathrm{K}}(q)$, and FD statistics, C_{K} for several values of q. The line is only a guide to the eyes.

of equation (17) for ϵ varying from 20 to 1000 did not show any deviation from the value $\zeta = 0.868$, contrary to what happens to its dependence with q. Therefore one can write for a general value of q:

$$\frac{1}{T_1} = C_{\mathrm{K}}(q)T; \quad C_{\mathrm{K}}(q) = C_{\mathrm{K}}\zeta(q). \tag{18}$$

Figure 2 shows the ratio $C_{\mathrm{K}}(q)/C_{\mathrm{K}}$ for several values of q. On the detail is shown how this ratio tends to 1 as $q \to 1$.

4 Conclusions

Various metallic properties were investigated on the framework of Tsallis generalized statistics. By deducing a "generalized Sommerfeld expansion", one finds that the temperature dependence of the chemical potential and the Pauli paramagnetic susceptibility exhibit a leading linear term, what does not happen if we use the FD statistics. The coefficient of the specific heat and the Korringa constant, on the opposite, do not depend on T, but only on the parameter q. The present results may possibly be tested by measuring some of these properties, for instance, the Pauli paramagnetic susceptibility in systems with metallic surfaces presenting fractal structure [16,17].

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