Correlated electrons and generalized statistics

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Abstract. Several important generalizations of Fermi-Dirac distribution are compared to numerical and experimental results for correlated electron systems. It is found that the quantum distributions based on incomplete information hypothesis can be useful for describing this kind of systems. We show that the additive incomplete fermion distribution gives very good description of weakly correlated electrons and that the nonadditive one is suitable to very strong correlated cases.

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71.10.-w Theories and models of many-electron systems – 71.27.+a Strongly correlated electron systems;
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1 Introduction

In this work, we attempt to relate generalized statistical theories to correlated electron or quasiparticle systems which, since 1980's, have been subjected to intensive theoretical and experimental studies due to their important roles in optical [1], mechanical [2], electric and magnetic [3–8] properties of metal compounds with partially filled d- or f-electrons. In general, with complex correlations, the conventional Boltzmann-Gibbs statistics (BGS) for free fermions is no longer valid. Most of the theoretical study up to now was numerical simulations based on approximate models including essential physics of the systems of interest. Although these theoretical works are very important and fruitful, the need of general understanding and theoretical formulation of the distribution laws begins to be felt. Due to the complexity of the correlations, we can conjecture that generalization of Fermi-Dirac (FD) theory may be useful. In this sense, some efforts have been made to understand localized electron behavior on the basis of fractal geometry (see [9] and references there-in), a generalization of normal space-time.

In what follows, I present a work in this direction based, not on the fractal or chaotic assumption, but on generalized statistical theories proposed for complex systems showing correlated phenomena. The theoretical results will be compared to numerical and experimental ones for correlated electrons. It is expected that this attempt can help to better understand different generalized theories and identify valid theories for this special circumstance.

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2 Some important generalizations of BGS and correlated electrons

Indeed, in the last decade, BGS theory has experienced a turbulent period with the rapid development of some anomalous theories to treat complex systems. These theories are anomalous in the sense that they may perturb our old conceptions concerning, *e.g.*, information, energy, quantum states, additivity etc. The main characters of these theories can be resumed as follows:
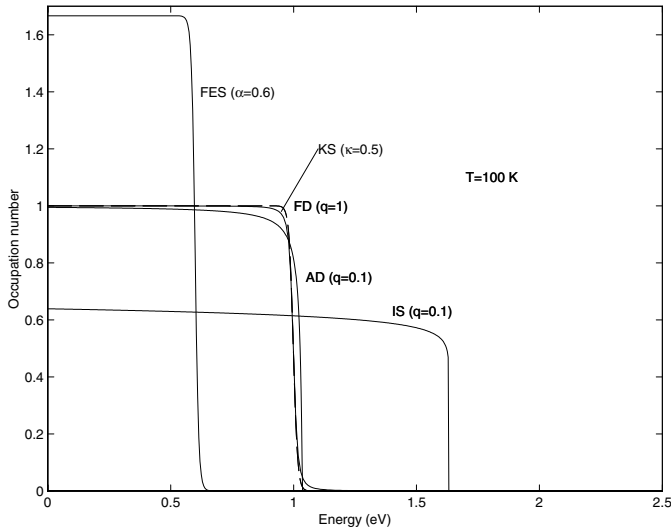
1) Consideration of nonadditivity in entropy, energy, quantum occupation number etc. depending on empirical parameters, *e.g.* $0 < q < \infty$ in Tsallis nonextensive statistical mechanics (NSM) [10] and in its incomplete statistics (IS) version [11–15] as well as in quantum group theory (QGT) [16,17], $\kappa \geq 0$ in κ-statistics (KS) [18].

2) Bosonization of fermions or fermionization of bosons allowing intermediate occupation number related to empirical parameter, *e.g.* $0 \leq \alpha \leq 1$ in fractional exclusion statistics(FES) [17,19–22] and $-1 \leq \eta \leq 1$ for the FES in the frame of KS [18].

3) The empirical parameters take some particular values when the theories recover BGS ($q = 1$, $\alpha = 0, 1$, $\kappa = 0$ and $\eta = -1, 0, 1$).

The philosophy of these generalizations, explicit or not, is to introduce empirical parameters to "absorb" the effects of complex correlations. So interacting systems can be mathematically treated as noninteracting or conventional ones. For example, the total energy of an interacting "free particle" can be written as $p^2/2m$ where p is the momentum and m the mass of the particle. The extra interaction energy is in this way "absorbed" in the

Fig. 1. Fermion distributions of FD, FES, AD, KS and nonextensive IS at 100 K. The fermion density is chosen to give $e_f^0 = 1$ eV for FD distribution at $T = 0$. We note that all these distributions show sharp n drop at Fermi energy e_f. In addition, AD and KS distributions are only slightly different from the FD one even with q very different from unity and maximal κ far from zero. On the other hand, the nonextensive IS distribution changes drastically with decreasing q. We notice a wide decrease of n and a strong increase of e_f with decreasing q. As $q \to 0$, the occupation number tends to 1/2 (zero) for all states below (above) e_f which increases up to 2 times e_{f_0}, a fact shown by numerical calculations for strong correlated electrons.

empirical parameter when they are different from the values corresponding to conventional cases.

About the generalization of FD statistics, Figure 1 shows the different fermion distributions at T=100 K of the generalized statistical mechanics mentioned above. We see that the discontinuity in occupation number n at Fermi energy e_f depends almost only on temperature for all these distributions. The sharp n-drop hardly changes for whatever value of the empirical parameters. In addition, we note that the approximate distribution (AD) $n = \frac{1}{[1+(q-1)\beta(e-e_f)]^{1/(q-1)}+1}$ ($0 < q \leq 1$ in order that the inverse temperature β can go to ∞) of NSM obtained with factorization approximation [22,23] by neglecting correlation energy between the particles is only slightly different from FD one. So its Fermi energy is almost identical to that of FD. The situation of KS is similar. At low temperature, the κ-distribution of standard fermion ($\eta = 1$) $n = \frac{1}{[\sqrt{1+\kappa^2\beta^2(e-e_f)^2}+\kappa\beta(e-e_f)]^{1/\kappa}+1}$ [18] is hardly different from FD for κ values which give finite internal energy (*e.g.* $0 \leq \kappa < 1/2$ for two dimensional fermion gas). For FES fermion distribution $(1/n - \alpha)^\alpha(1/n - \alpha + 1)^{1-\alpha} = e^{(e-e_f)/kT}$ [19] (or equivalently $n = \frac{1}{e^{q\beta(e-e_f)}-1} - \frac{(1+\alpha)/\alpha}{e^{q\beta(e-e_f)(1+\alpha)/\alpha}-1}$ [24]), the n-discontinuity depends only on temperature just as for FD. The influence of α smaller than unity (for FD) is to decrease e_f (α times) and to increase the maximal occupa-

tion number ($1/\alpha$). As for the nonextensive fermion distribution of IS $n = \frac{1}{[1+(q-1)\beta(e-e_f)]^{q/(q-1)}+1}$ [14,15], though n drop at e_f is always very sharp, e_f increase considerably as q decreases from unity. And consequently, there is an important wide n decrease with decreasing q. It was shown [15] that, for $q \to 0$, e_f can increase up to two times the e_f of FD with $n = 1/2$ ($n = 0$) for all energy below (above) e_f. Another common character of NSM and IS distributions is that, due to the energy cutoff with $q < 1$, there are few electrons above e_f at low temperature (large β).

Now let us see the distributions of correlated electrons. From some results of experiments and numerical simulations based on low dimension Kondo lattice models (KLM) [5–8], we notice two important effects of correlations. First, the wide decrease of n and the sharp n drop at e_f much larger than that without correlation have indeed been observed for very strongly correlated electrons (with the coupling parameter $J \geq 4$) [6,8] (see Figs. 3 and 4). So it is possible to describe correlated electron systems in strong coupling regime by IS fermion distribution with q very smaller than unity (close to zero) [15]. On the other hand, another effect of correlation, in the weak coupling regime, is the flattening of n drop at e_f [5–8]. That is that the correlation, even at low temperature, drives electrons above e_f so that the n discontinuity becomes less and less sharp as the correlation increases. Curiously, this flattening of n discontinuity at e_f, though confirmed by experimental results [5], is completely absent in the fermion distributions given by all the statistics, extensive (FES) or nonextensive (NSM, IS and KS), mentioned above.

Fermi surface plays an essential role in the physical properties of metals and metal compounds. So it is of great interest for generalized statistical theories to take into account the essential physics relevant to Fermi energy. In what follows, we will show that it is possible to cover the observed weak correlation effects upon e_f within an additive generalization of BGS based on the IS principles. The reader can find a complete review of IS theory in references [11–15].

3 Additive incomplete statistics

The concept of IS is inspired by incomplete probability distribution (*i.e.* $\text{Tr}\rho = Q \neq 1$) [25] as well as the theoretical difficulties one encounters with $\text{Tr}\rho^q \neq 1$ in NSM [10,13]. The basic assumption of IS is that our knowledge about physical systems is in general incomplete due to unknown interactions or their effects which can not be studied explicitly. In this case, there are always missing informations about the physical systems. So probability distribution is in general inexact and incomplete and can not sum to one. One should write $\text{Tr}(\rho/Q) = \text{Tr}F(\rho) = 1$ where F is certain function to be determined. In the case of complete or approximately complete distribution (such as BGS), F is identity function. In my previous paper, in order to keep Tsallis framework of NSM, I proposed $F(\rho) = \rho^q$ so that

$$\text{Tr}\rho^q = 1, \tag{1}$$

where q is Tsallis entropy index [11–13]. Since $\rho < 1$, we have to set $q \in [0, \infty]$. When $q = 1$, ρ becomes complete, which implies a complete or quasi-complete knowledge about the system of interest. The nonextensive IS formalism [11,13] on the basis of Tsallis entropy yields Tsallis q-exponential distributions and the fermion distribution [14,15] discussed above. An successful application of equation (1) to the study of some power laws on the basis of Rényi entropy [25] can be found in reference [26]. One can even find a plausible justification of equation (1) in a work of Tsallis on the probability distribution on some simple fractal supports like Koch or Cantor sets [27]. Indeed, the phase space of the systems including complex interactions is in general chaotic or fractal structure. In these structures, exact probability distribution is impossible due to the fact that, first, the structures are not differentiable and integrable, second, as mentioned above, some state points in the structures are not accessible. So the treatment of the incomplete distributions, not in the fractal space of d_f dimension, but in a differentiable and integrable d-dimension space, is inevitable. This consideration yields in a natural way the incomplete normalization equation (1) [15].

Now we suppose that the system of interest has additive information and physical quantities (e.g. $H = \sum_i H_i$ where H is the Hamiltonian of the compound system and H_i that of the ith subsystem). This case may happen if there are only weak and short range interactions, so that the Hartley formula $\ln(1/\rho)$ for information measure should apply. The entropy of the system can be defined à la Shannon as follows [12]:

$$S = k_B \text{Tr} \rho^q \ln(1/\rho). \tag{2}$$

S obviously becomes Gibbs-Shannon entropy (S_{GS}) when $q = 1$, which identifies k_B to Boltzmann constant. It is straightforward to see that S verifies all the properties of S_{GS}. For *microcanonical ensemble* ($\rho^q = \frac{1}{w}$), we have $S = \frac{k_B}{q} \ln w$ which decreases with increasing q value. In general, $\Delta S = S - S_{GS} < 0$ (or > 0) if $q > 1$ (or $q < 0$).

For *canonical ensemble*, we postulate

$$U = \text{Tr} \rho^q H \tag{3}$$

where H is the Hamiltonian and U the internal energy of the system. The maximum entropy of S with equation (1) and (3) as constraints leads to:

$$\rho = \frac{1}{Z} e^{-\beta H} \tag{4}$$

with $Z = (\text{Tr} e^{-q\beta H})^{1/q}$. The Lagrange parameter β can be determined by $\frac{\partial S_q}{\partial U_q} = k_B \beta = \frac{1}{T}$ where T is the absolute temperature. It is easy to see that all thermodynamic relations in this theory are identical to those in BGS.

We indicate in passing that this generalization of BGS is obviously the consequence of the "power-normalization" equation (1). Other useful normalizations, if any, of incomplete distributions may lead to different generalization of BGS. For example, if we use Hartley formula as
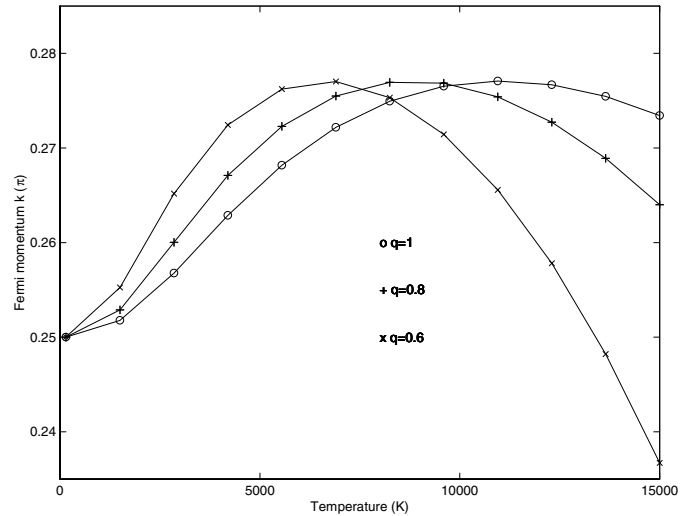
Fig. 2. T-dependence of Fermi momentum k_f of the extensive IS fermion distribution in present work. The density of fermions is chosen to give $k_{f_0} = 0.25\pi$ in the first Brillouin zone. The T-dependence of k_f is in general not monotonic, in contrast with the classical decreasing behavior of e_f with increasing temperature. We notice that, at low temperature, k_f shows an increase with increasing T.

information measure and define expectation value for additive entropy and energy with $F(p_i)$ satisfying $\frac{\partial \ln F(x)}{\partial x} = \frac{1/x}{\alpha - \ln x - (-\ln Zx)^{1/\gamma}}$ where γ is an empirical parameter, maximum entropy will lead to the famous *stretched exponential distribution* [28] $p_i = \frac{1}{Z} e^{-(\beta E_i)^\gamma}$ where E_i is positive energy of the system at state i, α and β the Lagrange multipliers related respectively to normalization and energy constraint $U = \sum_{i=1}^w F(p_i) E_i$. When $\gamma = 1$, we can recover $\frac{\partial \ln F(x)}{\partial x} = \frac{1}{x}$ as in BGS.
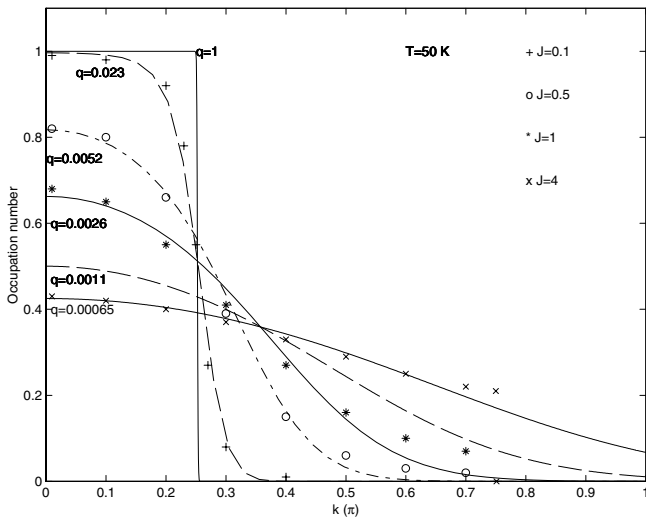
4 Additive IS fermion distribution

For *grand canonical ensemble*, the same machinery as above leads to

$$\rho = \frac{1}{Z} e^{-\beta(H - \mu N)} \tag{5}$$

with $Z = [\text{Tr} e^{-q\beta(H - \mu N)}]^{1/q}$. Supposing $U = \sum_j n_j e_j$ and $N = \sum_j n_j$ in accordance with the additivity assumption, the average occupation number n of one-particle state of energy e can be straightforwardly calculated [12]:

$$n = \frac{1}{e^{q(e - e_f)/k_B T} + 1} \tag{6}$$

which recovers FD distribution for $q = 1$. The Fermi energy can be calculated in the standard way. For 2-D systems, e.g., we have $e_f = e_{f_0} + k_q T \ln(1 - e^{-e_f/k_q T})$ where $k_q = \frac{k_B}{q}$. In Figure 2 is plotted the T-dependence of e_f for different q values for 1-D fermion systems. We see that e_f considerably changes with decreasing q. From

Fig. 3. Comparison of extensive IS fermion distribution (lines) with the numerical results (symbols) of Eder *et al.* on the basis of Kondo lattice $t - J$ model (KLM) for different coupling constant J [6]. The density of electrons is chosen to give $k_{f_0} = 0.25\pi$ in the first Brillouin zone. We note that IS distribution reproduces well the numerical results for about $J < 1$. When coupling is stronger, a long tail in the KLM distributions begins to develop at high energy. At the same time, a new Fermi surface at $k = k_{f_0} + \pi/2 = 0.75\pi$ starts to appear and a sharp n drop takes place at the new Fermi momentum. At $J = 4$, KLM distribution (x-marks) is very different from that of IS (*e.g.* $q = 0.0011$). The solid line fitting better the $J = 4$ KLM distribution is given by the IS version of fractional exclusion distribution $(1/n - \alpha)^{\alpha}(1/n - \alpha + 1)^{1-\alpha} = e^{q\beta(e-e_f)}$ [19,20] or $n = \frac{1}{e^{q\beta(e-e_f)}-1} - \frac{(1+\alpha)/\alpha}{e^{q\beta(e-e_f)(1+\alpha)/\alpha}-1}$ [24] with $1/\alpha = 0.85$ due to the KLM occupation number smaller than 0.5 at low momentum k.

equation (6), we see that q-dependence of e_f at given T will be similar to the T-dependence. The effect of q on other physical quantities (specific heat, electrical conductivity, susceptibility, effective mass etc.) is discussed in [12].

The n distribution around the Fermi momentum k_f can be estimated from equation (6) using $e = \hbar^2 k^2 / 2m$ (k is the momentum). We get:

$$n = \frac{1}{2}\left[1 + \frac{q}{k_B T}\frac{\hbar^2 k_f^2}{m}(k - k_f)\right] \qquad (7)$$

which is similar to the analog given by a Monte-Carlo calculation based on a tight-binding Kondo lattice (KL) [7]. A comparison with [7] leads to $Z = \frac{q\hbar k_f}{2}$, where Z is the quasiparticle weight of photoemission spectrum. Note that Z is k_f-dependent here. Equation (7) tells us that decreasing q yields a flattening of n drop at e_f.

In Figures 3 and 4, we compare the momentum distribution given by equation (6) for T=50 K to some numerical results of the momentum distribution of 1-D correlated electrons [6,8]. We see that, for about $J < 1$ and $q > 0.003$, KLM calculations can be well reproduced by equation (6). But for smaller q or stronger coupling with $J > 1$, a long
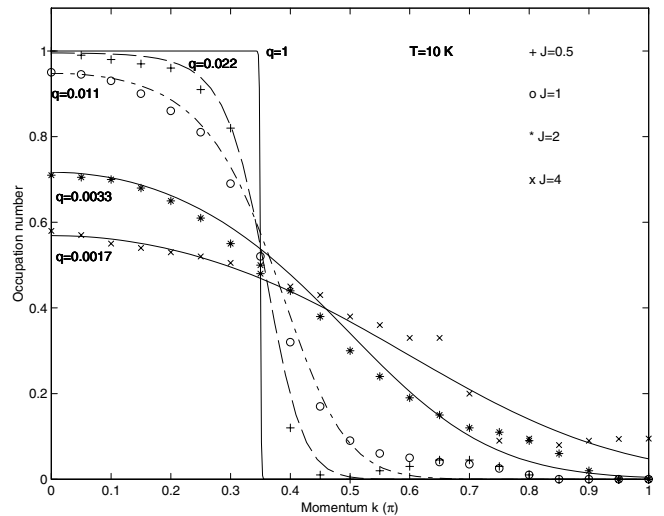
Fig. 4. Comparison of extensive IS fermion distribution (lines) with the numerical results (symbols) of Moukouri *et al.* on the basis of Kondo lattice $t - J$ model (KLM) for different coupling constant J [8]. The density of electrons is chosen to give $k_{f_0} = 0.35\pi$ in the first Brillouin zone. We note that IS distribution reproduces well the numerical results for about $J < 2$. When the coupling is stronger, a long tail in the KLM distributions begins to develop at high energy. A new Fermi surface with sharp n drop starts to appear at about $k = 0.7\pi$, an energy cutoff effect absent in the extensive IS fermion distribution.

tail in the KLM distributions begins to develop at high energy and can not be reproduced by equation (6). At the same time, a new Fermi surface at $k_f + \pi/2$ starts to appear and a sharp n drop (energy cutoff) takes place at the new Fermi momentum. All these strong correlation effects turn out to be completely absent within the present IS Fermion distribution. It is clear that this discrepancy marks the limit of this formalism and perhaps implies that nonextensivity is no more negligible in very strong-coupling case. It is worth noticing that the strong correlation effects, absent in additive IS fermion distribution, are just what we noted in nonextensive IS fermion distribution [15] plotted in Figure 1. This suggests that a combination of these two IS generalizations of BGS, representing respectively two different aspect of correlation, may be an interesting approach leading to more generally valid statistical mechanics suitable for correlated particle systems.

5 Conclusion

We have compared several important generalizations of FD distribution to numerical and experimental results for correlated electron systems. It is found that the generalized fermion distributions based on incomplete information can be useful for describing these systems. It is shown that the extensive IS fermion distribution gives a good description of correlated electrons in weak coupling regime. On the other hand, it fails to describe strongly correlated conduction electrons and localized f-electrons which are

possible to be described by the nonextensive IS fermion distribution. The latter, though powerless for the description of weakly correlated electrons, shows similar behavior as the heavy electrons in strong coupling regime: strong increase of e_f and n-cutoff accompanied by a general decrease in n at all energy up to e_f. In a current work, we are trying to combine these two partially valid generalizations. Further results will be presented in a future paper.

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