Statistical thermodynamics of strongly correlated electrons in a narrow band: Fermi liquid versus spin liquid

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We propose a novel statistical-mechanical approach to a system of strongly correlated electrons in a partially filled narrow band which reproduces rigorously the situation in the atomic limit. In this approach the doubly occupied configurations are excluded both in the real and in the reciprocal spaces. Employing this principle we calculate the thermodynamic properties of those electrons. The metallic state, corresponding to a partially-filled-band case, exhibits a Fermi-liquid–type behavior at low temperatures and transforms into a spin liquid at high temperatures. This feature of our results is reminiscent of the behavior in both magnetic metals and heavy-fermion systems. Additionally, the approach reproduces correctly the statistical properties of the system of localized moments in the limit of the half-filled band, corresponding to the Mott insulating phase. These results are not obtained if one starts from the Fermi-Dirac distribution for the quasiparticles. The last assertion is reinforced by an explicit derivation of a statistical distribution function for correlated electrons which reduces to the Fermi-Dirac distribution in the limit of weak interactions, as well as to the distribution for the spin liquid derived earlier in the limit of strong correlation between the particles.

The problem addressed in this paper can be formulated as follows: Suppose we have a correlated metal represented by a half-filled ($n=1$) narrow band.[1] As the ratio U/W of the intra-atomic Coulomb interaction U to the bare bandwidth W increases, the system transforms either continuously[2] (at temperature $T=0$) or discontinuously[3] (at $T>0$) into the lattice of localized magnetic moments (for $U>U_c\sim W$). The metallic phase near the transition may be represented by an almost localized Fermi liquid,[4] while the insulating phase has an entropy $S\equiv S_L=R\ln 2$ per mole. For the case of partially filled band ($n<1$) the ground state is always metallic because charge transport takes place via holes in the lowest Mott-Hubbard subband.[5] However, one may inquire into the nature of the correlated liquid for $U>U_c(n)$ (herein after called briefly the spin liquid, *SL*) corresponding to the spin lattice for $n=1$. Will this liquid differ from the Fermi-liquid state? This type of question is of fundamental importance for its own sake. Additionally, it is relevant to the heavy-fermion systems, since it has recently[6] been proposed to represent them via an almost half-filled and very narrow band of strongly correlated electrons. It is this particular situation of an almost half-filled narrow band we concentrate on here.

The difference between the correlated electron liquid (SL) and the Fermi liquid (*FL*) can be characterized easily in the high-temperature regime $U\gg k_BT\gg W^*=\Phi W$, where W is the quasiparticle bandwidth and Φ is the band-narrowing factor.[7] Namely, if we have N_e electrons and N states available then the number of configuration for *SL* state (with the double occupancies of each state excluded) is $2^{N_e}N!/[N_e!(N-N_e)!]$ which yields the molar entropy

$$S_L=R\,[n\ln 2-n\ln n-(1-n)\ln(1-n)]\,, \tag{1}$$

with $n=N_e/N$. It reduces to $S_L=R\ln 2$ for $n=1$. By contrast, the corresponding entropy for the Fermi liquid is

$$S_F=R\,[2\ln 2-n\ln n-(2-n)\ln(2-n)]\,. \tag{2}$$

Hence, for $n=1$, $S_F=2S_L$. One should emphasize that only Eq. (1) correctly reproduces the value of S in the atomic limit. The purpose of this paper is to propose the statistical distribution function of the energy levels for the quasiparticle states which reproduces correctly the behavior of electrons in both the atomic limit and for the arbitrary filling, as well as the properties of localized spins in the Mott insulating phase, corresponding to the half-filled band case. These features are absent when we start from the Fermi-Dirac distribution, as illustrated in Appendices A and B.

To describe SL state at low temperatures (e.g., $S_L\to 0$ for $T\to 0$) we make a basic assumption that for a strongly correlated electron liquid ($U/W\to\infty$) the double occupancies are excluded not only in real space but also in reciprocal ($\mathbf{k}$) space. This is because the quasiparticle states representing the two Mott-Hubbard subbands with energies $\{\epsilon\}$ and $\{\epsilon+U\}$ are separated energetically, as has been demonstrated with the example of a Lorentzian density of states (DOS) in the bare band.[5] In other words, the energy manifolds $\{\epsilon_i\}$ and $\{\epsilon_i+U\}$ for $U/W\gg 1$ are disjoint, independent of the quantum-mechanical representation $\{i\}$ labelling these energies. One can also use a phase-space type of argument by noting that for $U/W\gg 1$ the doubly-occupied (spin-compensated) configurations should be projected out

from the physical space,[8] independently of the representation (Bloch or Wannier) chosen to describe the single-particle states. In other words, the same number of degrees of freedom, corresponding to compensated spin configurations, must be removed from either **k** space or real space. For $n=1$ (i.e., for the Mott-insulator case) this amounts to removing N configurations out of available $2N$ states. Implementation of this principle will lead to corrections to the Fermi-Dirac distribution, since the latter contains no correlation between the quasiparticles. Hence, our approach differs at the outset from the Fermi-liquid perturbative approach to the interacting electrons. The nonperturbative nature of the ground *SL* state derives from the qualitative difference (for $n=1$) between the metallic and Mott insulating states. We assume this difference persists also for $n<1$, i.e., the screening effects are insufficient to reduce drastically U.

The number of configurations for the system of $\{N_k\}$ fermions distributed over $\{g_k\}$ states and with the double occupancies excluded is

$$W=\prod_k \begin{bmatrix} g_K \\ N_k \end{bmatrix} \frac{N_k!}{N_{k\uparrow}!N_{K\downarrow}!} , \tag{3}$$

where $N_{k\sigma}$ is the number of electrons with spin σ,

$$N_k=N_{K\uparrow}+N_{k\downarrow} ,$$

and

$$\begin{bmatrix} g_k \\ N_k \end{bmatrix}=\frac{g_k!}{N_k!}[(g_k-N_k)!]^{-1} .$$

This leads to the expression for the entropy (per site)

$$S_L=-\frac{R}{N}\sum_k [(1-n_k)\ln(1-n_k)+n_{k\uparrow}\ln n_{k\uparrow} +n_{k\downarrow}\ln n_{k\downarrow}] , \tag{4}$$

where $n_{k\sigma}=N_{k\sigma}/N$, and $n_k=n_{k\uparrow}+n_{k\downarrow}$. This expression should be compared with that for noninteracting fermions

$$S_F=-\frac{R}{N}\sum_{k,\sigma} [(1-n_{k\sigma})\ln(1-n_{k\sigma})+n_{k\sigma}\ln n_{k\sigma}] , \tag{5}$$

for which the doubly occupied states $|k\uparrow\downarrow\rangle$ have not been excluded from the phase space.

Taking Eq. (4) as a starting point and using the method of the most probable distribution one obtains the set of optimal occupation numbers $\{\bar{n}_{k\sigma}\}$ in the form

$$\bar{n}_{k\sigma}=(1-\bar{n}_{k-\sigma})\frac{1}{1+\exp[\beta(E_{k\sigma}-\mu)]} , \tag{6}$$

where $E_{k\sigma}$ denotes the quasiparticle energy, μ is the chemical potential determined from the condition $(1/N)\sum_{k,\sigma}\bar{n}_{k\sigma}=n$, and $\beta=(k_BT)^{-1}$. This distribution function differs from the ordinary Fermi-Dirac formula by the factor $1-\bar{n}_{k-\sigma}$ which expresses the conditional probability that there is no second particle with spin $-\sigma$ if the state σ is already occupied. If $E_{k\sigma}=E_k$ we find that either $\bar{n}_{k\uparrow}+\bar{n}_{k\downarrow}=1$, or

$$\bar{n}_k=\frac{1}{1+(\frac{1}{2})\exp[\beta(E_k-\mu)]} . \tag{7}$$

For $T=0$ each occupied state is singly occupied. This is the principal feature by which the present formula differs from the Fermi-Dirac distribution, as is illuminated in Fig. 1. It leads also to the doubling of the volume enclosed by the Fermi surface in the *SL* state compared to that for the FL state.[9(a)] Hence, the Luttinger theorem[9(b)] is violated, since we regard the *SL* state as the one which *cannot* be obtained perturbatively, start-

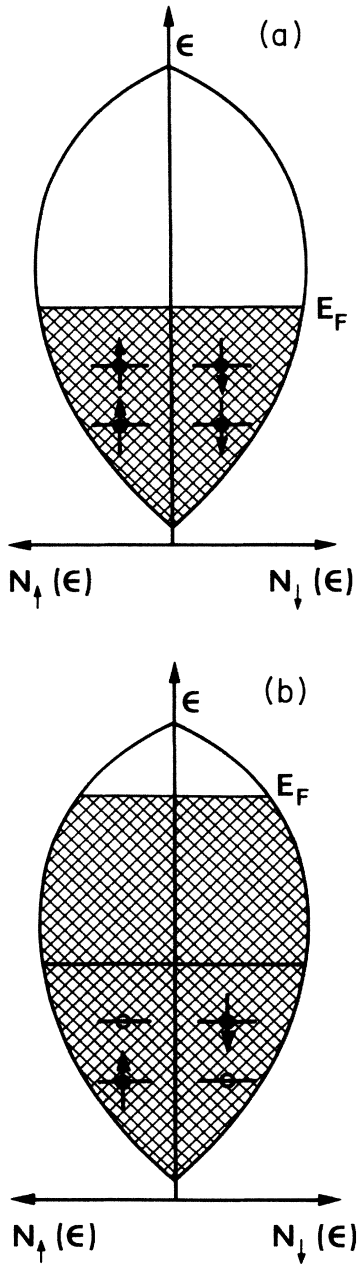

FIG. 1. Schematic representation of the difference in the k-space occupation for the ordinary fermions (top) and the strongly correlated electrons (bottom). The spin subbands are not symmetric in the magnetized state. This distortion does not appear in the paramagnetic state.

ing from the Fermi-Dirac statistic. Also, it is worth noting that one obtains the distribution (7) when considering the statistics of single-electron donors, with the difference that $\{k\sigma\}$ then labels the donors in real space. Hence, one can say that the proposed function (6) describes the statistical distribution of particles near the atomic limit in the same way as does the Fermi-Dirac distribution in the complementary regime of weakly interacting quasiparticles describing the Landau-Fermi liquid state. In other words, our basic equation (3) expresses directly the localized-moment behavior at high temperatures and as such assumed to hold true also at low temperatures. Thus, the function (6) describes correctly $T\to 0$ and $T\to\infty$ limits. It may represent a first step towards the correct formula for the entropy of the strongly interacting electron liquid. It is natural, that we have called the liquid it describes the spin liquid state, since it incorporates some of the properties of both the Fermi liquid and of the localized (spin) moments.

In order to calculate thermodynamic properties we must specify the quasiparticle energies which we take to be in the form[3,7,10]

$$E_{k\sigma}=\Phi_\sigma\epsilon_k-\mu_B H_a\sigma \ ,$$

where

$$\Phi_\sigma=(1-n)/(1-n_\sigma) \ , \quad n_\sigma=N^{-1}\sum_k \bar{n}_{k\sigma}$$

μ_B is the Bohr magneton, H_a is the applied magnetic field, and ϵ_k the energy of electron in a bare band. The internal energy is then

$$E(T)=\sum_{k,\sigma} E_{k\sigma}\bar{n}_{k\sigma} \ ,$$

and the specific heat $C_v=\partial E(t)/\partial T$. Explicitly, for $H_a=0$ we find

$$E(T)=\sum_{k,\sigma}\epsilon_k \bar{f}\left[\frac{\Phi\epsilon_k-\bar{\mu}}{k_B T}\right] , \tag{8}$$

$\bar{f}(x)$ being the Fermi-Dirac function with the shifted chemical potential for the spin liquid $\bar{\mu}=\mu+k_B T\ln 2$, determined from

$$\frac{1}{N}\sum_k \bar{f}\left[\frac{\Phi\epsilon_k-\mu}{k_B T}\right]=n \ , \tag{9}$$

We see that Eqs. (8) and (9) formally coincide with those for either nN spinless fermions or with those for the Fermi liquid containing $2nN$ particles but with Φ corresponding to nN particles in the system.

The Eqs. (8) and (9) require an explanation. First, we use the identity

$$\frac{1}{1+(\frac{1}{2})\exp[\beta(E-\mu)]}\equiv\frac{1}{1+\exp[\beta(E-\bar{\mu})]} \ ,$$

with $\bar{\mu}\equiv\mu+k_B T\ln 2$. This is to show a formal connection of the distribution function derived here with the ordinary Fermi-Dirac function. Second, strictly speaking the quantity $\bar{n}_k$ describes the number of electrons in the singly occupied configuration. So the operators $n_{k\sigma}$ correspond to the entity $n^0_{k\sigma}(1-n^0_{k-\sigma})$ in the terms of Fermi operations $n^0_{k\sigma}=C^\dagger_{k\sigma}C_{k\sigma}$, in the same way as the atomic-operator representation $b_{i\sigma}=C_{i\sigma}(1-n^0_{1-\sigma})$, $b^\dagger_{i\sigma}b_{i\sigma}=C^\dagger_{i\sigma}C_{i\sigma}(1-C^\dagger_{i-\sigma}C_{i-\sigma})$ corresponds to the fermion operators $(C_{i\sigma},n^0_{i\sigma})$ in the real space.[8,9(a)] Hence, one can say that in Eqs. (8) and (9) the summation is over singly occupied configurations in the reciprocal space rather than over independent Fermi quasiparticle states.

The temperature dependence of C_v and C_v/T is shown in Figs. 2(a) and 2(b), respectively. The rectangular form of DOS in the bare band has been used. The specific heat has a pronounced maximum below which the linear dependence,

$$C_v=(\pi^2/3)R\rho^0(\mu_0)(k_B T/W)\Phi^{-1}=\gamma T \ , \tag{10}$$

is obtained [$\rho^0(\mu_0)$ is the density of bare states at $\mu_0=\mu/\Phi$]. The value of γ is enhanced by the factor $\Phi^{-1}=(1-n/2)(1-n)$. The position of the maximum of C_v is determined by the width of the unoccupied part of

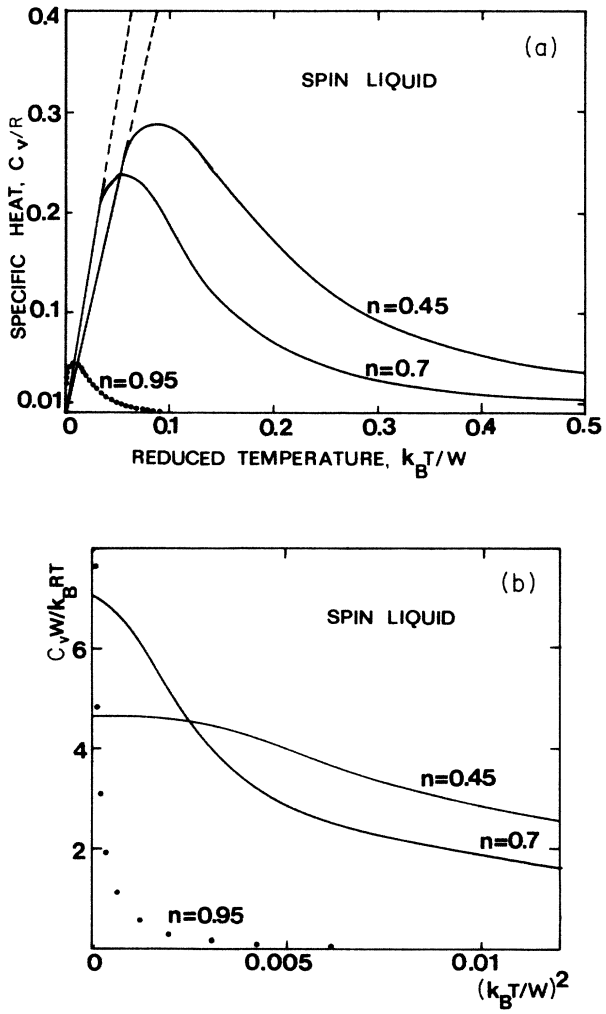

FIG. 2. (a) Temperature dependence of the specific heat c_v for strongly correlated electrons for the band fillings $n=0.45$, 0.7, and 0.95. The dashed lines indicate the linear T dependence at low temperatures. (b) C_v/T as a function of T^2 in dimensionless units.

the band, $W\Phi/2-\mu$. Thus the distribution (7) leads to an enhanced linear specific heat particularly for $n\rightarrow 1$ which is of the same type as for *FL* state[10] (except for the additional factor due to the exclusion of half of the configurations). For comparison, in Figs. 3(a) and 3(b) we have plotted C_v and C_v/T for the Fermi-Dirac distribution case. The maximum is connected with the existence upper band limit $[(W/2)\Phi]$ for the thermal excitation of the electrons.

One of the features of SL is the value of the entropy in the regime $k_B T \gg W\Phi$. In Fig. 4(a) we have plotted the value of $S_L(T\rightarrow\infty)$ as a function of n [cf. also Eq. (1)], while in Fig. 4(b) the dependence $S_L(T)$ is drawn. The temperature dependence of the entropy for the Fermi gas is shown in Fig. 4(c). One should notice that $S_L(T\rightarrow\infty)$ per mole grows rapidly from the value R ln2 as soon as n starts deviating from unity. However, for $T=0$, $\bar{n}_{k\sigma}=0$ or 1 (cf. Fig. 1) and hence $S_L(0)=0$. Thus, $S_L(T)$ expresses both the Fermi-liquid behavior for $T\rightarrow 0$ (where $S_L\sim T$), and localized-moment behavior for $n=1$ (where $S_L=R$ ln2) of the *SL* state. Despite these similarities in this particular situation one should be aware of the basic difference for $n\neq 1$ of the spin liquid with either the *FL* (for $T\rightarrow\infty$) or with the system of localized paramagnetic moments [for $T\rightarrow 0$, cf. Figs.

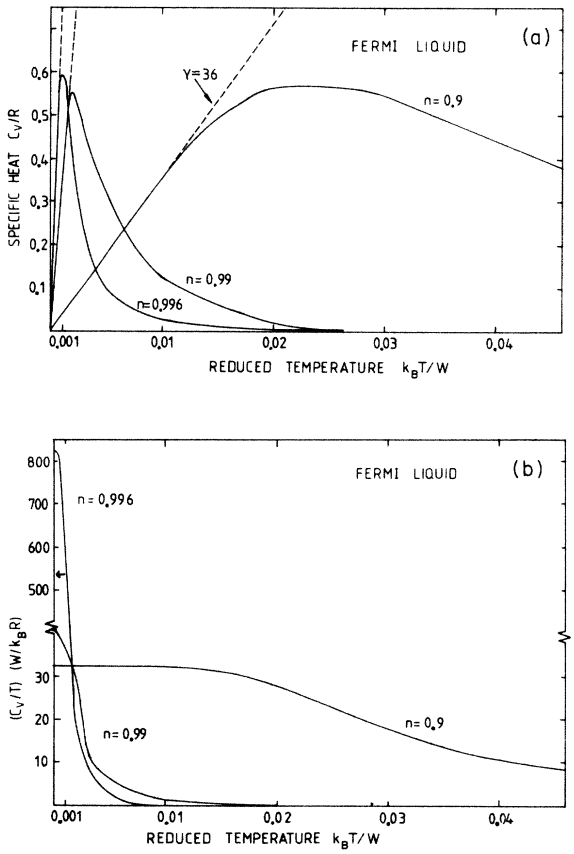

FIG. 3. (a) Same as in Fig. 2(a) but for the Fermi liquid with the same band narrowing factor (Φ) and for the same DOS in the bare band (rectangular). (b) Same as in Fig. 2(b) but for the Fermi liquid with same characteristics: Φ and DOS.

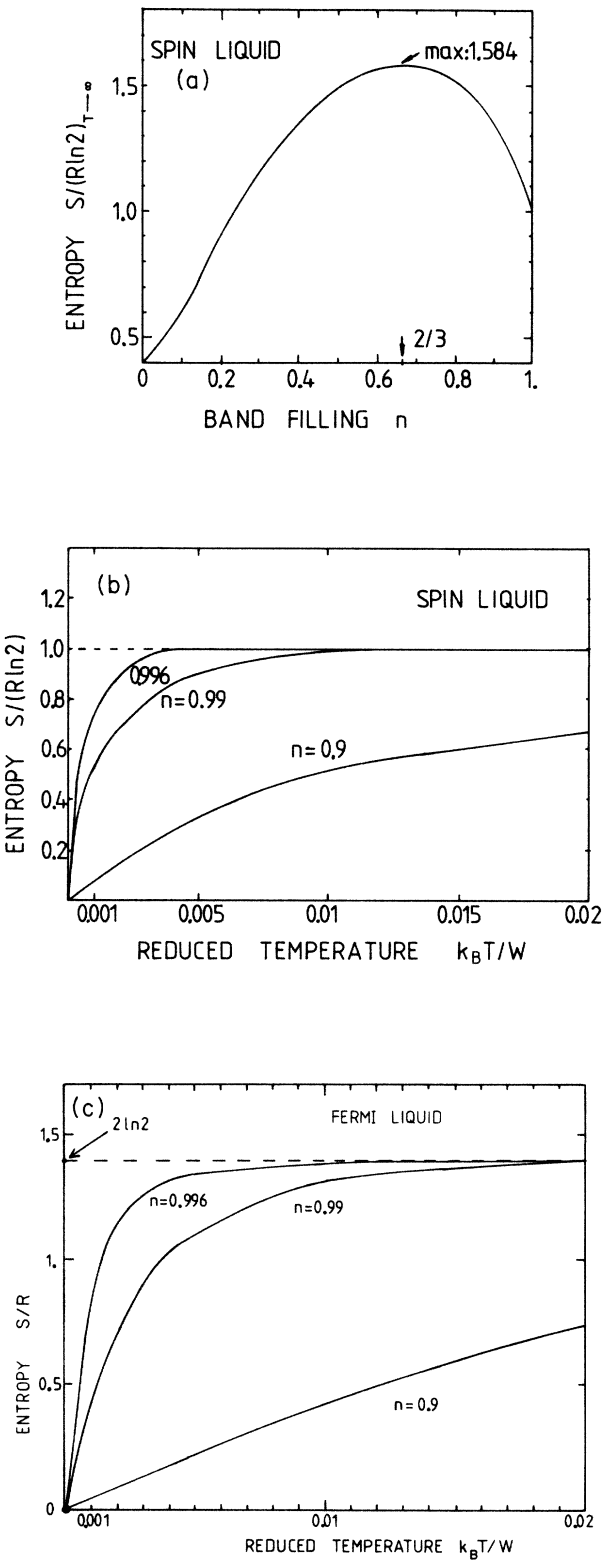

FIG. 4. (a) Limiting value of the entropy $S_L(T\rightarrow\infty)$ as a function of the band filling for the strongly correlated electrons. (b) Temperature dependence of the entropy for the SL state. Note the asymptotic limit $S_L/R\sim\ln 2$ as $T\rightarrow\infty$. (c) The temperature dependence of the entropy S (in dimensionless units) as a function of temperature for the Fermi liquid. Note the asymptotic limit $S_F/R\sim 2\ln 2$ as $T\rightarrow\infty$.

1 and 3(b)]. The full entropy of *FL* is recovered in the limit $k_B T \gg U$, here regarded as unphysically large.

The correlated liquid responds to the magnetic field both by changing the population of the spin subbands (as in *FL*) and by distorting the subbands due to the spin-dependent band narrowing factor Φ_σ. Namely, the subband with the moment $\mathbf{M} \| \mathbf{H}_a$ becomes broader for growing H_a, eventually recovering the full bandwidth W of the bare band for $\mu_B H_a \gtrsim Wn$. This broadening is responsible for the linear dependence $M \sim H_a$ over a wide field range. It also leads to decrease of the specific heat coefficient γ with the field for strong fields.

Quantitatively, introducing the factor Φ_σ into the quasiparticle energy for $H_a \neq 0$, we obtain the following formula for the zero-field susceptibility (per site)

$$\chi = \frac{\mu_B^2}{k_B T} n \left[1 + \frac{E_B (2-n/2)}{2(1-n/2) k_B T} \right]^{-1}, \tag{11}$$

where $E_B = \Phi_0 \int_{W/2}^{W/2} d\epsilon \rho_0(\epsilon) \bar{f}(\epsilon)$ is the band energy of quasiparticles. As the temperature decreases, the system approaches ferromagnetic instability, in agreement with the rigorous Nagaoka result[11] for $U = \infty$. This instability disappears if the kinetic exchange interaction[8] between the correlated electrons is included for large but finite U (see the comment under Ref. 12). In the opposite limit $T \to \infty$ we get the Curie law $\chi = n\mu_B^2/(k_B T)$, i.e., the value for the system of localized spins.

Finally, we discuss briefly the relevance of our results to the heavy-fermion systems, in terms of the strongly correlated (*SL*) liquid. We have shown before that the *SL* state is stable with respect to the *FL* state in the low T range. The high-temperature value of $S \sim R \ln 2$ has been observed in UBe_{13} and interpreted by introducing a phenomenological correction to the entropy of fermions.[6(a)] This value follows naturally from our approach for $n \to 1$. Furthermore, it has been argued very recently[13] that the value of $S(T \to \infty)$ for this system can be substantially higher than $R \ln 2$. This feature can be explained by noting that the saturation value for the entropy depends on n, as shown in Fig. 4(a). We believe that the filling of an extremely narrow band can be perturbed easily by a technological process; hence, the difference in the results. Furthermore, if the f^n configuration is recovered at high temperature then the entropy will approach the limit $R \ln(2J+1) > R \ln 2$, where J is the effective angular momentum.

In summary, we have proposed a novel description of strongly correlated electrons based on the removal of the compensated spin configurations from the phase space for the quasiparticles. The description combines normal Fermi-liquid behavior for $T \to 0$ (i.e., enhanced Pauli susceptibility, large γ, entropy $\sim T$, $M \sim H_a$) and localized-moment type of behavior of $T \to \infty$ (the Curie-Weiss law for susceptibility,[14] $S \sim R \ln 2$). It would be of interest to develop a more microscopic justification for those systems, e.g., by an identification of the large or divergent values of the Landau parameters[15] with the exclusion of some of the quasiparticle states assumed in the present work. Also, an application of the distributions (6) or (7) to the description of the superconducting state would be of interest,

From the theoretical point of view our model treats the correlated narrow-band electrons in a different way compared to the approach in Ref. 6(a). Namely, the authors in Ref. 6(a) correct in a phenomenological way the entropy in order to reproduce the limiting, value $R \ln 2$ as $T \to \infty$. This amounts (in statistical-mechanical treatment) to the removal of the doubly-occupied configurations for the excited quasiparticle states only. In this paper, the doubly occupied (spin-compensated) configurations have been explicitly removed from both the ground and the excited configurations. Under this sole assumption we reproduce an overall behavior of the entropy and the specific heat for the correlated (e.g., heavy-fermion) system in the full temperature range.[16] Despite the principal difference between the statistical approach presented here and that of Refs. 6(a) and 18, the obtained results are similar. This is because at low temperature the same low lying excitations contribute to thermodynamics in both cases [cf. Figs. 1(a) and 1(b)]. The difference in the basic assumptions concerning the statistical treatment of the quasiparticles in the two approaches follows from the lack of knowledge of the detailed value of U for those systems. Namely, since in heavy-fermion systems hybridization is quite important[17] in forming the effective narrow f band, the value of U may be much smaller than that in the atomic limit. In any case, we have assumed that it is far above the value needed for the Mott localization of the corresponding states.

As has been stated above, our approach reproduces the statistical mechanics of electrons in the localized states. In Appendix A we derived the equation for the magnetization for localized electrons. It is also easy to show that the distribution (6) describes correctly the statistics of single donors.[18] In Appendix B we propose a more general distribution function for the correlated electrons which reduces both to the Fermi-Dirac distribution function in the limit of weak interactions, as well as to the new distribution function introduced in this paper in the limit of strong correlations between the particles. This analysis provides a further support for the physical concepts proposed.

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APPENDIX A: MAGNETIZATION IN THE LOCALIZED-MOMENT LIMIT

In this Appendix we make a simple observation about the localized-moment limit, viewed as a limiting situation of either the system of particles obeying the Fermi-Dirac distribution or the distribution (6). For that purpose we define the magnetization per particle.

$$\bar{S}^z = \frac{1}{2N} \sum_k \frac{\bar{n}_{k\uparrow} - \bar{n}_{k\downarrow}}{\bar{n}_{k\uparrow} + \bar{n}_{k\downarrow}} . \tag{A1}$$

In the localized-moment limit corresponding to Mott insulator we have $n \to 1$ (and $\eta = 0$), and hence $E_{k\sigma} = \Phi_\sigma \varepsilon_k - \mu_B H_a \sigma \to -\mu_B H_a \sigma$. Substituting this value for E to the distribution (6) we obtain

$$\bar{S}^z = \tfrac{1}{2} \tanh\left[\frac{\mu_B H_a}{k_B T}\right], \tag{A2}$$

while for the case of the Fermi-Dirac distribution we have

$$(\bar{S}^z)_{\mathrm{FD}} = \tfrac{1}{2} \tanh\left[\frac{\mu_B H_a}{2 k_B T}\right]. \tag{A3}$$

Only the result (A2) is correct for system of localized spins. The additional factor $\frac{1}{2}$ in (A3) comes from the circumstance that for noninteracting fermions two configurations appear which are absent for the lattice of localized spins. These are the configurations with no particle and two particles in the same state. One has to notice that the result (A2) has been derived starting from statistical distribution in the k space. Usually, one derives it starting from the canonical distribution of individual moment directions ($\sigma = \pm 1$) in magnetic field.

APPENDIX B: GENERALIZATON OF THE DISTRIBUTION FUNCTION

Let us assume we have N_{kd} doubly occupancies of N_k particles distributed among g_k states. Then, the number of physically distinct configurations for the whole system is

$$W = \prod_k \frac{g_k!}{(N_{k\uparrow} - N_{kd})!(N_{k\downarrow} - N_{kd})! N_{kd}! (g_k - N_k + N_{kd})!}. \tag{B1}$$

By applying the same procedure of maximization of W as in the main text with respect to $\{N_{k\sigma}\}$, we obtain the most probable distribution of the particles in the form

$$\bar{n}_{k\sigma} = \frac{1 - \bar{n}_{k-\sigma}}{1 + \exp[\beta(E_{k\sigma} - \mu)]} + n_{kd}, \tag{B2}$$

where $n_{kd} = N_{kd}/g_k$. We recover distribution function (6) for the spin liquid in the limit $n_{kd} = 0$. Also, in the limit of weakly interacting particles, i.e., for $n_{kd} = \bar{n}_{kd} = \bar{n}_{k\uparrow}\bar{n}_{k\downarrow}$, the distribution function reduces to the ordinary Fermi-Dirac distribution function, and the entropy (per site) of correlated liquid

$$S = -\frac{R}{N} \sum_k \left[\sum_\sigma (\bar{n}_{k\sigma} - \bar{n}_{kd}) \ln(\bar{n}_{k\sigma} - \bar{n}_{kd}) + \bar{n}_{kd} \ln \bar{n}_{kd} + (1 - \bar{n}_k + \bar{n}_{kd}) \ln(1 - \bar{n}_k + \bar{n}_{kd}) \right], \tag{B3}$$

to the entropy (5) for the Fermi gas.

In the limit $E_{k\sigma} = E_k$ we have that

$$\bar{n}_k = \frac{1 + n_{kd}\left[1 + \exp\left[\frac{E_k - \mu}{k_B T}\right]\right]}{1 + (\frac{1}{2}) \exp\left[\frac{E_k - \mu}{k_B T}\right]}. \tag{B4}$$

For $n_{kd} = 0$ it reduces to the distribution (7).

Depending on the value of n_{kd} we recover either Fermi-Dirac distribution or that for the spin liquid. Hence, n_{kd} is an extra variable which should be determined variationally by minimizing the free energy

$$F(T)/N = (1/N) \sum_{k,\sigma} E_{k\sigma} \bar{n}_{k\sigma} - TS/N. \tag{B5}$$

For that purpose we need an expression for the quasiparticle energies $E_{k\sigma} = E_{k\sigma}\{n_{k\sigma}, n_{kd}\}$, representing the correlated electrons. This poses a problem at the moment. The simple minded type of estimate of n_{kd} can be achieved by noting that we must have that

$$\sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle = \sum_k \bar{n}_{kd}.$$

In other words, the average number of spin-compensated pair states is independent of the representation. Noting that $\sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle = \eta N$, where $\eta \equiv \langle n_{i\uparrow} n_{i\downarrow} \rangle$, we have

$$\eta = \frac{1}{N} \sum_k \bar{n}_{kd}.$$

For the sake of simplicity we assume that for sufficiently large U, $n_{kd} \simeq \bar{n}_d$, i.e., is independent of k. Then $\eta = \bar{n}_d$. This means that $\bar{n}_d$ can be determined from the approach devised before,[7,3] equivalent in the paramagnetic case to the Gutzwiller approach[2,4]. In particular, for the Mott insulating state $\eta = \bar{n}_d = 0$, as assumed in the paper. Moreover, from (B2) we have that

$$\bar{n}_{k\sigma} = (1 - \bar{n}_{k-\sigma}) \bar{n}^{\,0}_{k\sigma} + \bar{n}_d, \tag{B6}$$

where $\bar{n}^{\,0}_{k\sigma}$ is the Fermi-Dirac function. In other words, the statistical distribution function for $k < k_F$ is diminished by the k-dependent factor $1 - \bar{n}_{k-\sigma}$, superposed on k-independent value $\bar{n}_d$. For $\bar{n}_d = 0$ the Fermi volume is twice of that for noninteracting fermions (cf. Fig. 1). All of these features can be obtained also within the Gutzwiller approach, as has been demonstrated recently.[19] So, there is a similarity between the two approaches. However, one should keep in mind that our simple approach is equally valid for both $T = 0$ and $T > 0$ situations.

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[1] We refer often to the Hubbard model as representing correlated electrons in a narrow band, here analyzed in $U \to \infty$ limit. However, the main results in this paper are independent of the particular model chosen, since they are obtained under the only assumption that some configurations are projected out from the physical space.

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