Almost localized fermions in a magnetic field: Properties at the metamagnetic transition

Jozef Spałek and Paweł Korbel
Institute of Physics, Jagiellonian University, ulica Reymonta 4, 30-059 Kraków, Poland

Włodzimierz Wójcik
Institute of Physics, Technical University, ulica Podchorążych 1, 30-084 Kraków, Poland

(Received 6 February 1996; revised manuscript received 8 January 1997)

We present applied magnetic-field dependences of the magnetization, linear specific heat, and de Haas–van Alphen oscillations for the almost-localized Fermi liquid (ALFL) close to the metamagnetic transition. The analysis is performed within the mean-field slave-boson approach, which provides a realistic description in the strong applied-field limit. The Fermi liquid is thermodynamically unstable at the metamagnetic point, at which it is proposed that the system transforms into a statistical spin liquid (SSL) in the partially-filled-band case. This transition corresponds to the Mott-Hubbard localization in the half-filled band situation. The effective mass in the ALFL phase is spin dependent and large, whereas it is spin independent and has a band value in the SSL phase. [S0163-1829(97)04227-6]

In this paper we discuss one of the physical consequences coming from the presence of spin-dependent effective masses and of the nonlinear molecular field for almost localized fermions,[1] namely, a magnetic-field-induced transformation of the almost localized Fermi liquid (ALFL) into a correlated fermionic liquid, hereafter referred to as the statistical spin liquid (SSL).[2] In other words, we predict the existence of anomalous low-temperature magnetic-field-dependent phenomena for fermions in a non-half-filled narrow band, which should be observed experimentally if the mean-field slave boson approach is a correct starting point for those systems. The importance of our predictions is validated by the assumed presence of a strong applied magnetic field, which suppresses quantum-spin-fluctuation contribution to the dynamic properties of almost localized fermions. Thus the present communication supplements the recently achieved quasiparticle picture of ALFL with its generic instability in an applied magnetic field. This instability reduces to the Mott localization at a metamagnetic point in the half-filled band case, and was discussed earlier.[3,4] Also, in the limit of magnetic saturation SSL reduces to the saturated Fermi gas. Here we concentrate on the partially filled band case (with filling $n<1$), i.e., we deal with quantum liquids on both sides of the transition and study the transformation (or crossover behavior) as a function of an applied magnetic field.

The mean-field quasiparticle picture of ALFL we use to calculate the physical properties of ALFL was formulated before.[4,1] It involves both the concepts of band narrowing factor q_σ, the inverse of which specifies the spin-dependent renormalization of the effective band mass ($m_\sigma = m_B/q_\sigma$), and the nonlinear molecular field β_m, each of them calculated self-consistently within the slave-boson approach. In effect, the quasiparticle energy $E_{\mathbf{k}\sigma}$ is related to the bare particle energy $\epsilon_{\mathbf{k}}$ through the relation $E_{\mathbf{k}\sigma} = q_\sigma \epsilon_{\mathbf{k}} - (\mu_B H_a - \sigma \lambda_\sigma^{(2)})\sigma$. This expression was obtained by solving a modified version[4] of the spin rotationally invariant version[5] of the slave-boson approach to the Hubbard model by keeping the spin operator in the fermion representation. The quasiparticle energy contains both the spin-split effective mass renormalization ($m_\sigma / m_B = 1/q_\sigma$) (where m_B is the band mass), and the nonlinear molecular field ($\beta_m \equiv (\lambda_\uparrow^{(2)} - \lambda_\downarrow^{(2)}/2$. Note that both spin-dependent masses and the molecular field are absent in a standard Fermi-liquid theory, although it can be introduced in the situation when the time-reversal symmetry for the Landau scattering amplitude $f_{\mathbf{kk}'}^{\sigma\sigma'}$ is *not* assumed.

The free-energy functional for the Fermi quasiparticles takes the form[1,4,5]

$$\frac{F_{\mathrm{FL}}}{N} = -k_B T \frac{1}{N} \sum_{\mathbf{k}\sigma} \ln\left[1 + \exp\left(\frac{\mu - E_{\mathbf{k}\sigma}}{k_B T}\right)\right] - \lambda^{(1)}(e^2 + d^2 + p_\uparrow^2 + p_\downarrow^2 - 1) - \lambda_\uparrow^{(2)}(p_\uparrow^2 + d^2) - \lambda_\downarrow^{(2)}(p_\downarrow^2 + d^2) + U d^2 + \mu n, \tag{1}$$

where T is the temperature, U is the magnitude of the intra-atomic (Hubbard) interaction, $n = n_\uparrow + n_\downarrow$ is the band filling, N the number of atoms, and $\lambda^{(1)}$ and $\lambda_\sigma^{(2)}$ are the Lagrange multipliers expressing respectively the completeness condition ($e^2 + d^2 + p_\uparrow^2 + p_\downarrow^2 = 1$), the particle-number conservation ($n = p_\uparrow^2 + p_\downarrow^2 + 2d^2$), and the equivalence of the fermion and boson representation of the spin operator S^z component ($n_\uparrow - n_\downarrow = \Sigma_\sigma \sigma p_\sigma^+ p_\sigma$). The factor q_σ is expressed in terms of auxiliary fields as follows:

$$q_\sigma = \frac{e^2 p_\sigma^2 + d^2 p_{\bar\sigma}^2 + 2 e d p_\sigma p_{\bar\sigma}}{(1 - d^2 - p_\sigma^2)(1 - e^2 - p_{\bar\sigma}^2)}. \tag{2}$$

Equation (1) represents the *Landau-type free-energy functional* for the almost localized fermions in a magnetic field and as such must be minimized with respect to the auxiliary fields ($e, d, p_\sigma, \lambda^{(1)}, \lambda_\sigma^{(2)}$), as well as with respect to magnetization $m \equiv n_\uparrow - n_\downarrow$, and the chemical potential μ. This has been performed for constant density of states. In particular, we obtain the relation

$$m^2=h^2(n-2d^2)^2/[h^2+d^2(1-n)+d^4], \qquad (3)$$

where $h=\mu_B H_a/W$, and W is the bandwidth of the bare particles. For $d=0$, $m=n$ and a saturated ferromagnetic state is reached. In that state the majority spin electrons acquire the bare band mass m_B, and their ground-state energy takes the form $E_G/WN=-hm-n(1-n)/2$. This state is reached either via metamagnetic or continuous transitions, at $T=0$ at a critical field $h=h_c$.[1] In the saturated state the correlations induced by the intra-atomic interactions are completely suppressed, since all the particles have the same spin direction.

An interesting question arises as to what happens at $T>0$, when the ALFL is unstable for $H_a>H_c$, even in the regime $U/U_c<1$, where U_c is the critical value of interaction for the Mott-Hubbard localization for $n=1$.[6] This can be seen easily by computing d^2 for $n<1$ and noting that $d^2(H_a>H_c)<0$, a clearly unphysical result. Therefore, to describe consistently the metallic phase in the regime with $d^2\equiv 0$ we invoke the concept of statistical spin liquid,[2] for which double occupancies are totally excluded. To describe this state with antiparallel-spin double occupancies excluded, we assume that the double occupancy probability $\langle n_{\mathbf{k}\uparrow} n_{\mathbf{k}\downarrow}\rangle$ vanishes identically for all **k** values in this new state. Physically, the SSL is the simplest type of strongly correlated state, which is represented by the itinerant spins and encompasses naturally both the localized-moment limit as a $n\rightarrow 1$, and the limit of magnetically saturated Fermi-gas state for $m\rightarrow 1$. Therefore, SSL represents a natural choice for describing the doped Mott insulator, when the holes are itinerant (here we assume additionally that the intersite magnetic interactions are not important). The properties of this liquid have been studied before;[2] we summarize next its features needed to analyze in detail the ALFL→SSL transformation.

First, the exclusion of double occupancies in the momentum space leads to a modified statistical distribution function:

$$\overline{n_{\mathbf{k}}}=1/\{1+a\exp[\beta(\epsilon_{\mathbf{k}}-\mu)]\},$$

with

$$a=[2\cosh(\beta\mu_B H_a)]^{-1},$$

where μ is the chemical potential, and $\beta=(k_BT)^{-1}$. Second, the magnetic moment per atom $m\equiv\langle n_{i\uparrow}-n_{i\downarrow}\rangle$ changes with field according to $m=\tanh(\beta\mu_B H_a)$, i.e., it has the same shape as in the localized-moment case. Additionally, in the low-T limit and for a constant density of states in the band with energies in the interval $[-W/2,W/2]$ the chemical potential is given by

$$\mu=\frac{W}{2}-k_BT\ln\{\exp[\beta W(1-n)]-1\}$$
$$-k_BT\ln[2\cosh(\beta\mu_B H_a)]. \qquad (4)$$

As $T\rightarrow 0$, we find that $\mu(T=0)=W(n-1/2)-\mu_B H_a$. This value of μ coincides with that for ALFL in the saturated state. However, the Luttinger theorem concerning the constant value of the volume encompassed by the Fermi surface is violated at the ALFL→SSL transition, as it is at the Mott-Hubbard transition. Namely, this volume is increased at the transition, since the double occupancies in the **k** space are excluded. Finally, the Helmholtz free energy per site is determined from the expression

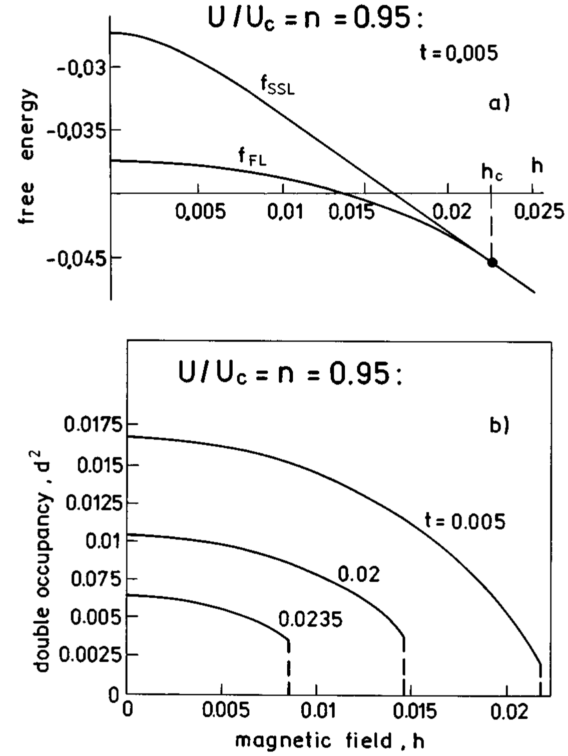

FIG. 1. (a) Field dependence of the free energies for an almost localized Fermi liquid $f_{\rm FL}$ and for the correlated liquid ($f_{\rm SSL}$). The ALFL is unstable for $h>h_c$; (b) the variation of the double occupancy probability.

$$F_{\rm SSL}=-k_BT\int_{-W/2}^{W/2}d\epsilon\ln\left(1+\frac{1}{a}\exp[-\beta(\epsilon-\mu)]\right)+\mu n, \qquad (5)$$

which for $n<1$ reduces to

$$f_{\rm SSL}\equiv\frac{F}{W}=-\frac{1}{2}n(1-n)-\frac{\pi^2}{6}t^2-nt\ln[2\cosh(h/t)], \qquad (6)$$

where $t\equiv k_BT/W$.

The transition is determined from the coexistence condition $F_{\rm FL}=F_{\rm SSL}$. In Fig. 1(a), we display the free energies of the ALFL (as represented by $f_{\rm FL}=F_{\rm FL}/W$) and SSL states for $n=U/U_c=0.95$ and $t=5\times 10^{-3}$. The two energies coincide exactly at H_c. In other words, at H_c the Fermi liquid transforms thermodynamically into a gas of hopping spins with a band mass but with the changed statistical distribution. For comparison, in the ALFL the saturated state $m_\uparrow=m_B$ also, but then the distribution is still provided by the Fermi-Dirac function. In Fig. 1(b) the field dependence of d^2 in the ALFL state.

The resultant magnetization curve in the regime of the ALFL-SSL coexistence is shown in Fig. 2 for the parameters ($n=U/U_c=0.95$), for which *metamagnetism* occurs (the inset provides the temperature variation of the critical field). For $n>n_c\sim 0.973$ the magnetization will exhibit only an up-

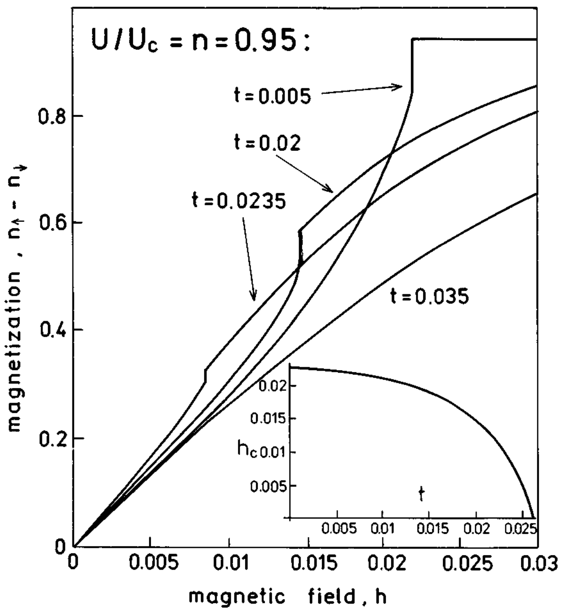

FIG. 2. The theoretical magnetization curve; the inset shows the temperature dependence of the metamagnetic field h_c.

ward turn without a subsequent jump; this behavior will be called, in the following, the *metamagnetic or crossover behavior*.[1]

To model the field dependence of the linear coefficient γ of the specific heat C we have calculated numerically $\gamma \equiv C/T$ as a function of h shown in Fig. 3. Since $\gamma \sim m^*$, the $\gamma(h)$ curve models the field dependence of the total mass enhancement, which in the present situation contains two (spin-dependent) parts: $m^*/m_B = \frac{1}{2}(1/q_\uparrow + 1/q_\downarrow)$. Thus, both γ and the average effective mass m^* can have a cusplike behavior as a function of applied field H_a. Note that the left parts in Figs. 2 and 3 describe the properties of ALFL, while the right parts those for SSL.

In Figs. 4(a) and 4(b) we exhibit the shape of the $T=0$ de Haas–van Alphen oscillations for ALFL, which is calculated in two regimes. Figure 4(a) is representative of the Fermi liquid when H_a is substantially lower than H_c. Under these

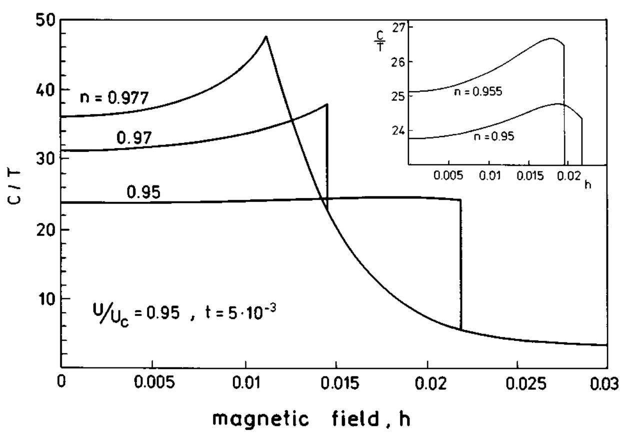

FIG. 3. Field dependence of the linear specific-heat coefficient (in units of $k_B^{-2}W$) for the specified parameters; note the cusp at $h-h_c$. The inset illustrates a rapid change of the $\gamma(h)$ curve with band filling n in the nearly half-filled-band situation.

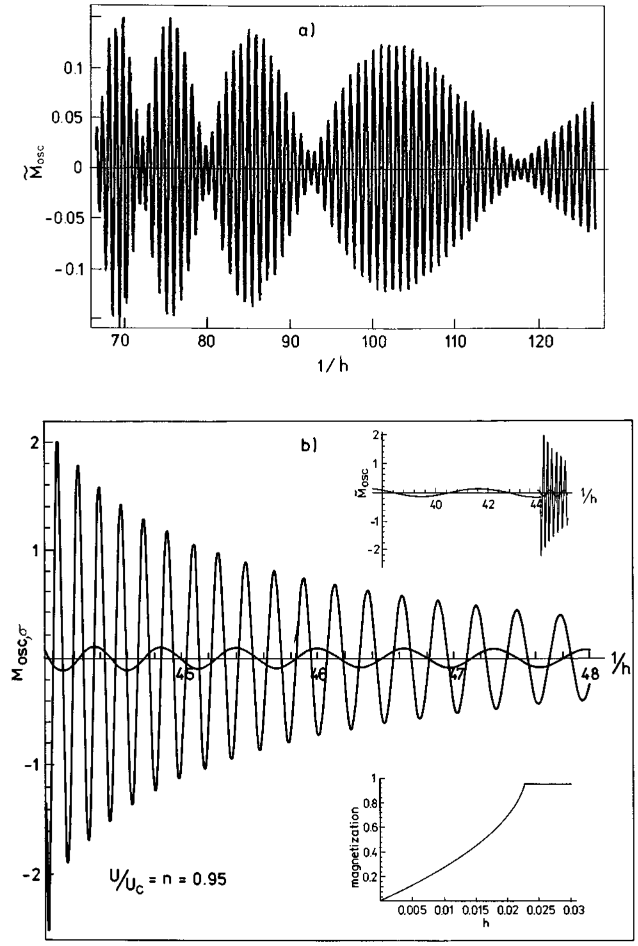

FIG. 4. The shape of the oscillatory component of magnetization vs $1/h$ in the Fermi-liquid regime (a), and near the ALFL $\rightarrow$SSL transition. (b) The upper inset illustrates the evolution of the de Haas–van Alphen oscillations across the metamagnetic transition whereas the lower specifies the shape of the magnetization curve in this case.

conditions the de Haas–van Alphen amplitudes calculated with spin-split masses are almost the same for both majority and minority spin electrons. Also, the cyclotron frequencies $\omega_\sigma = eH_a/(2m_\sigma c)$ are similar. In that situation the spin-resolved components of the oscillating magnetization $M_{\mathrm{osc},\sigma}$ interfere with each other and produce one spectacular quantum beat in the total magnetization $\tilde{M}_{\mathrm{osc}} = \Sigma_\sigma M_{\mathrm{osc},\sigma}$. By contrast, close to the metamagnetic point [Fig. 4(b) and insets], the spin-resolved signals differ significantly and, hence, do not produce beats. Eventually, for $h > h_c$ [cf. the upper inset in Fig. 4(b)] only the majority spin component is present (with the bare band mass); the oscillations become very small and decrease with $1/h$ in the standard manner. The temperature dependence of the oscillations requires a separate analysis. Let us only mention that the transition is reached for $T>0$ for a lower field than that required for $T=0$.

In view of the above quantitative analysis we conclude that a crossover from the Fermi-liquid (albeit almost localized) to the hopping-spins regime is signalled by a cusplike behavior of γ and by a qualitative change of the de Haas–van Alphen oscillation with growing applied field. Both effects accompany the metamagnetic transition or behavior of $m(h)$. Obviously, a direct confirmation would involve the determination of the spin-split effective masses. Concerning this point, note that when $d^2 \rightarrow 0$ the effective masses in the ALFL phase are given by $m_\sigma/m_0 = (1-n/2)/\delta - \sigma m/(2\delta)$, where $\delta = 1-n$. Therefore, *the mass difference grows linearly with magnetization*, i.e., $m_\downarrow - m_\uparrow \approx m/\delta$.

In summary, we have introduced a *physical model* of the transformation of a Fermi liquid of almost localized quasiparticles into a SSL. An interesting feature of this model is that it encompasses both the transition of the first order and a crossover behavior. The microscopic model considered for ALFL was the Hubbard model for $H_a < H_c$, with electron correlations treated for $U \rightarrow U_c$ in the mean-field approximation. On the contrary, the SSL state was introduced to reproduce localized-moment properties for $n \rightarrow 1$ and an exclusion of spin-singlet configurations in a strong applied field.

Note added in proof. Recently, we became aware of the works discussing the metamagnetic behavior for the Hubbard model in the limit of infinite dimensions $d = \propto$) and for $n = 1$. The paper by L. Laloux *et al.* [Phys. Rev. B **50**, 3092 (1994)] analyzes a type of metamagnetic behavior discussed here for $n < 1$; the results are in variance with those obtained earlier[3] in the Gutzwiller approximation. Suprisingly, the magnetization curve has been calculated also for *the-stable-in-this-case* antiferromagnetic phase and does not show any prominent metamagnetic behavior [cf. T. Saso and T. Hayashi, J. Phys. Soc. Jpn. **63**, 401 (1993); A. Giesekus and U. Brandt, Phys. Rev. B **48**, 10 311 (1994)]. However, the phase diagram on the H_a-T plane obtained by the Monte Carlo method by K. Held *et al.*, Mod. Phys. Lett. B **10**, 22203 (1996), exhfibits a number of phases and critical points. Our work in this respect presents the field dependence of the physical properties (C/T, m_σ, m) for $n < 1$, when antiferromagnetic moment becomes totally suppressed. One should emphasize that our results reproduce nicely the main features of the observed behavior of the $CeRu_2Si_2$ heavy-fermion system in the field [for review of magnetic properties see J. Flouquet *et al.*, Physica B **215**, 77 (1995); C/T is provided in C. Paulsen *et al.*, J. Low Temp. Phys. **81**, 317 (1990); the field-dependent masses and the quantum beats are presented in M. Takashita *et al.*, J. Phys. Soc. Jpn. **65**, 515 (1996)].

This research was supported by KBN Grants No. 2P302 093 05 and No. 2 PO3B 129 12. J. S. thanks Professor D. Vollhardt for a discussion on metamagnetism.

[1] P. Korbel, J. Spałek, W. Wójcik, and M. Acquarone, Phys. Rev. B **52**, R2213 (1995); the spin-split masses were introduced in J. Spałek and P. Gopalan, Phys. Rev. Lett. **64**, 2823 (1990).

[2] J. Spałek, Phys. Rev. B **40**, 5180 (1989); Physica B **163**, 521 (1989); J. Spałek and W. Wójcik, Phys. Rev. B **37**, 1532 (1988); K. Byczuk and J. Spałek, *ibid.* **51**, 7934 (1995).

[3] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).

[4] J. Spałek and W. Wójcik, in *Spectroscopy of the Mott Insulators and Correlated Metals*, Springer Series in Solid State Sciences Vol. 119 (Springer-Verlag, Berlin, 1995), pp. 41–65.

[5] R. Frésard and P. Wölfe, Int. J. Mod. Phys. B **6**, 237 (1992); **6**, 3087(E) (1992). In the saddle-point approximation this formulation reduces to the earlier approach discussed in G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986). However, in the approach developed in the last paper only the S^z component of the spin operator is defined properly [$S_i^z = (P_{i\uparrow}^+ P_{i\uparrow}^+ - P_{i\downarrow}^+ P_{i\downarrow})/2$; for a detailed discussion, see Ref. 4].

[6] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970); J. Spałek, A. Datta, and J. M. Honig, Phys. Rev. Lett. **59**, 728 (1987); for review see e.g., J. Spałek, J. Solid State Chem. **88**, 70 (1990); A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).