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Spin-split masses and metamagnetic behavior of almost-localized fermions

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We discuss specific features of quasiparticles in a strong applied magnetic field and near the Mott-Hubbard localization: the strong spin dependence of the de Haas–van Alphen oscillations, the maximum in the field dependence of the linear specific-heat coefficient, and metamagnetic behavior. These properties are obtained within the approach involving auxiliary (slave boson) fields that provides both the Gutzwiller band narrowing and a nonlinear molecular field. The simultaneous observation of all three properties provides a consistent set of predictions of the mean-field approach to the almost-localized Fermi liquid. The situation for heavy fermion system $CeRu_2Si_2$ is briefly discussed.

Almost-localized systems of strongly correlated fermions comprise Mott-Hubbard systems [e.g., pure and doped V_2O_3 (Ref. 1) or $La_{1-x}Sr_xTiO_3$ (Ref. 2)], heavy-fermion systems [such as UPt_3, URu_2Si_2, or $CeRu_2Si_2$ (Ref. 3)], liquid ^3He close to solidification,[4] and high-temperature superconducting materials near the antiferromagnetic insulating state [e.g., $La_{2-x}Sr_xCuO_4$ for $x \sim 0.05$ (Ref. 5) and $YBa_2Cu_3O_{6+x}$ for $x \sim 0.3$–0.4]. The first three classes of materials are frequently considered as *Fermi liquids of almost localized quasiparticles*, i.e., the liquids bordering on a state with localized magnetic moments. The Fermi-liquid nature of their electronic or atomic (in the case of ^3He) states should not be taken for granted, since close to the localization, regarded as a well-defined phase transition, one may encounter a soliton or other non-Fermi-liquid types of single-particle excitations. The purpose of this paper is to propose a consistent set of experimentally verifiable predictions that determine the specific behavior of an almost-localized Fermi liquid in an applied magnetic field, treated within a simple single-particle approach.[6] The lifetime effects for temperatures $T>0$, as well as the detailed applications to heavy-fermion systems, will be discussed separately.[7]

In systems close to the Mott-Hubbard localization the band energy of quasiparticles is small (the effective mass $m^* \rightarrow \infty$) and almost compensated by the short-range repulsive interaction among the carriers.[8] In effect, the system is very susceptible to much weaker perturbations such as the exchange interactions (which lead to a spin-density wave formation on the itinerant side, and to antiferromagnetism on the insulating side), thermal noise (causing the disruption of a coherent band motion and a formation of localized moments at elevated temperature[9]), and applied magnetic field. The main goal of this paper is to show that the applied magnetic field induces a set experimentally verifiable new effects, namely, (i) a spectacular spin dependence of the effective mass as exhibited, e.g., in de Haas–van Alphen oscillations, (ii) quasimetamagnetic behavior for the non-half-filled band case, and (iii) a strong and nonmonotonic magnetic field dependence of the linear specific-heat coefficient γ. These effects should appear concurrently at low temperature.

We start from the quasiparticle picture of almost-localized fermions in a narrow band modeled by the Hubbard model and treated within the rotationally invariant slave-boson approach.[10,11] In this approach in the mean-field approximation, the essential features of the Gutzwiller approach are reproduced[11] as well as quantum fluctuations can be incorporated.[12] Here we discuss the physical results for $T=0$, leaving a detailed formal analysis to a separate publication.[13] Explicitly, we have the quasiparticle energies in the applied magnetic field $h\equiv\mu_B H_a$ of the form

$$E_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}R_\sigma^2[(e+d)q_0+(e-d)q_3]^2+\sigma(\beta-h)+\beta_0, \quad (1)$$

where $\epsilon_{\mathbf{k}}$ is the bare particle energy, e, d, q_0, and q_3 are the average amplitudes of the auxiliary (slave-boson) fields, expressing the empty (e), double occupied (d), and singly occupied (scalar q_0 and the z component of the vector field q_3) configurations, respectively. The constants β_0 and β are the Lagrange multipliers expressing the constraints on the slave-boson representation,[10,11] and $R_\sigma^2=1/[n_\sigma(1-n_\sigma)]$ is an additional renormalization factor introduced to recover properly the limit of uncorrelated electrons, namely, $E_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}-\sigma h$ (n_σ is the average particle number $\langle n_{i\sigma}\rangle$ per site with spin σ). The parameters e, d, q_0, q_3, β, and β_0, together with the chemical potential μ and the magnetic moment (per site) $m\equiv n_\uparrow-n_\downarrow$, are determined by minimization of the free-energy functional for fermions, which is

$$\frac{F}{N}=-k_BT\frac{1}{N}\sum_{\mathbf{k}\sigma}\ln\left[1+\exp\left(\frac{\mu-E_{\mathbf{k}\sigma}}{k_BT}\right)\right]+\alpha(e^2+d^2+q_0^2+q_3^2-1)+\beta_0(q_0^2+q_3^2+2d^2)-2\beta q_0q_3+Ud^2+\mu n, \quad (2)$$

where T is the temperature, U is the magnitude of intra-atomic (Hubbard) interaction, $n=n_\uparrow+n_\downarrow$ is the band filling, N is the number of sites, and α is an additional Lagrange multiplier, minimization with respect of which provides the completeness condition $e^2+d^2+q_0^2+q_3^2=1$. By choosing the representation $p_\sigma\equiv(q_0+\sigma q_3)/\sqrt{2}$, we can write the minimum conditions with respect to β_0 and β in the forms $n_\sigma+n_{\bar\sigma}=p_\sigma^2+p_{\bar\sigma}^2+2d^2$, and $n_\sigma-n_{\bar\sigma}=\sigma(p_\sigma^2-p_{\bar\sigma}^2)$, with

$$n_\sigma=(1/N)\sum_{\mathbf{k}}[1+\exp(\{E_{\mathbf{k}\sigma}-\mu\}/k_BT)]^{-1}.$$

Using the above relations one can eliminate the fields e and p_σ entirely, and obtain the quasiparticle energies in the form $E_{\mathbf{k}\sigma}=q_\sigma\epsilon_{\mathbf{k}}-\sigma(h-\beta)+\beta_0$, and the function (2) in the form

$$F/N=-k_BT\sum_{\mathbf{k}\sigma}\ln[1+\exp(\{\mu-E_{\mathbf{k}\sigma}\}/k_BT)]-\beta_0 n-\beta m+Ud^2+\mu n. \quad (3)$$

The quantity q_σ is the Gutzwiller band narrowing factor[14]

$$q_\sigma=\frac{1}{n_\sigma(1-n_\sigma)}[d\sqrt{n_{\bar\sigma}-d^2}+\sqrt{n_\sigma-d^2}\sqrt{1-n+d^2}]^2, \quad (4)$$

and β is the molecular field. Furthermore, we can express the remaining fields via m, d, and n as follows: $e=(d^2+\delta)^{1/2}$, $q_{0,3}^2=\{n-2d^2\pm[(n-2d^2)^2-m^2]^{1/2}\}/2$, $\approx[n\pm(n^2-m^2)^{1/2}]/2$. Also, $\beta_0=U/2$ and $\beta=h-B$, where B is a complicated function of m and d, rendering the molecular field highly nonlinear in m. Expression (3) essentially represents the free energy for noninteracting fermions subjected to self-consistently adjusted fields (i.e., via the minimization with respect to d and m). Therefore, $E_{\mathbf{k}\sigma}$ represents the quasiparticle energy; the effective mass enhancement for those quasiparticles is defined through the relation

$$m^*/m_0\equiv m_\sigma/m_0=1/q_\sigma. \quad (5)$$

The effective mass m_σ is explicitly spin dependent in an applied field even when the stable state for $h=0$ is paramagnetic. Finally,

$$\mu=\beta_0-\frac{W(1-n)q_\uparrow q_\downarrow}{q_\uparrow+q_\downarrow}+(h-\beta)\frac{q_\uparrow-q_\downarrow}{q_\uparrow+q_\downarrow}. \quad (6)$$

Since q_σ still involves the field d, which is obtained by minimizing the balance between the single-particle and the interaction (Ud^2) contributions to the total energy, the present approach differs from the Landau Fermi-liquid theory, but the methodology is similar to that involving the concept of statistical quasiparticles.[15] Physically, the present approach depends on the number of doubly occupied sites d^2N, which plays the role of the order parameter distinguishing *the Fermi liquid (metallic) state (when $d^2\neq0$) from the local moment bearing state (when $d^2=0$ and $m=n$)*. For $n=1$ the latter state describes the Mott insulator in the mean-field approximation without the exchange interactions.[8]

In the remaining part we discuss our results. To make our argument simple we adopt a constant bare density of states of width W and within the energy interval $-W/2\leqslant\epsilon<W/2$; the gravity center of the band is chosen at zero energy. Then the ground state energy is

$$E_G/WN=2ud^2-hm-(n-2d^2)(1-n+2d^2)/2-\{[d^2(1-n)+d^4][(n-2d^2)^2-m^2]\}^{1/2}, \quad (7)$$

where $u\equiv U/U_c$ and $U_c=2W$ is the critical value of the interaction for Mott-Hubbard localization. We have also set now $h=\mu_BH_a/W$. Minimization of (7) with respect to m provides the relation

$$m^2=h^2(n-2d^2)^2/[h^2+d^2(1-n)+d^4]. \quad (8)$$

Substituting (8) to (7) and minimizing the resulting expression with respect to d, we obtain a following third-order equation with respect to $x=d^2$:

$$-64ux^3+x^2(-80u+96nu-16u^2)+x(-4+16h^2+8n-4n^2-16u-64h^2u+48nu-32n^2u-16u^2+16nu^2)-4h^2+16h^4+8h^2n+n^2-8h^2n^2-2n^3+n^4-16h^2u+32h^2nu-16h^2u^2=0.$$

In Fig. 1 we have displayed m and d^2, both as a function of h, for u = 0.99 and n = 0.99, 0.95, and 0.9. The inset displays the metamagnetism for $n=1$ discussed in detail by Vollhardt.[4] The first-order metamagnetic transition disappears very rapidly when n deviates from unity. Nonetheless, metamagnetic behavior, displayed by an upward turn of $m(h)$ curves, persists over a substantial range of the filling. The metamagnetism is caused by a change in the nature of the ground state from the Fermi-liquid state of heavy fermi-

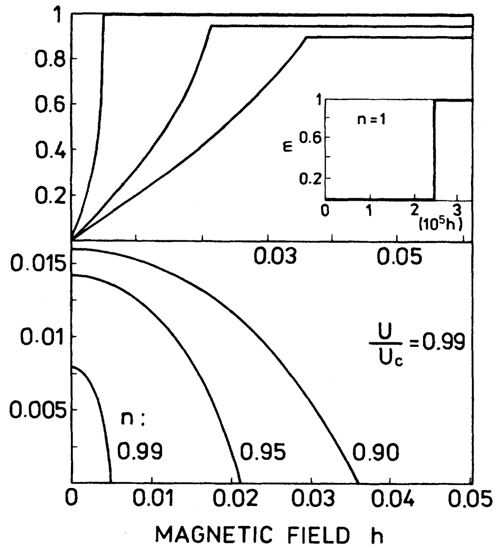

FIG. 1. Field dependent magnetization (top) and double occupancy (bottom), for three band fillings $n=$ 0.90, 0.95, and 0.99. The inset displays the metamagnetism for the half-filled ($n=1$) case.

ons to a state of itinerant (for $n<1$) or localized (for $n=1$) spins. The discontinuity in $\chi \equiv dm/dh$ for $m \rightarrow 1$ is smeared out for $T>0$, and the susceptibility then has a maximum when the system approaches magnetic saturation. The critical field for saturation is strongly reduced as $n \rightarrow 1$, making this phenomenon observable for the extremely narrow band systems such as heavy fermions or liquid ^{3}He. In ^{3}He a small number $\delta \sim 0.01$ of zero-point vacancies is sufficient to render the the magnetization curve continuous.

In Fig. 2 we have summarized the type of magnetic behavior in the applied field assuming that the paramagnetic state is stable for $h=0$.[16] The upper panel characterizes the magnetic saturation field h_c if the magnetization process is continuous. This profile does not reflect the actual situation when a metamagnetic transition takes place, as specified by the dark area in the lower panel. True metamagnetism occurs only for $n \geqslant 0.8$ and for $u \geqslant 0.28$. At low fillings and for small values of u one recovers the normal Fermi-liquid behavior, since the interaction part diminishes roughly as $Un^2/4$.

The crucial quantity in the present paper is the spin-dependent effective mass m_σ. The field dependence of the two mass enhancement factors $1/q_\sigma$ is displayed in Fig. 3. Close to the Mott localization both factors grow with increasing h. In effect, the quantity $(1/q_\uparrow + 1/q_\downarrow)$, proportional to the total density of states, also increases sharply with increasing magnetic field until the saturation point is reached. At that point the minority spin subband becomes empty and all the particles have the same spin and acquire the bare band mass, since the Hubbard interaction $\sim U n_{i\uparrow} n_{i\downarrow}$ is then totally suppressed. This type of behavior manifests itself in the field dependence of the linear specific heat coefficient γ which is proportional to the total density of states at the Fermi energy, i.e., $\gamma = (1/3)\pi^2 \rho(\epsilon_F) \times k_B^2 (1/q_\uparrow + 1/q_\downarrow)$, where $\rho(\epsilon_F)$ is the density of bare states.

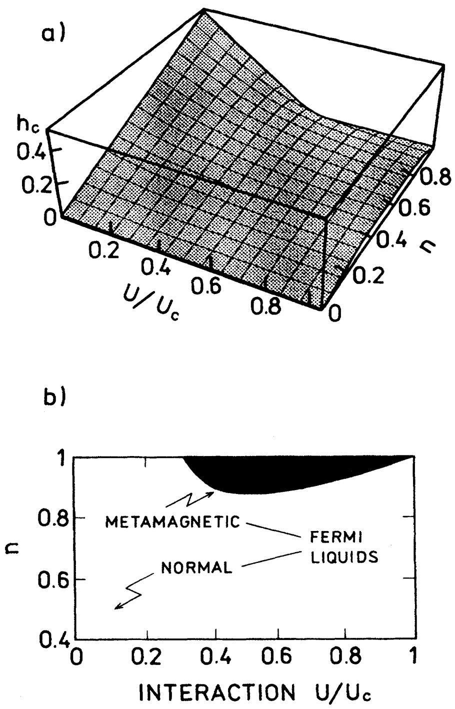

FIG. 2. Critical field for magnetic saturation via a continuous magnetization (top) and the regime of metamagnetism (dark area in the bottom part). All points are drawn for $T=0$.

The quasiparticle masses are determined directly in the de Haas–van Alphen effect. To calculate the spin-resolved signal for the almost-localized charged fermions with spin dependent masses one can adopt the Lifshitz-Kosevich approach.[16] The oscillating part of the magnetization can be expressed as follows:

$$\tilde{M}_2 = -\frac{V}{8\pi^4\hbar^3}\left(\frac{e\hbar}{c}\right)^{3/2} H_a^{\frac{1}{2}} \sum_{l,\sigma} \frac{S_l^\sigma}{m_\sigma} \sum_{k=1}^{\infty} \frac{\psi(k\lambda^\sigma)}{k^{5/2}} A_\sigma \times \sin\left(k\frac{cS_l^\sigma}{e\hbar H_a} + \sigma k\pi\frac{m^\sigma}{m_0} \pm \frac{\pi}{4}\right), \qquad (9)$$

where the area of the mth extremal orbit is $S_l^\sigma = (e\hbar H_a/c) n_{m\sigma} = \pi(2m_\sigma\epsilon_\sigma - p_z^2)$, with $\epsilon_\sigma \equiv \mu + \sigma h$, $\psi(z) \equiv z/\sinh z$, $\lambda_\sigma = (2\pi^2 k_B T c m_\sigma / e\hbar H_a)$, and

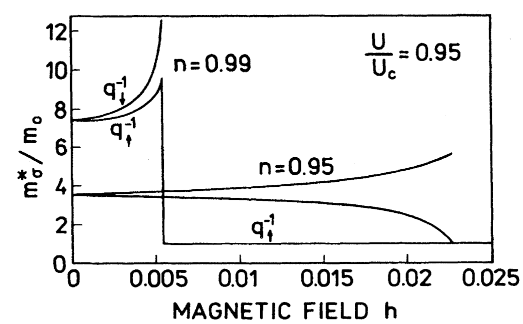

FIG. 3. Applied field dependences of the effective mass enhancement factors $1/q_\uparrow$ and $1/q_\downarrow$, for two different fillings $n=$ 0.99 and 0.95.

$$A_\sigma = 1 - \sigma \frac{\pi}{m_0} \frac{e\hbar}{c} \frac{H_a^2}{S_l^\sigma} \frac{\partial m_\sigma}{\partial H_a} - \frac{H_a}{S_l^\sigma} \frac{\partial S_l^\sigma}{\partial H_a}. \tag{10}$$

Other symbols are standard.[16] For each l we have two periodicities determined by the difference $\Delta(1/H_a)$ in the inverse applied field.

One can easily estimate the amplitudes of the signal by considering the electron gas as having the effective masses m_σ. In that case, $S^\sigma = 2\pi m_\sigma \mu_\sigma$. Additionally, for $d^2 < \delta$ one has $m_\sigma \simeq (1-n_\sigma)/\delta$, where $\delta = 1-n$. Explicitly, $m_\sigma = (1-n/2)/\delta - \sigma m/(2\delta)$. In other words, *the effective mass is approximately a linear function of magnetization.* From this dependence one can estimate the amplitude ratio of the periodic signal for the two spin directions, $\alpha_\uparrow/\alpha_\downarrow$, which for $T \to 0$ can be expressed as

$$[1 + \tfrac{1}{2} H_a \chi(H_a)/\delta][1 - \tfrac{1}{2} H_a \chi(H_a)], \tag{11}$$

where $\chi(H_a) \equiv \partial m/\partial H_a$ is the differential susceptibility [the slope of the $m(H_a)$ curve]. As the saturation or the metamagnetic point is approached, χ exhibits a sharp maximum. Therefore, the amplitude of the majority spin signal should increase or diminish in accord with the behavior of the quantity $H_a\chi(H_a)$. Furthermore, the majority spin subband provides the dominant contribution to the signal. Also, the effective mass should have a cusplike behavior as a function of applied field (cf. Fig. 3). Finally, both the signal amplitude and the effective mass should depend on temperature via the quantities $m = m(H_a, T)$ and $\chi = \chi(H_a, T)$. The detailed behavior is outside the scope of the present paper. It is also clear that the field dependence of the effective mass m_σ obtained from the de Haas–van Alphen oscillations does not exactly follow the field dependence of γ, since the latter quantity involves their sum $(m_\uparrow + m_\downarrow)$.

The theoretical results discussed above correlate very well with experimental observations for the heavy-fermion system $CeRu_2Si_2$. Namely, the metamagnetic behavior and the cusplike field dependence of χ have been observed by Haen *et al.*,[18] while the cusplike behavior of γ was reported by Paulsen *et al.*[19] The maxima in χ and γ correspond to the inflection point in $m(H_a)$, which we identify with the field saturating the magnetization, since we have made the calculations for $T=0$. At $T>0$ this point corresponds to the metamagnetic point. Additionally, the cusplike behavior of $m_\sigma^*(H_a)$ has been detected recently,[20] together with the nonmonotonic field dependence of the de Haas–van Alphen signal amplitude. The decrease in signal frequency with temperature can be attributed to the fact that $S^\sigma \sim m_\sigma \sim m(H_a, T)$, i.e., it is proportional to the orbit area S^σ, which in turn is proportional to m_σ. Obviously, quantitative analysis requires a generalization of the present approach to nonzero temperatures. In general, the present single-band model applies to the heavy fermions if only both the Zeeman energy $g\mu_B H_a$ and the cyclotron frequencies $\omega_\sigma = eH_a/m_\sigma c$ are substantially smaller than the Kondo temperature $k_B T_K$,[21] which characterizes both the width of the peak in the lower quasiparticle band and the hybridization gap.

In summary, we have discussed the metamagnetic behavior of almost localized fermions in a non-half-filled band case, as well as its relation to the nonmonotonic behavior of both spin-split effective masses and to the linear specific-heat coefficient. The results match the experimental observations for the heavy-fermion system $CeRu_2Si_2$.

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