Pis'ma v ZhETF, vol. 82, iss. 4, pp. 234 – 238 © 2005 August 25

Hall coefficient in heavy fermion metals

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Submitted 30 June 2005

Experimental studies of the antiferromagnetic (AF) heavy fermion metal $YbRh_2Si_2$ in a magnetic field B indicate the presence of a jump in the Hall coefficient at a magnetic-field tuned quantum state in the zero temperature limit. This quantum state occurs at $B \geq B_{c0}$ and induces the jump even though the change of the magnetic field at $B = B_{c0}$ is infinitesimal. We investigate this by using the model of heavy electron liquid with the fermion condensate. Within this model the jump takes place when the magnetic field reaches the critical value B_{c0} at which the ordering temperature $T_N(B = B_{c0})$ of the AF transition vanishes. We show that at $B \to B_{c0}$, this second order AF phase transition becomes the first order one, making the corresponding quantum and thermal critical fluctuations vanish at the jump. At $T \to 0$ and $B = B_{c0}$, the Grüneisen ratio as a function of temperature T diverges. We demonstrate that both the divergence and the jump are determined by the specific low temperature behavior of the entropy $S(T) \propto S_0 + a\sqrt{T} + bT$ with S_0, a and b are temperature independent constants.

PACS: 71.10.Hf, 71.27.+a, 74.72.–h

The most outstanding puzzle of heavy fermion (HF) metals is what determines their universal behavior which drastically differs from the behavior of ordinary metals. It is wide accepted that the fundamental physics observed in the HF metals is controlled by quantum phase transitions. A quantum phase transition is driven by control parameters such as composition, pressure, number density x of electrons (holes), magnetic field B, etc, and takes place at a quantum critical point (QCP) when the temperature $T = 0$. In the case of conventional quantum phase transitions (CQPT) the physics is dominated by thermal and quantum fluctuations near CQP. This critical state is characterized by the absence of quasiparticles. It is believed that the absence of quasiparticle-like excitations is the main cause of the non-Fermi liquid (NFL) behavior, see e.g. [1]. However, theories based on CQPT fail to explain the experimental observations of the universal behavior related to the divergence of the effective mass M^* at the magnetic field tuned QCP, the specific behavior of the spin susceptibility, its scaling properties, etc.

It is possible to explain the observed universal behavior of the HF metals on the basis of the fermion condensation quantum phase transition (FCQPT) which takes place at $x = x_{FC}$ and allows the existence of the Landau quasiparticles down to the lowest temperatures [2]. It is the quasiparticles which define the universal behavior of the HF metals at low temperatures [2, 3]. In contrast to the conventional Landau quasiparticles, these are characterized by the effective mass which strongly depends on temperature T, applied magnetic field B and the number density x of the heavy electron liquid of HF metal. Thus, we come back again to the key role of the of the effective mass.

On the other hand, it is plausible to probe the other properties of the heavy electron liquid which are not directly determined by the effective mass. Behind the point of FCPT when $x < x_{FC}$, the heavy electron liquid possesses unique features directly determined by its quasiparticle distribution function $n_0(\mathbf{p})$ formed by the presence of the fermion condensate (FC) [4]. Therefore, the function $n_0(\mathbf{p})$ drastically differs from the quasiparticle distribution function of a typical Landau Fermi liquid (LFL) [5]. For example, it was predicted that at low temperatures the tunneling differential conductivity between HF metal with FC and a simple metallic point can be noticeably dissymmetrical with respect to the change of voltage bias [6]. As we shall see below, the magnetic field dependence of the Hall coefficient $R_H(B)$ can also provide information about electronic systems with FC.

Recent experiments have shown that the Hall coefficient in the antiferromagnetic (AF) HF metal $YbRh_2Si_2$ in a magnetic field B undergoes a jump in the zero temperature limit upon magnetic-field tuning the metal from AF to a paramagnetic state [7]. At some critical value B_{c0}, the magnetic field B induces the jump even though the change of the magnetic field at at the critical value B_{c0} is infinitesimal.

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In this letter, we show that the abrupt change in the Hall coefficient is determined by the presence of FC and investigate this jump by using the model of the heavy electron liquid with FC which is represented by an uniform electron liquid near FCQPT. Within this model the jump takes place when magnetic field reaches the critical value B_{c0} at which the Néel temperature $T_N(B = B_{c0})$ of the AF transition vanishes. At some temperature $T_{\rm crit}$ when $B \to B_{c0}$, this second order AF phase transition becomes the first order one, making the corresponding quantum and thermal critical fluctuations vanish at the point where $T_N(B = B_{c0}) \to 0$. At $T \to 0$ and $B = B_{c0}$, the Grüneisen ratio $\Gamma(\mathrm{T}) = \alpha(\mathrm{T})/\mathrm{C}(\mathrm{T})$ as a function of temperature T diverges. Here, $\alpha(T)$ is the thermal expansion coefficient and $C(T)$ is the specific heat. We show that both the divergence and the jump are determined by the specific low temperature behavior of the entropy $S(T) \simeq S_0 + a\sqrt{T/T_f} + bT/T_f$ with S_0, a and b being temperature independent constants, and T_f is the temperature at which the influence of FC vanishes.

To study the universal behavior of the HF metals at low temperatures, we use the heavy electron liquid model in order to get rid of the specific peculiarities of a HF metal. It is possible since we consider processes related to the power-low divergences of the corresponding physical quantities. These divergences are determined by small momenta transferred as compared to momenta of the order of the reciprocal lattice, therefore, the contribution coming from the lattice can be ignored. On the other hand, we can simply use the common concept of the applicability of the LFL theory when describing electronic properties of metals [5]. Thus, we may safely ignore the complications due to the anisotropy of the lattice regarding the medium as the homogeneous heavy electron isotropic liquid.

At first, we briefly describe the heavy electron liquid with FC. Dealing with FCQPT, we have to put $T = 0$. In that case, the ground state energy E_{gs} of a system in the superconducting state is given by the BSC theory formula

$$E_{gs}[\kappa(\mathbf{p})] = E[n(\mathbf{p})] + E_{sc}[\kappa(\mathbf{p})], \tag{1}$$

where the occupation numbers $n(\mathbf{p})$ are connected to the factors $v(\mathbf{p})$, $u(\mathbf{p})$ and the order parameter $\kappa(\mathbf{p})$

$$\begin{gathered} n(\mathbf{p}) = v^2(\mathbf{p}); \;\; v^2(\mathbf{p}) + u^2(\mathbf{p}) = 1; \\ \kappa(\mathbf{p}) = v(\mathbf{p})u(\mathbf{p}) = \sqrt{n(\mathbf{p})(1 - n(\mathbf{p}))}. \end{gathered} \tag{2}$$

The second term $E_{sc}[\kappa_p]$ on the right hand side of Eq. (1) is defined by the superconducting contribution which in the simplest case of the weak coupling regime is of the form

$$E_{sc}[\kappa_p] = \lambda \int V_{pp}(\mathbf{p}_1, \mathbf{p}_2)\kappa(\mathbf{p}_1)\kappa^*(\mathbf{p}_2)\frac{d\mathbf{p}_1 d\mathbf{p}_2}{(2\pi)^4}, \tag{3}$$

where $\lambda V_{pp}(\mathbf{p}, \mathbf{p}_1)$ is the pairing interaction. Varying E_{gs} given by Eq. (1) with respect to $v(\mathbf{p})$ one finds

$$\varepsilon(\mathbf{p}) - \mu = \Delta(\mathbf{p})\frac{1 - 2v^2(\mathbf{p})}{2\kappa(\mathbf{p})}. \tag{4}$$

Here $\varepsilon(\mathbf{p})$ is defined by the Landau equation $\delta E[n(\mathbf{p})]/\delta n(\mathbf{p}) = \varepsilon(\mathbf{p})$, μ is chemical potential, and the gap

$$\Delta(\mathbf{p}) = -\lambda \int V_{pp}(\mathbf{p}, \mathbf{p}_1)\sqrt{n(\mathbf{p}_1)(1 - n(\mathbf{p}_1))}\frac{d\mathbf{p}_1}{4\pi^2}. \tag{5}$$

If $\lambda \to 0$, then $\Delta(\mathbf{p}) \to 0$, and Eq. (4) reduces to the equation

$$\frac{\delta E[n(\mathbf{p})]}{\delta n(\mathbf{p})} - \mu = \varepsilon(\mathbf{p}) - \mu = 0, \text{ if } \kappa(\mathbf{p}) \neq 0. \tag{6}$$

As a result, at $x < x_{FC}$, the function $n(\mathbf{p})$ is determined by the standard equation to search the minimum of functional $E[n(\mathbf{p})]$ [8, 9]. Equation (6) determines the quasiparticle distribution function $n_0(\mathbf{p})$ which delivers the minimum value to the ground state energy E. The function $n_0(\mathbf{p})$ being the signature of the new state of quantum liquids [10] does not coincide with the step function in the region $(p_f - p_i)$ where $\kappa(\mathbf{p}) \neq 0$, so that $0 < n_0(\mathbf{p}) < 1$ and $p_i < p_F < p_f$, with $p_F = (3\pi^2 x)^{1/3}$ is the Fermi momentum. We note the remarkable peculiarity of FCQPT at $T = 0$: this transition is related to spontaneous breaking of gauge symmetry, when the superconducting order parameter $\kappa(\mathbf{p}) = \sqrt{n_0(\mathbf{p})(1 - n_0(\mathbf{p}))}$ has a nonzero value over the region occupied by the fermion condensate, with the entropy $S = 0$ [2, 9], while the gap $\Delta(\mathbf{p})$ vanishes provided that $\lambda \to 0$ [8, 9]. Thus the state with FC cannot exist at any finite temperatures and driven by the parameter x: at $x > x_{FC}$ the system is on the disordered side of FCQPT; at $x = x_{FC}$, Eq. (6) possesses the non-trivial solutions $n_0(\mathbf{p})$ with $p_i = p_F = p_f$; at $x < x_{FC}$, the system is on the ordered side [2].

At finite temperatures $0 < T \ll T_f$, the function $n_0(\mathbf{p})$ determines the entropy $S_{NFL}(T)$ of the heavy electron liquid in its NFL state

$$S_{NFL}[n(p)] = -2\int [n(\mathbf{p}, T)\ln n(\mathbf{p}, T) + (1 - n(\mathbf{p}, T)) \times \ln(1 - n(\mathbf{p}, T))]\frac{d\mathbf{p}}{(2\pi)^3}, \tag{7}$$

with T_f being the temperature at which the influence of FC vanishes [8, 9]. Inserting into Eq. (7) the function $n_0(\mathbf{p})$, one can check that behind the point of FCQPT there is a temperature independent contribution $S_0(r) \propto \propto (p_f - p_F) \propto |r|$, where $r = x_{FC} - x$. Another specific contribution is related to the spectrum $\varepsilon(\mathbf{p})$ which insures the connection between the dispersionless region $(p_f - p_i)$ occupied by FC and the normal quasiparticles located at $p < p_i$ and at $p > p_f$, and therefore it is of the form $\varepsilon(\mathbf{p}) \sim (p - p_f)^2 \sim (p_i - p)^2$. Such a form of the spectrum can be verified in exactly solvable models for systems with FC and leads to the contribution of this spectrum to the specific heat $C \sim \sqrt{T/T_f}$ [4]. Thus at $0 < T \ll T_f$, the entropy can be approximated as

$$S_{NFL}(T) \simeq S_0(r) + a\sqrt{\frac{T}{T_f}} + b\frac{T}{T_f}, \qquad (8)$$

with a and b are constants. The third term on the right hand side of Eq. (8) comes from the contribution of the temperature independent part of the spectrum $\varepsilon(\mathbf{p})$ and gives a relatively small contribution to the entropy.

The temperature independent term $S_0(r)$ determines the specific NFL behavior of the system. For example, the thermal expansion coefficient $\alpha(T) \propto x\partial(S/x)/\partial x$ determined mainly by the contribution coming from $S_0(r)$ becomes constant at $T \to 0$ [11], while the specific heat $C = T\partial S(T)/\partial T \simeq (a/2)\sqrt{T/T_f})$. As a result, the Grüneisen ratio $\Gamma(T)$ diverges as $\Gamma(T) = \alpha(T)/C(T) \propto \propto \sqrt{T_f/T}$.

We see that at $0 < T \ll T_f$, the heavy electron liquid behaves as if it were placed at QCP, in fact it is placed at the quantum critical line $x < x_{FC}$, that is the critical behavior is observed at $T \to 0$ for all $x \leq x_{FC}$. At $T \to 0$, the heavy electron liquid undergoes a first-order quantum phase transition because the entropy is not a continuous function: at finite temperatures the entropy is given by Eq. (8), while $S(T = 0) = 0$. Therefore, the entropy undergoes a sudden jump $\delta S = S_0(r)$ in the zero temperature limit. We make up a conclusion that due to the first order phase transition, the critical fluctuations are suppressed at the quantum critical line and the corresponding divergences, for example the divergence of $\Gamma(T)$, are determined by the quasiparticles rather than by the critical fluctuations as one could expect in the case of CQPT, see e.g. [1]. Note that according to the well known inequality, $\delta Q \leq T\delta S$, the heat δQ of the transition from the ordered phase to the disordered one is equal to zero, because $\delta Q \leq S_0(r)T \to 0$ at $T \to 0$.

To study the nature of the abrupt change in the Hall coefficient, we consider the case when the LFL behavior arises by the suppression of the AF phase upon applying a magnetic field B, for example, as it takes place in the HF metals $YbRh_2Si_2$ and $YbRh_2(Si_{0.95}Ge_{0.05})_2$ [12, 13]. The AF phase is represented by the heavy electron LFL, with the entropy vanishing as $T \to 0$. For magnetic fields exceeding the critical value B_{c0} at which the Néel temperature $T_N(B \to B_{c0}) \to 0$ the weakly ordered AF phase transforms into weakly polarized heavy electron LFL. At $T = 0$, the application of the magnetic field B splits the FC state occupying the region $(p_f - p_i)$ into the Landau levels and suppresses the superconducting order parameter $\kappa(\mathbf{p})$ destroying the FC state. Such a state is given by the multiconnected Fermi sphere, where the smooth quasiparticle distribution function $n_0(\mathbf{p})$ in the $(p_F - p_i)$ range is replaced by a multiconnected distribution. Therefore the LFL behavior is restored being represented by the weakly polarized heavy electron LFL and characterized by quasiparticles with the effective mass $M^*(B)$ [2, 14]

$$M^*(B) \propto \frac{1}{\sqrt{B - B_{c0}}}. \qquad (9)$$

At elevated temperatures $T > T^*(B - B_{c0}) \propto \sqrt{B - B_{c0}}$, the NFL state is restored and the entropy of the heavy electron liquid is given by Eq. (8). This behavior is displayed in the $T - B$ phase diagram shown in Fig.1.

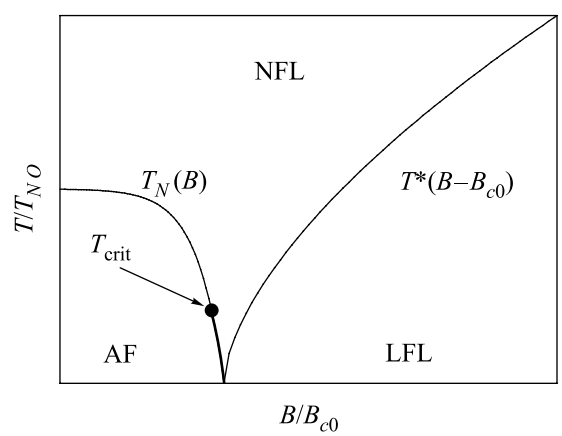

Fig.1. $T - B$ phase diagram of the heavy electron liquid. The $T_N(B)$ curve represents the field dependence of the Néel temperature. Line separating the AF and the NFL state is a guide to the eye. The black dot at $T = T_{crit}$ shown by the arrow is the critical temperature at which the second order AF phase transition becomes the first one. At $T < T_{crit}$, the thick solid line represents the field dependence of the Néel temperature when the AF phase transition is of the first order. The NFL state is characterized by the entropy S_{NFL} given by Eq. (8). Line separating the NFL state and the weakly polarized heavy electron LFL is $T^*(B - B_{c0}) \propto \sqrt{B - B_{c0}}$

In accordance with experimental facts we assume that at relatively high temperatures $T/T_{NO} \sim 1$ the AF phase transition is of the second order [12]. Where T_{NO} is the Néel temperature in the absence of the magnetic field. In that case, the entropy and the other thermodynamic functions are continuous functions at the transition temperature $T_N(B)$. This means that the entropy of the AF phase $S_{AF}(T)$ coincides with the entropy of the NFL state given by Eq. (8),

$$S_{AF}(T \to T_N(B)) = S_{NFL}(T \to T_N(B)). \qquad (10)$$

Since the AF phase demonstrates the LFL behavior, that is $S_{AF}(T \to 0) \to 0$, Eq. (10) cannot be satisfied at sufficiently low temperatures $T \leq T_{\text{crit}}$ due to the temperature-independent term $S_0(r)$, see Eq. (8). Thus, the second order AF phase transition becomes the first order one at $T = T_{\text{crit}}$ as it is shown in Fig.1. At $T = 0$, the critical field B_{c0} at which the AF phase becomes the heavy LFL is determined by the condition that the ground state energy of the AF phase coincides with the ground state energy $E[n_0(\mathbf{p})]$ of the heavy LFL, that is the ground state of the AF phase becomes degenerated at $B = B_{c0}$. Therefore, the Néel temperature $T_N(B \to B_{c0}) \to 0$, and the behavior of the effective mass $M^*(B \geq B_{c0})$ is given by Eq. (9), that is $M^*(B)$ diverges when $B \to B_{c0}$. We note that the corresponding quantum and thermal critical fluctuations vanish at $T < T_{\text{crit}}$ because we are dealing with the first order AF phase transition. We can also safely conclude that the critical behavior observed at $T \to 0$ and $B \to B_{c0}$ is determined by the corresponding quasiparticles rather than by the critical fluctuations accompanying second order phase transitions. When $r \to 0$ the heavy electron liquid approaches FCQPT from the ordered phase. Obviously, $T_{\text{crit}} \to 0$ at the point $r = 0$, and we are led to the conclusion that the Néel temperature vanishes at the point when the AF second order phase transition becomes the first order one. As a result, one can expect that the contributions coming from the corresponding critical fluctuations can only lead to the logarithmic corrections to the Landau theory of the phase transitions [15], and the power low critical behavior is again defined by the corresponding quasiparticles.

Now we are in position to consider the recently observed jump in the Hall coefficient at $B \to B_{c0}$ in the zero temperature limit [7]. At $T = 0$, the application of the critical magnetic field B_{c0} suppressing the AF phase (with the Fermi momentum $p_{AF} \simeq p_F$) restores the LFL with the Fermi momentum $p_f > p_F$. At $B < B_{c0}$, the ground state energy of the AF phase is lower then that of the heavy LFL, while at $B > B_{c0}$, we are dealing with the opposite case, and the heavy LFL wins the competition. At $B = B_{c0}$, both AF and LFL have the same ground state energy being degenerated . Thus, at $T = 0$ and $B = B_{c0}$, the infinitesimal change in the magnetic field B leads to the finite jump in the Fermi momentum. In response the Hall coefficient $R_H(B) \propto 1/x$ undergoes the corresponding sudden jump. Here we have assumed that the low temperature $R_H(B)$ can be considered as a measure of the Fermi volume and, therefore, as a measure of the Fermi momentum [7]. As a result, we obtain

$$\frac{R_H(B = B_{c0} - \delta)}{R_H(B = B_{c0} + \delta)} \simeq 1 + 3\frac{p_f - p_F}{p_F} \simeq 1 + d\frac{S_0(r)}{x_{FC}}. \qquad (11)$$

Here δ is infinitesimal magnetic field, $S_0(r)/x_{FC}$ is the entropy per one heavy electron, and d is a constant, $d \sim 5$. It follows from Eq. (11) that the abrupt change in the Hall coefficient tends to zero when $r \to 0$ and vanishes when the system in question is on the disordered side of FCQPT.

As an application of the above consideration we study the $T-B$ phase diagram for the HF metal $YbRh_2Si_2$ [12] shown in Fig.2. The LFL behavior is characterized by

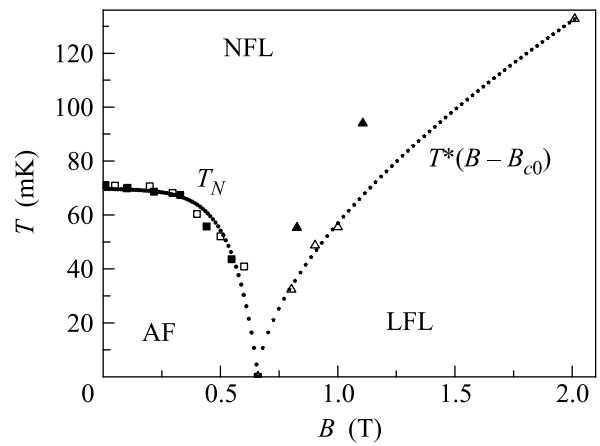

Fig.2. $T - B$-phase diagram for $YbRh_2Si_2$. The T_N curve represents the field dependence of the Néel temperature. Line separating the AF and the NFL state is a guide to the eye. The NFL state is characterized by the entropy S_{NFL} given by Eq. (8). Line separating the NFL state and the LFL is $T^*(B - B_{c0}) = c\sqrt{B - B_{c0}}$, with c being an adjustable factor

the effective mass $M^*(B)$ which diverges as $1/\sqrt{B - B_{c0}}$ [12]. We can conclude that Eq. (9) gives good description of this experimental fact, and $M^*(B)$ diverges at the point $B \to B_{c0}$ with $T_N(B = B_{c0}) = 0$. It is seen from Fig.2, that the line separating the LFL state and NFL can be approximated by the function $c\sqrt{B - B_{c0}}$ with c being a parameter. Taking into account that the behavior of $YbRh_2Si_2$ strongly resembles the behavior of $YbRh_2(Si_{0.95}Ge_{0.05})_2$ [13, 16, 17], we can conclude

that in the NFL state the thermal expansion coefficient $\alpha(T)$ does not depend on T and the Grüneisen ratio as a function of temperature T diverges [13]. We are led to the conclusion that the entropy of the NFL state is given by Eq. (8). Taking into account that at relatively high temperatures the AF phase transition is of the second order [12], we predict that at lower temperatures this becomes the first order phase transition. Then, the described behavior of the Hall coefficient $R_H(B)$ is in good agreement with experimental facts [7].

In summary, we have shown that the $T-B$ phase diagram of the heavy electron liquid with FC is in good agreement with the experimental $T-B$ phase diagram obtained in measurements on the HF metals $YbRh_2Si_2$ and $YbRh_2(Si_{0.95}Ge_{0.05})_2$. We have also demonstrated that the abrupt jump in the Hall coefficient $R_H(B)$ is determined by the presence of FC. We observed that at decreasing temperatures $T \leq T_{\rm crit}$, the second order AF phase transition becomes the first order one, making the corresponding quantum and thermal critical fluctuations vanish at the jump. Therefore, the abrupt jump and the divergence of the effective mass taking place at $T_N \to 0$ are defined by the behavior of quasiparticles rather than by the corresponding thermal and quantum critical fluctuations.

This work was supported by Russian Foundation for Basic Research, Grant # 05-02-16085.

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