Low-temperature thermodynamics of the heavy-fermion metal YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ within a topological scenario for the quantum critical point

V A Khodel$^{1,2}$, J W Clark$^2$ and M V Zverev$^1$

$^1$ Russian Research Centre Kurchatov Institute, Moscow, 123182, Russia
$^2$ McDonnell Center for the Space Sciences & Department of Physics, Washington University, St. Louis, MO 63130, USA

E-mail: vak@wuphys.wustl.edu, jwc@wuphys.wustl.edu, zverev@mbslab.kiae.ru

Abstract. We describe a topological scenario for the quantum critical point signaled by a divergent density of states at zero temperature, in which the Landau quasiparticle picture survives but the topology of the Fermi surface is altered. Predictions of this scenario for thermodynamic properties of the heavy-fermion metal YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ are shown to be in agreement with available experimental data, whereas the conventional scenario based on critical fluctuations of a collective mode fails to explain these properties.

According to the theory of second-order magnetic phase transitions, when the temperature is close to the critical value $T_N$, the Sommerfeld ratio $\gamma(T) = C(T) / T$ has a singular part behaving as $(T - T_N)^{-\alpha}$ that is universal across different materials. The critical index $\alpha$ becomes positive in the domain of a quantum phase transition [1] in which quantum fluctuations come into play. If this behavior holds as $T_N \to 0$, then the end point belongs to a family of quantum critical points (QCP) where $\gamma(T = 0)$ diverges.

On the other hand, at $T \to 0$ the properties of metals whose ground states exhibit no symmetry violation must obey Fermi liquid (FL) theory. In homogeneous matter, $\gamma(T \to 0)$ is a constant proportional to the density of states $N(0)$, or equivalently the effective mass $M^*$. It is a commonly accepted view, dating back to Ref. [2], that $M^*$ diverges at points of $T = 0$ second-order phase transitions due to vanishing of the quasiparticle weight $z$ in single-particle states at the Fermi surface. However, the derivations of this result ignore the scattering of the fluctuations themselves, an effect of crucial importance at the transition point [3, 4].

There exists alternative scenario, in which the Fermi velocity $v_F \sim 1 / M^*$ vanishes and changes its sign at a critical density $\rho_\infty$, while $z$ remains finite. (For more detail, see Ref. [3] and references therein.) Consequently, beyond the QCP the number of roots of the equation $\epsilon(p) = 0$ increases from the single solution $p = p_F$, giving rise to a rearrangement of the Fermi surface. (As is convenient, the single-particle energy $\epsilon(p)$ is measured from the Fermi surface.) The choice between this topological scenario and the conventional picture based on critical fluctuations can in principle be informed by analysis of the experimental data on selective materials. However, such data is scarce, except for measurements of excellent quality on a family of Yb-based heavy-fermion metals [5, 6, 7, 8, 9, 10].

We focus here on a compound YbRh$_2$(Si$_{1-x}$Ge$_x$)$_2$ located extremely close to the QCP, i.e., the
end point of the line $T_N(B)$, with $T_N(B_{c0}) = 0$ corresponding to $B_{c0} = 0.027$ T [5]. We restrict the analysis to thermodynamic properties, which depend primarily on heavy carriers relevant to the QCP. We employ a model in which 2D electron liquid moves in a quadratic lattice, assuming the electron Fermi line to be approximately a circle with the origin shifted to $(\pi/a, \pi/a)$.

In this anisotropic case, the normal component $v_n(p)$ of the group velocity $v = \partial \epsilon(p)/\partial p$, having direct bearing on the QCP, is determined by the Landau equation[11]

$$\frac{\partial \epsilon(p)}{\partial p_n} = \frac{\partial \epsilon_0^p}{\partial p_n} + \int f(p, p_1) \frac{\partial n(p_1)}{\partial p_{1n}} d\tau, \quad (1)$$

where $\epsilon_0^p$ is the bare single-particle spectrum, $f(p, p_1)$ is the spin-independent component of the interaction function, and $d\tau$ is the volume element in momentum space. At the topological QCP, $v_n(p)$ vanishes at a momentum with coordinates $p = p_\infty$, $\phi = 0$. Close to the QCP one finds

$$v_n(p, \phi; \rho) = a_p (p - p_\infty)^2 + a_\phi \phi^2 + a_\rho (\rho - \rho_\infty), \quad (2)$$

wherein the terms linear in $p - p_\infty$ and $\phi$ are absent for the normal component of the group velocity to vanish for the first time at $\rho = \rho_\infty$, while the last term ensures FL behavior on the disordered side of the QCP. The constants $a_p, a_\phi$, and $a_\rho$ are calculated numerically.

The specific heat $C(T) = T dS/dT \sim T N(T)$, thermal expansion coefficient $\beta(T) \sim -\partial S(T, \rho)/\partial P \sim -T \partial N(T, \rho)/\partial \rho$, and Gr"uneisen ratio $\Gamma(T, \rho_\infty) = \beta(T, \rho_\infty)/C(T, \rho_\infty)$ are all determined by the density-of-states integral

$$N(T, \rho) \propto \int n(\epsilon) (1 - n(\epsilon)) \frac{d\epsilon}{v_n(\epsilon, \phi; \rho)}, \quad (3)$$

where $n(\epsilon) = [1 + \exp(\epsilon/T)]^{-1}$. The overwhelming contributions to this integral come from a domain of small $\epsilon$ and $\phi$, yielding $N(T) \propto T^{-1/3}$; accordingly, we find

$$C(T, \rho_\infty) \propto T^{2/3}, \quad \beta(T, \rho_\infty) \propto O(1), \quad \Gamma(T, \rho_\infty) \propto T^{-2/3}. \quad (4)$$

In obtaining these results we employ the results $p(\epsilon, \phi = 0) - p_\infty \sim \epsilon^{1/3}$ and $v_n(\epsilon, \phi = 0) \sim \epsilon^{2/3}$, derived from Eq. (2). This extends an analogous result derived for the isotropic FL [12] to the present anisotropic case. We emphasize that the agreement between the predicted theoretical behaviors (4) and those discovered experimentally [6] is a primary requirement for the viability of the anisotropic model (2) and provides a strong basis for its choice over competing models.

Imposition of an external magnetic field $B$ splits the original Fermi line into two lines determined by the equations

$$\epsilon(p^\pm(\phi)) \pm \mu_e B = 0. \quad (5)$$

Field-free FL relations such as Eq. (3) are modified through replacement of the quantity $v_n^{-1}$ by the sum of quantities $(\partial \epsilon(p, \phi)/\partial p_n)^{-1}$, evaluated at $\epsilon(p, \phi) \pm \mu_e B$.

We analyze only the FL side of the QCP, assuming $B > B_c$. In this case, at $r = \mu_e B/T \ll 1$, terms in Eq. (3) linear in $r$ cancel each other upon integration over $\phi$ [4]. In particular, one finds $\partial \beta/\partial B \propto r$ and $\partial S/\partial B = \partial M/\partial T \sim r$, where $M$ is the magnetization. Thus at high $T$ where $C(T, B) \propto T$, one obtains

$$\Gamma_{\text{mag}}(T, r \ll 1) \propto T^{-1} r = B T^{-2} \quad (6)$$

for the magnetic Gr"uneisen ratio $\Gamma_{\text{mag}}(T, B) = - (\partial S(T, B)/\partial B)/C(T, B)$.

In the opposite limit $T \rightarrow 0$, the density of states $N(T = 0, B)$ diverges at $B_\infty > 0$ provided the function $v_n(p, \phi, T = 0, B_\infty)$ vanishes on one of the two Fermi lines, say at $p^+(\phi)$ with
\( \phi = 0 \). At \( T = 0, B > B_\infty \), the critical quantity \( v_n(\epsilon = 0, p^+(\phi = 0); T = 0, B) = v_n^+(b) \), with \( b = B - B_\infty \), becomes positive, and FL behavior is recovered, as in the isotropic case [13, 12]. In the present case, integration over \( \phi \) yields \( N(T = 0, b) \approx 1/\sqrt{v_n^+(b)} \). To evaluate \( v_n^+(b) \), we write Eq. (1) twice, first at \( B \) and then at \( B_\infty \), where \( v_n^+(0) = 0 \). Subtracting one result from the other we have
\[
\frac{v_n^+(b)}{\sqrt{v_n^+(b)}} = \int (F(\phi, b) - F(\phi, 0)) \frac{d\phi}{2\pi},
\]
where \( F(\phi, b) = f(p^+(\phi = 0, b), p^+(\phi, b))p^+(\phi, b) \). On the r.h.s. of this equation, we retain only a leading term proportional to \( p^+(\phi, b) - p^+(\phi, 0) \). Then, replacing this difference from Eq. (5) by \( b/(v_n^+(b) + a_\phi \phi^2) \), the angular integration can be performed analytically to find \( v_n^+(b) \propto b/\sqrt{v_n^+(b)} \), yielding \( v_n^+(b) \propto b^{-3/2} \). Thus we arrive at
\[
N(0, b) \propto b^{-1/3}, \quad C(T \to 0, b) = S(T \to 0, b) \propto T b^{-1/3}.
\]
We also find \( \partial S(T \to 0, b)/\partial B = T/3 b^{4/3} \) and
\[
\Gamma_{\text{mag}}(T \to 0, b) = \frac{1}{3} b^{-1}.
\]
Such a divergence was first predicted within scaling theory [14], in which the peak of \( \Gamma_{\text{mag}}(T \to 0, B) \) is located at \( B_{c0} \). In principle, \( B_\infty \) may not coincide with \( B_{c0} \); this issue will be considered in further work.

At finite \( T \), the equation for the critical quantity \( v_n^+(T, b) \) becomes
\[
v_n^+(T, b) = v_n^+(T, 0) + b/\sqrt{v_n^+(T, b)},
\]
where the finite value of \( v_n^+(T, 0) \propto T^{2/3} \) comes from the term in the group velocity \( v^+(\epsilon, \phi, 0) \propto \epsilon^{2/3} \). Consequently, the density of states \( N(T \neq 0, B_\infty) \) ceases to diverge. The term \( v_n^+(T, 0) \) becomes comparable with the original one at \( T \approx \mu_e b \), with \( \mu_e \approx 4.5 \mu_B \). The line \( T = \mu_e b \) separates two regions of NFL behavior (cf. Fig. 2 of Ref. [15]). At \( \mu_e b \leq T \) the NFL behavior exhibits itself in the \( T \)-dependence of thermodynamics quantities, while at \( \mu_e b \leq T \) such behavior shows up in their dependence on \( B - B_\infty \). With further increase of \( B \), the magnitude of NFL effects declines. As seen from the analysis of the experimental data, these effects die out at \( B \geq 0.3 \mathrm{T} \).

Finally, we examine the magnetic susceptibility \( \chi(T, B) = \partial \mathcal{M}/\partial B \propto N(T, B)(1 + g_0 N)^{-1} \), where \( g_0 \) is the spin-spin component of the interaction function. In the present case, one deals with a long-wavelength antiferromagnetic phase transition, the Stoner factor \( (1 + g_0 N)^{-1} \) being enhanced. Still, it remains finite at the QCP in spite of the divergence (8) of \( N(T = 0, b) \sim b^{-1/3} \), implying that \( g_0(b) \propto b^{1/3} \). Retaining in \( N \) a leading correction independent of \( b \), one finds that before the Stoner factor saturates, it behaves as \( b^{-1/3} \), giving rise to \( \chi(T \to 0, b) \propto b^{-2/3} \) and \( \mathcal{M}(T \to 0, b) \propto b^{1/3} \). These results together with (6), (8), and (9) are in agreement with the available experimental data [6, 7, 8, 9, 10].

These data also provide a test of modern phenomenological scaling theories of the QCP [14]. The outcome of this test, as aired in Ref. [9], is that none of the models based on 2D or 3D fluctuations can describe the data. Thus, while the spin-fluctuation mechanism remains applicable at finite \( T \) close to \( T_N(B) \), it becomes inadequate at the QCP itself.

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