# On the superconducting dome near antiferromagnetic quantum critical points

Mucio A. Continentino*
*Instituto de Física, Universidade Federal Fluminense,*
*Campus da Praia Vermelha, 24210-340, Niterói, RJ, Brazil*

(Dated: December 4, 2018)

One of the most exciting discoveries in strongly correlated systems has been the existence of a superconducting dome on heavy fermions close to the quantum critical point where antiferromagnetic order disappears. It is hard even for the most skeptical not to admit that the excitations which bind the electrons in the Cooper pairs have a magnetic origin. As a system moves away from an antiferromagnetic quantum critical point, (AFQCP) the correlation length of the fluctuations decreases and the system goes into a local quantum critical regime. The attractive interaction mediated by the non-local part of these excitations vanishes and this allows to obtain an upper bound to the superconducting dome around an AFQCP.

## I. INTRODUCTION

The study of heavy fermion materials is an exciting area in physics motivating sophisticated experimental work and giving rise to many new concepts and ideas[1]. In particular the fact that heavy fermions are close to a magnetic quantum critical point[2] has brought a new range of possibilities to this field, both theoretically and experimentally.

On the course of their investigations, as experimentalists aim to reach closer to the AFQCP at even lower temperatures, came out the exciting discovery of a superconducting dome encircling a putative AFQCP[3]. The region of superconductivity in the phase diagram is restricted to a close neighborhood of the AFQCP. Even for the most skeptical it is hard not to admit that in this case superconductivity is due to quantum antiferromagnetic fluctuations associated with the QCP[4].

The theory of superconductivity mediated by spin fluctuations has progressed very much in the last decades mostly due to its relevance for high temperature superconductivity[5,6,7,8,9]. In these theories, the paramagnon propagator describing critical antiferromagnetic fluctuations close to an AFQCP can be written in the scaling form[6],

$$\chi(q,\omega) = \frac{\chi_S}{i\omega\tau + q^2\xi^2 + 1} \tag{1}$$

where $\chi_S = \chi_0/|g|$ is the staggered susceptibility, $\xi = \sqrt{A/|g|}$ and $\tau = \tau_0 \xi^z$ the correlation length and critical relaxation time, respectively. The quantity $g$ measures the distance (in energy scale) to the AFQCP (at $g=0$), $A$ is the stiffness of the spin fluctuations, $\tau_0 = 1/A$ and the dynamic exponent $z=2$. We are interested here in quantum phase transitions which occur in three ($d=3$) or two dimensions ($d=2$). Since the dynamic exponent associated with an AFQCP takes the value[10] $z=2$, the effective dimension associated with the antiferromagnetic quantum phase transition is $d_{eff} = d+2$. Then, for $2d$ and $3d$ systems the effective dimension coincides or is above the upper critical dimension $d_c = 4$, respectively. This implies that the transition at $T=0$, $g=0$ is described by Gaussian or mean-field exponents[11] with logarithmic corrections in the marginal case ($d=2$). Then for $d_{eff} \geq d_c$ the Gaussian exponents, $\gamma = 1$, for the staggered susceptibility and $\nu = 1/2$, for the correlation length turn out to describe correctly the quantum critical behavior of the AFQCP.

The Gaussian free energy close to the AFQCP can be written as $(k_B = 1)$[12,13],

$$f = -\frac{3}{\pi}\sum_q T\int_0^\infty \frac{d\lambda}{e^\lambda - 1}\tan^{-1}\left[\frac{2\pi\lambda T\xi^z}{A(1+q^2\xi^2)}\right] \tag{2}$$

For temperatures $T << T_{coh}$ the free energy is given by,

$$f = -\frac{\pi^2 T^2 \xi^{z-d}}{A}\left(\frac{L}{2\pi}\right)^d S_d \int_0^{q_c\xi} dy \frac{y^{d-1}}{1+y^2} \tag{3}$$

where $q_c$ is a cut-off. The coherence temperature, $T_{coh} = |g|^{\nu z} = |g|$ is that introduced by Continentino et al.[2] and marks the entrance of the system in the Fermi liquid regime. $S_d$ is the surface of a d-dimensional sphere with unit radius. The specific heat $C/T = -\partial^2 f/\partial T^2$ in the Fermi liquid regime, $T << T_{coh}$, is easily obtained,

$$C/T = \frac{V/\xi}{A} q_c\xi\left(1 - \frac{\tan^{-1} q_c\xi}{q_c\xi}\right) \tag{4}$$

in $3d$ and,

$$C/T = \frac{\pi S_2}{2A}\ln\left(1 + q_c^2\xi^2\right) \tag{5}$$

in $2d$. In the critical regime $q_c\xi \gg 1$, we get that $\gamma = C/T$ is constant in $3d$ and logarithmically divergent in $2d$[12]. We can also define[13,14] a *local limit*, $q_c\xi < 1$, in which case the specific heat is given by,

$$C/T = \frac{2\pi^2 N}{T_{coh}} \tag{6}$$

independent of dimension. This result can be obtained directly from Eq. 2 neglecting its q-dependence and replacing $\sum_q \to N$. The propagator associated with these local spin fluctuations is given by,

$$\chi_L(\omega) = \frac{\chi_S}{i\omega\tau + 1} \tag{7}$$

with $\chi_S = \chi_0/|g|$ and $\tau = \tau_0\xi^z$. It is remarkable that in spite of the local character of the fluctuations in this regime, the system is still *aware* of the quantum phase transition through the dependence of $\tau$ and $\chi_S$ on $g$. Indeed, in this regime the fluctuations are local in space but correlated along the *time directions*. The theory of this regime can be described as a critical theory in $d_{eff} = z = 2$ but with Euclidean dimension $d = 0$. The properties of the system for $q_c\xi < 1$ have been described in Ref.[13]. They can all be expressed in terms of a single parameter, the coherence temperature[13].

## II. RELATION TO SUPERCONDUCTIVITY

The q-dependent propagator given by Eq. 1 provides an attractive interaction in the singlet channel among quasi-particles in neighboring sites. Thus, antiferromagnetic paramagnons can give rise to d-wave pairing with $d_{x^2-y^2}$ symmetry[6], for $q_c\xi \gg 1$. What about local spin fluctuations?

The spatial dependence of the dynamic susceptibility can be obtained from the Fourier transform of the $q$ and $\omega$ dependent propagator,

$$\chi(r,\omega) = \sum_q \chi(q,\omega) e^{iq.r}. \tag{8}$$

In the case of local spin fluctuations, the relevant propagator is given by Eq. 7, such that,

$$\Re e \chi_L(\omega) = \frac{\chi_S}{1+\omega^2\tau^2}, \tag{9}$$

and,

$$\Re e \chi_L(\omega = 0) = \chi_S.$$

Then,

$$\chi(r) = \chi_S \sum_q e^{iq.r} = 2\pi\chi_S \int dq d\theta q^2 \sin\theta e^{iqr\cos\theta}.$$

The interaction among the quasi-particles according to Monthoux et al.[4] is given by:

$$\begin{aligned} U(r) &= -\lambda^2 \chi(r) S_1.S_2 \qquad (10)\\ &= -\lambda^2(-1)\frac{8\pi^4\chi_S}{a^3}\frac{1}{(\frac{\pi r}{a})^3}\left\{\sin\frac{\pi r}{a} - \frac{\pi r}{a}\cos\frac{\pi r}{a}\right\}. \end{aligned}$$

For small $r$ this yields,

$$\begin{aligned} U(r\to 0) &= 8\pi\frac{\lambda^2}{r^3}\chi_S\frac{1}{3}\frac{\pi^3}{a^3}r^3 = \frac{8}{3}\frac{\pi^4}{a^3}\lambda^2\chi_S\\ U(a) &= 8\frac{\pi^2}{a^3}\lambda^2\chi_S\\ U(2a) &= -2\frac{\pi^2}{a^3}\lambda^2\chi_S \end{aligned} \tag{11}$$

If we are dealing with a lattice then we have a delta-function at the origin. The potential is repulsive at the origin and zero everywhere else in the singlet channel.

Also, it is interesting to obtain the results in the case the local propagator is associated with density fluctuations. In this case[6],

$$U(r) = -\lambda^2\chi(r)$$

and we obtain,

$$\begin{aligned} U(r\to 0) &= -8\pi\frac{\lambda^2}{r^3}\chi_S\frac{1}{3}\frac{\pi^3}{a^3}r^3 = -\frac{8}{3}\frac{\pi^4}{a^3}\lambda^2\chi_S\\ U(a) &= -8\frac{\pi^2}{a^3}\lambda^2\chi_S\\ U(2a) &= 2\frac{\pi^2}{a^3}\lambda^2\chi_S \end{aligned} \tag{12}$$

where $\chi_S$ in this case is the compressibility. In the case of a lattice the interaction is attractive at the origin and zero everywhere else in the singlet channel.

In the magnetic case, Eqs. 11 show that the on-site and nearest neighbor quasi-particle interaction mediated by critical local spin fluctuations are repulsive in the singlet channel and do not lead to Cooper pair formation. Then, as the system moves away from the AFQCP, the correlation length of the spin fluctuations decreases and for $q_c\xi \sim 1$ the relevant interactions mediated by these fluctuations become repulsive everywhere destroying superconductivity. On the other hand, local charge fluctuations can still mediate an attractive local interaction.

The condition

$$q_c\xi = 1 \tag{13}$$

puts an upper limit to the region of the phase diagram around the AFQCP where superconductivity mediated by spin fluctuations can exist. At zero temperature this implies that superconductivity survives up to a critical coupling $|g|_S = Aq_c^2$.

In order to extend Eq. 13 to finite temperatures ($T$), we consider the scaling form of the correlation length, $\xi = \sqrt{A}|g|^{-\nu}F[T/T_{coh}]$, where $F[t]$ is a scaling function and $T_{coh} = |g|^{\nu z}$. In this case Eq. 13 can be written as,

$$F\left[\frac{T_D}{|g|^{\nu z}}\right] = \frac{\sqrt{|g|}}{\sqrt{A}q_c} \tag{14}$$

where $T_D(g)$ represents an upper limit for superconductivity around the AFQCP.

The scaling function $F(t)$ has a well known behavior in two limiting cases. First, $F(t\to 0) \propto 1-t^2+O\left(t^4\right)$, such that $F(0) = 1$ and for $t \ll 1$, i.e., $T \ll T_{coh}$ this yields a Fermi liquid behavior for the staggered susceptibility which in the spin fluctuation theory is used to define the correlation length[12]. Also, neglecting the effect of dangerously irrelevant interactions (to be discussed below), $F(t\to\infty) \propto t^x$ where the exponent $x$ is determined by the condition that the dependence of the correlation

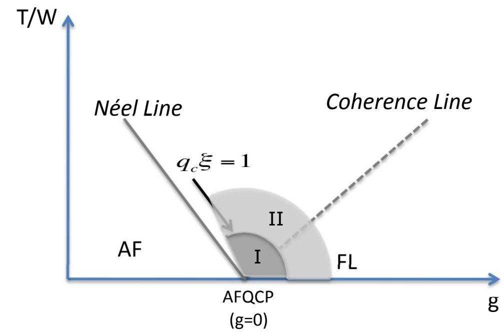


FIG. 1: (Color online) The line $q_c\xi(T_D) = 1$ represents an upper limit where superconductivity induced by antiferromagnetic spin fluctuations can occur. It's equation is $T_D = |g|^{\nu z} G^{-1}[|g|/Aq_c^2]$ (see equation 14) and is plotted schematically in the figure. It separates region I with $q_c\xi \gg 1$ from region (II) of local quantum criticality where fluctuations are critical in the time directions but local in space. The latter gives rise to repulsive, on-site and nearest neighbors interactions (see text).

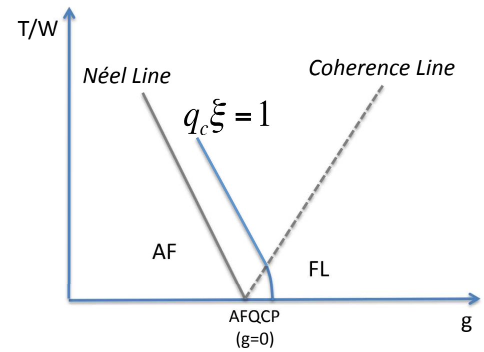


FIG. 2: (Color online) Line of constant correlation length ($q_c\xi = 1$) when thermal or interacting antiferromagnetic spin fluctuations are taken into account.

length on $g$ cancels out. This yields $x = -1/z$, such that, at the quantum critical trajectory ($g = 0$, $T \to 0$), the correlation length diverges as $\xi \propto T^{-1/z}$. We can also show using this asymptotic behavior of the scaling function that the point in the phase diagram at which the superconducting temperature can attain its maximum value is just above the AFQCP, i.e., at $g = 0$. In fact $dT_D/dg \propto |g|^{z/2}$ and vanishes at $g = 0$.

An interpolation formula for the scaling function which gives correct results on both limits ($t \to 0$ and $\infty$) is given by,

$$F(t) = \frac{1}{(1+t^2)^{1/4}}, \tag{15}$$

where we used the value of the exponents $\nu = 1/2$ and $z = 2$. Using this expression for the scaling function, Eq. 13 can be written as,

$$\sqrt{T_D^2 + |g|^2} = Aq_c^2. \tag{16}$$

This has the form of a dome as shown in Fig. 1. This equation provides a reasonable interpolation for the lines of constant correlation length in the region of the phase diagram $g \geq 0$. For negative ($g < 0$), there may be thermal fluctuations that change the scaling behavior of the correlation length, as will be discussed below. The physical significance of $T_D$ is now quite clear. It provides an upper limit to the region where superconductivity induced by quantum antiferromagnetic spin fluctuations can exist. While for $T \approx 0$ this may provide a reasonable estimate of the actual superconducting region and its shape, for larger temperatures thermal fluctuations should reduce the critical temperature $T_s$ to values well below $T_D$.

In the theory of the AFQCP for $d_{eff} \geq d_c$, the quartic interaction $u$ is *dangerously irrelevant*[15]. It determines the shape of the Neel line and changes the value of the shift exponent $\psi$ from the expected scaling result, $\psi = \nu z$, to $\psi = z/(d + z - 2)$ (for the AFQCP in 3d, $\psi = 2/3$)[15]. The scaling expression for the correlation length can be immediately generalized to include the effect of the quartic interaction $u$. It is given by[11]

$$\xi = \sqrt{A}|g(T)|^{-\nu} G\left[\frac{T}{|g(T)|^{\nu z}}\right] \tag{17}$$

In this equation $g(T) = g - uT^{1/\psi}$, such that, $g(T_N) = 0$ gives the equation for the Néel line. The scaling function $G(t)$ has the following asymptotic behaviors; $G(t = 0) = 1$ to reproduce the previous zero temperature results, and $G(t \to \infty) = t^{\frac{\tilde{\nu}-\nu}{\nu z}}$. The latter guarantees the correct behavior close to the critical Néel line $g(T_N) = 0$, i.e., $\xi = Q(T)|g(T))|^{-\tilde{\nu}}$, with the amplitude $Q(T) = \sqrt{A}T^{\frac{\tilde{\nu}-\nu}{\nu z}}$. When $T \to T_N$, $g(T) \to 0$ and the correlation length diverges with the thermal correlation length exponent $\tilde{\nu}$. Assuming[15], $\tilde{\nu} = \nu = 1/2$, we get at $g = 0$,

$$\xi = \sqrt{\frac{A}{u}}T^{-1/3} \tag{18}$$

For $g = 0$, this yields a temperature for the dome at $g = 0$, $T_D^u(g = 0) = \left(Aq_c^2/u\right)^{3/2}$, to be compared with $T_D(g = 0) = Aq_c^2$, obtained previously. This leads to $T_D = u(T_D^u)^{2/3}$ and since $u$ is a small number, we expect that in general $T_D \ll T_D^u$, such that, non-Gaussian fluctuations allow in principle for larger critical superconducting temperatures just above the AFQCP. However, in this case the lines of constant $\xi$ satisfying Eq. 13 should follow closely the Néel line as in Fig.2. The experimental results show however that the superconducting region has a dome shape[3]. Then, they seem to imply that only purely Gaussian quantum fluctuations are effective in pairing the quasi-particles. Also notice that along the Néel line, for $T \neq 0$, the quartic interaction is a *relevant* interaction[11]. Then, as the spin fluctuations start to interact they apparently loose their efficacy in pairing the quasi-particles. At least this is what the experiments seem to imply.

In some heavy fermion systems as one moves away from the AFQCP, for example, applying pressure in the system there is a second superconducting dome[17,18]. This is generally attributed to pairing due to charge fluctuations associated with a valence transition[18]. This second dome is larger than that associated with the AFQCP extending in a wider region of pressures and temperature. As pointed out before in the case of pairing by charge fluctuations the interaction is attractive when the system is in the regime of local quantum criticality. So, we expected that in this case, superconductivity can occur in a larger region of the phase diagram around the relevant quantum critical point, as is in fact observed.

The energy scale of the *magnetic glue* that fixes the region where superconductivity can exist is given by $Aq_c^2$. $A$ is the stiffness of the spin fluctuations and $q_c$ a cutoff appropriate for a hydrodynamic description of these modes. This quantity plays a role similar to the Debye energy in BCS superconductors.

The region of the phase diagram just above the limiting superconducting dome is a state of *local quantum criticality.* This state is characterized by a single energy scale, the coherence temperature, $T_{coh} = |g|^{\nu z}$. It has a resistivity which scales as $\rho \propto (T/T_{coh})^2$ for $T \ll T_{coh}$ and as $\rho \propto (T/T_{coh})$ for $T \gg T_{coh}$. In the case of anisotropic lattices, the crossover to the local regime occurs in stages. For a tetragonal system with a spectrum of spin fluctuations given by, $a_{xy}q_x^2 + a_{xy}q_y^2 + a_z q_z^2$, as the system moves away from the AFQCP it goes from $d = 3$ to $d = 2$ and finally to $d = 0$ quantum critical behavior.

The dome shape of the superconducting region seems to indicate that the interaction between the spin fluctuations acts in detriment of superconductivity. It can not be excluded that interacting spin fluctuations can still provide a pairing mechanism to produce, for example, a pseudo-gap state, but not superconductivity. We have shown quite generally that if Gaussian quantum spin fluctuations give rise to superconductivity, the maximum allowed $T_c$ can be found just above the AFQCP. Finally, our results strongly support the proposal that the second superconducting dome observed in some heavy fermions systems is due to pairing by charge fluctuations. Since even in the local quantum regime, charge fluctuations give rise to attractive interactions, superconductivity in this case can extend over a wider region of the phase diagram.

Our results are appropriate to describe the system in the paramagnetic region. In the long range ordered magnetic phase of the diagram there are new excitations, the spin waves, associated with transverse modes. Then in this region the present approach does not provide any insight.

**Acknowledgments**

I would like to thank Dr. P. Monthoux for invaluable discussions. This work is partially supported by the Brazilian agencies CNPq and FAPERJ.

---

[*] Electronic address: mucio@if.uff.br


[1] Philipp Gegenwart, Qimiao Si, Frank Steglich, Nature Physics **4**, 186 (2008); Tuson Park, F. Ronning, H. Q. Yuan, M. B. Salamon, R. Movshovich, J. L. Sarrao, J. D. Thompson, Nature **440**, 65 (2006).

[2] M. A. Continentino, G. Japiassu, A. Troper, Phys. Rev. B 39, 9734 (1989); M. A. Continentino, J. de Physique, **I**, 693 (1991); M.A. Continentino, Phys. Rev. B 47, 11587 (1993); M. A. Continentino, Phys. Rep. 239, 179 (1994); M.A. Continentino, Zeitschrift für Physik B 101, 197 (1996).

[3] N. D. Mathur, F. M. Grosche, S. R. Julian, I. R. Walker, D. M. Freye, R. K. W. Haselwimmer, G. G. Lonzarich, Nature 394, 39 (1998).

[4] P. Monthoux, D. Pines and G. G. Lonzarich, Nature, **450**, 1177 (2007).

[5] P. Monthoux, A. V. Baltsky, D. Pines, Phys. Rev. Lett. 67, 3448 (1991); Phys. Rev. B 46, 14803 (1992); P. Monthoux and G.G. Lonzarich, Phys. Rev. **B 59**, 14 598 (1999).

[6] P. Monthoux and G.G. Lonzarich, Phys. Rev. **B 63**, 054529 (2001).

[7] P. Monthoux and G. G. Lonzarich, Phys. Rev. **B 69**, 064517 (2004).

[8] P. Monthoux and G. G. Lonzarich, Phys. Rev. **B 66**, 224504 (2002).

[9] Hisashi Kondo, Tôru Moriya, arXiv:0809.4825v2 [cond-mat.str-el], and J. Phys. Soc. Jpn. 78, 013704 (2009); Tetsuya Takimoto and Tôru Moriya, Phys. Rev. **B 66**, 134516 (2002).

[10] John A. Hertz, Phys. Rev. B14, 1165 (1976).

[11] M. A. Continentino, *Quantum Scaling in Many-Body Systems*, WorldScientic, Singapore,(2001); M. A. Continentino, Phys. Rev. B 47, 11587 (1993).

[12] T. Moriya, in *Spin Fluctuations in Itinerant Electron Magnetism* (Springer-Verlag, Berlin Heidelberg, 1985); T. Moriya, T. Takimoto, J. Phys. Soc. Jap. 64, 960 (1995).

[13] M. A. Continentino, Eur. Phys. J. **B 13**, 31 (2000); ibid, JMMM 272-276, 231 (2004); ibid, Phys. Rev. B 57, 5966 (1998).

[14] C. Pinettes and C. Lacroix, J. Phys.-Cond. Matter 6, 10093 (1994); C. Lacroix and C. Pinettes, Physica B 206-207, 11 (1995).

[15] A. J. Millis, Phys. Rev. B 48, 7183 (1993).

[16] In the original spin fluctuation theory of the QCP[12], the coherence temperature is never explicitly introduced. However, it is clearly there, with the same significance that it was first introduced in Ref.[2], as marking the onset of Fermi liquid behavior.

[17] J. Flouquet in W. I. Halperin (Ed.), Progress in Low Temperature Physics, Vol. 15, p.139, Elsevier, Amsterdam (2005).

[18] A. T. Holmes, D. Jaccard and K. Miyake, Phys. Rev. B 69, 024508 (2004).

[19] A. Kopp and S. Chakravarty, Nature Physics 1, 53 (2005).