Possible origin of the pseudogap end point in the high-Tc cuprates

Tao Li
Department of Physics, Renmin University of China, Beijing 100872, P.R.China
(Dated: May 17, 2018)

Recent experiments find that the pseudogap phase of the high-Tc cuprates ends suddenly at an electron doping $x^*$ when the Fermi surface change its shape from hole-like to electron-like. In this short note, we argue that the antiferromagnetic(AF) spin correlation of the system should drop abruptly at the same doping. At the same time, we argue that the critical behavior observed at $x^*$ in the specific heat measurement should be attributed to the strong renormalization of the quasiparticle excitation in the anti-nodal region by the critical AF spin fluctuation.

PACS numbers:

![Graph](image-url)

**FIG. 1:** (Color on-line) The Fermi surfaces for several different values of $x$ around the pseudogap end point $x^*$. The Fermi surface changes its shape from hole-like to electron-like at $x^*$. The red line marks the boundary of the AF Brillouin zone, which intersects the Fermi surface at the hot spots (denoted by blue dots). The hot spots move towards the VHS at $M=(0, \pi)$ or $(\pi, 0)$ as we increase $x$ and disappear altogether when $x > x^*$.

Here $\epsilon_k$ is the dispersion of the quasiparticle. $\vec{s}_i = \frac{1}{2} \sum_{\alpha, \beta} c^\dagger_{i, \alpha} \sigma_{\alpha, \beta} c_{i, \beta}$ is the spin density operator of the itinerant electron. $\vec{S}_i$ is the local moment operator. The dynamics of the local moment is assumed to be described by a phenomenological (inverse) propagator $\chi(q, \omega)$, which peaks at the AF wave vector $Q=(\pi, \pi)$. $g$ is a phenomenological coupling constant between the quasiparticle system and the local moment system, which is expected to be ferromagnetic.

In the spin-Fermion model, the magnetic susceptibility of the system is determined by the coupled response of the local moment system and the quasiparticle degree of freedom. In the spirit of the random phase approximation, the magnetic susceptibility of the system is given by

$$\chi(q, \omega) = \frac{\chi_l + \chi_i - 2g\chi_l\chi_i}{1 - g^2\chi_l\chi_i}.$$
susceptibility of the quasiparticle system at the AF wave vector caused by the scattering off critical AF fluctuation. quasiparticle renormalization effect in the anti-nodal region. We argue that the suppression of quasiparticle excitation will be strongly suppressed when the Fermi surface change its shape from hole-like to electron-like. Indeed, the calculated susceptibility at the AF wave vector, which is plotted in Figure 2, drops abruptly for $x > x^*$. The logarithmic divergence of the AF susceptibility at $x^*$ is caused by the divergence in the effective mass at the VHS. The local moment system by itself is far away from magnetic criticality for $x = x^*$. However, through its coupling to the quasiparticle system, the magnetic response of the local moment system at $x = x^*$ will also be driven into critical. At the same time, the abrupt drop in the AF response of the quasiparticle system for $x > x^*$ will significantly reduce of AF response of the whole system. If the AF fluctuation is indeed the ultimate origin of the pseudogap phenomena, as we argued for in previous work, then the suppression of the AF correlation for $x > x^*$ is very likely the origin of the pseudogap end point at $x^*$. At the same time, the divergence of the AF response of the quasiparticle system at $x^*$ will greatly enhance its coupling to the local moment system, resulting in divergent self-energy correction for the quasiparticle excitation in the anti-nodal region. We believe this is at the origin of the observed critical behavior in the specific heat coefficient at $x^*$. However, we note that the anti-nodal quasiparticle under the scattering of the AF fluctuation is a genuine strongly coupled system as a result of the divergence of effective mass at the VHS. The proximity to the VHS also renders the Migdal theorem strongly violated in the anti-nodal region. These features pose a big challenge for any analytical effort to understand the critical behavior at $x^*$. To make further progress, we now derive a low energy effective theory for the system at $x^*$. The action of the effective theory is given by $S = S_\psi + S_\varphi$, in which

$$S_\psi = \int d\tau d\mathbf{k} \sum_{\alpha=1,2} \psi_{\alpha,\mathbf{k}}^\dagger [\partial_\tau - \epsilon_\alpha(\mathbf{k})] \psi_{\alpha,\mathbf{k}}$$

and

$$S_\varphi = \int d\tau d\mathbf{q} \varphi_{-\mathbf{q}}^\dagger \cdot (\psi_{2,\mathbf{k}+\mathbf{q}}^\dagger \sigma \psi_{1,\mathbf{k}} + \psi_{1,\mathbf{k}+\mathbf{q}}^\dagger \sigma \psi_{2,\mathbf{k}})$$

denotes the effective action of the anti-nodal Fermions. Here we have approximated the Fermion field around the two VHSs at $(0, \pi)$ and $(\pi, 0)$ as independent degree of freedoms. $\psi_{1,\mathbf{k}} = (\psi_{1,\mathbf{k},\uparrow}, \psi_{1,\mathbf{k},\downarrow})^T$ denotes the Fermion field around the $(0, 0)$ point, whose dispersion is given by $\epsilon_1(\mathbf{k}) = (t - 2t')k_x^2 - (t + 2t')k_y^2$, $\psi_{2,\mathbf{k}} = (\psi_{2,\mathbf{k},\uparrow}, \psi_{2,\mathbf{k},\downarrow})^T$ denotes the Fermion field around the $(0, 0)$ point, whose dispersion is given by $\epsilon_2(\mathbf{k}) = (t + 2t')k_x^2 - (t - 2t')k_y^2$. Here the momentum $\mathbf{k}$ is defined with respect to the corresponding VHSs and $\epsilon_\alpha(\mathbf{k})$ is approximated to the second order in $\mathbf{k}$. $\varphi_{\mathbf{q}}$ is the field of the AF spin fluctuation, whose effective action is given by

$$S_\varphi = \int d\mathbf{r} d\mathbf{r}' d\mathbf{q} \chi^{-1}_{\mathbf{q}}(\mathbf{r}, \tau - \tau') \varphi(\mathbf{q}, \tau) \cdot \varphi(-\mathbf{q}, \tau').$$

Here $\chi^{-1}_{\mathbf{q}}(\mathbf{r}, \tau)$ is the inverse of the dynamical susceptibility of the local moment system. The momentum $\mathbf{q}$ of
the spin fluctuation field is now defined with respect to the AF wave vector \( Q = (\pi, \pi) \).

The effective theory presented above has exactly the same structure as the model proposed by Berg et al.\(^{23}\), which is free of the sign problem in quantum Monte Carlo (QMC) simulation. We thus expect that the QMC simulation can also be used to understand the observed critical behavior at \( x^* \).

In conclusion, we argued that the sudden end of the pseudogap phase at \( x^* \) and the observed critical behavior at the same doping can be understood in the framework of the spin-Fermion model, in which the magnetism is carried by both itinerant quasiparticles and local moments with dominating AF correlation.

---

1. S. Badoux, W. Tabis, F. Lalibert, G. Grissonnanche, B. Vignolle, D. Vignolles, J. Bard, D. A. Bonn, W. N. Hardy, R. Liang, N. Doiron-Leyraud, Louis Taillefer, and Cyril Proust, Nature 531, 210 (2016).
2. N. Doiron-Leyraud, O. Cyr-Choinire, S. Badoux, A. Ataei, C. Collignon, A. Gourgout, S. Dufour-Beausjour, F.F. Tafti, F. Lalibert, M.-E. Boulanger, M. Matusiak, D. Graf, M. Kim, J.-S. Zhou, N. Momono, T. Kurosawa, H. Takagi and Louis Taillefer, Nat. Comm. 8, 2044 (2017).
3. B. Loret, S. Sakai, S. Benhabib, Y. Gallais, M. Cazayous, M. A. Measson, R. D. Zhong, J. Schneeloch, G. D. Gu, A. Forget, D. Colson, I. Paul, M. Civelli and A. Sacuto, Phys. Rev. B 96, 094525 (2017).
4. B. Michon, C. Girod, S. Badoux, J. Kamark, Q. Ma, M. Dragomir, H. A. Dabkowska, B. D. Gaulin, J.-S. Zhou, S. Pyon, T. Takayama, H. Takagi, S. Verret, N. Doiron-Leyraud, C. Marcenat, L. Taillefer and T. Klein, arXiv:1804.08502.
5. H. V. Lohneysen et al., Phys. Rev. Lett. 72, 3262 (1994).
6. P. Walmsley et al., Phys. Rev. Lett. 110, 257002 (2013).
7. H. Braganca, S. Sakai, M. C. O. Aguiar and M. Civelli, Phys. Rev. Lett. 120, 067002 (2018).
8. P. Monthoux, A. V. Balatsky and D. Pines, Phys. Rev. Lett. 67, 3448 (1991).
9. P. Monthoux and D. Pines: Phys. Rev. Lett. 69, 961 (1992).
10. A. V. Chubukov, D. Pines and J. Schmalian, arXiv:0201140.
11. J. Schmalian, D. Pines, and B. Stojkovi, Phys. Rev. Lett. 80, 3839 (1998); Phys. Rev. B 60, 667 (1999).
12. Tao Li and Da-Wei Yao, arXiv:1803.08226.
13. Tao Li and Da-Wei Yao, arXiv:1805.04883.
14. Tao Li and Da-Wei Yao, arXiv:1805.05530.
15. M. Le Tacon, G. Ghiringhelli, J. Chaloupka, M. M. Sala, V. Hinkov, M. W. Haverkort, M. Minola, M. Bakr, K. J. Zhou, S. Blanco-Canosa, C. Monney, Y. T. Song, G. L. Sun, C. T. Lin, G. M. De Luca, M. Salluzzo, G. Khaliullin, T. Schmitt, L. Braicovich, and B. Keimer, Nat. Phys. 7, 725 (2011).
16. M. P. M. Dean, R. S. Springell, C. Monney, K. J. Zhou, J. Pereire, I. Božović, B. Dalla Piazza, H. M. Romnow, E. Morenzoni, J. van den Brink, T. Schmitt, and J. P. Hill, Nat. Mater. 11, 850 (2012).
17. M. P. M. Dean, A. J. A. James, R. S. Springell, X. Liu, C. Monney, K. J. Zhou, R. M. Konik, J. S. Wen, Z. J. Xu, G. D. Gu, V. N. Strocov, T. Schmitt, and J. P. Hill, Phys. Rev. Lett. 110, 147001 (2013).
18. M. Le Tacon, M. Minola, D. C. Peets, M. Moretti Sala, S. Blanco-Canosa, V. Hinkov, R. Liang, D. A. Bonn, W. N. Hardy, C. T. Lin, T. Schmitt, L. Braicovich, G. Ghiringhelli, and B. Keimer, Phys. Rev. B 88, 020501(R) (2013).
19. M. P. M. Dean, G. Dellea, R. S. Springell, F. Yakhou-Harris, K. Kummer, N. B. Brookes, X. Liu, Y.-J. Sun, J. Strle, T. Schmitt, L. Braicovich, G. Ghiringhelli, I. Bozovic, and J. P. Hill, Nat. Mater. 12, 1019-2023 (2013).
20. M. P. M. Dean, G. Dellea, M. Minola, S. B. Wilkins, R. M. Konik, G. D. Gu, M. Le Tacon, N. B. Brookes, F. Yakhou-Harris, K. Kummer, J. P. Hill, L. Braicovich, and G. Ghiringhelli, Phys. Rev. B 88, 020403(R) (2013).
21. A. Abanov, A. V. Chubukov, and J. Schmalian, Advances in Physics 52, 119(2003).
22. The ferromagnetic nature of the coupling constant \( g \) can be most easily seen from the following identity of the Hubbard interaction, namely, \( U n_{i\uparrow} n_{i\downarrow} = -\frac{U}{2} \hat{s}_i \cdot \hat{s}_i + const. \) In the spirit of the auxiliary field path integral formulation, one can interpret one of the spin operator \( \hat{s}_i \) as the operator for the local moment.
23. E. Berg, M. A. Metlitski and S. Sachdev, Science 338, 1606 (2012).