Novel antiferromagnetic quantum phase transition in underdoped cuprates

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(September 12, 2018)

We investigate a zero-temperature itinerant antiferromagnetic transition where the fermions possess a $d$-wave gap. This problem pertains to both the nodal liquid insulating phase and the $d$-wave superconducting phase of the underdoped cuprates. We find that a non-trivial quantum phase transition exists, and that the quantum critical point is dominated by a long-ranged interaction $(|x - y|^{-2d})$ of the Néel order parameter, which is induced by the Dirac-like fermions near gap nodes. We formulate a Ginzburg-Landau functional and estimate the critical exponents via the large-$\eta$ expansion method.

PACS numbers: 75.40.-s, 74.20.De, 75.50.Ee, 11.10.Hi

Recent experiments have revealed that underdoped cuprate materials exhibit an exotic pseudogap phase under a characteristic temperature $T^*$. There is ample evidence of the pseudogap phase above the superconducting critical temperature $T_c$; even a low-temperature pseudogap may exist in vortex cores in the mixed states. Although the underlying microscopic mechanism of the pseudogap phenomena is not understood, we may nevertheless study the effective theory and its phenomenologies. Based on the smallness of the superfluid density in underdoped cuprates, the pseudogap phase may be described as a superconductor whose phase coherence is destroyed by strong thermal phase fluctuations but where the gap amplitude is robust. As a possible zero-temperature analog of the pseudogap state, the idea of nodal liquid has been proposed, as a superconductor which is quantum disordered by quantum phase fluctuations. The nodal liquid is a non-magnetic insulating spin-liquid state, which can be effectively described by charge-neutral fermionic quasiparticles with a $d$-wave gap, but with a non-zero insulating gap in terms of the charge-ful electrons. This exotic state can be an intervening phase between the undoped antiferromagnetic (AF) insulating state and the the $d$-wave superconducting state. Further experimental and theoretical studies on the insulating and AF phases are needed to confirm this idea.

In this report, a distinctive consequence of the nodal liquid state is presented: We show that quasiparticles with a $d$-wave gap cause a characteristic critical behavior of quantum phase transitions in the nodal liquid phase, which is distinct from that of the conventional Fermi liquid. More specifically, we study an itinerant AF transition at zero temperature. We expect, however, that without much modification the same is true of certain classes of itinerant magnetic transitions in a superconducting state of unconventional symmetry. The origin of the characteristic scaling is the long-ranged interaction between the order parameter which is induced by massless Dirac-like fermions near gap nodes; after integrating out the fermionic degrees of freedom, a term of the form $N(x) \cdot N(y)/|x - y|^{2d}$ is induced, where $N$ is the Néel order parameter, $d$ is the spatial dimension, and $x$, $y$ are $(d + 1)$-dimensional space-time vectors. We show that a non-trivial quantum critical point exists at the transition and that the abovementioned long-ranged interaction dominates the critical behavior. The same argument holds without modification for a zero-temperature AF transition in the $d$-wave superconductor although it is uncertain whether such a transition takes place in the superconducting state of cuprates. This long-rangedness of the order parameter is similar to the case of itinerant ferromagnetic transition where non-critical soft modes of the Fermi liquid induce such non-trivial interactions. The difference is that in the case of Dirac fermions, additional soft modes are not needed to generate the long-ranged order parameter interactions.

First, we construct an effective theory of nodal fermions with commensurate AF exchange interaction. We will not discuss AF ordered phase in this paper. Here and throughout we do not make a distinction between quasiparticles in the $d$-wave superconducting state and charge-neutral nodal quasiparticles in the nodal liquid phase. We consider a system close to half-filling where the gap nodes are located on the nested Fermi surface. (See Fig. 1) Since we are only interested in the low-energy properties, we integrate out the fast momentum degrees of freedom and retain only the momenta.

![FIG. 1. Schematic geometry of the Fermi surface and the $d$-wave gap. The solid line is the nested Fermi surface, and the dashed line represents the gap in the quasiparticle spectrum. $Q$ depicts an AF ordering wave-vector.](http://example.com/fig1.png)
near the Fermi surface. Assuming that we can construct such a low-energy effective theory of the Hubbard model near half-filling, we may express the effective action $S = S_0 + S_{\text{AF}}$ in the following form:

$$S_0 = T \sum_{\omega} \sum_{\mathbf{k}} \left[ \psi^\dagger_{\alpha}(\mathbf{k}; \omega) (i\omega - \xi_{\mathbf{k}}) \psi^\alpha(\mathbf{k}; \omega) + \Delta_{\mathbf{k}} \psi^\dagger(\mathbf{k}; \omega) \psi^\alpha(-\mathbf{k}; -\omega) + \text{c.c.} \right],$$

$$S_{\text{AF}} = \frac{1}{2} J \int d\tau \sum_{\mathbf{q}} \mathbf{n}_Q(\mathbf{q}, \tau) \cdot \mathbf{n}_Q(-\mathbf{q}, \tau),$$

where $\mathbf{n}_Q(\mathbf{q}, \tau) = \sum_{\mathbf{k}} \frac{1}{2} \psi^\dagger_{\alpha}(\mathbf{k}, \tau) \sigma^\alpha_{\beta} \psi^\beta(\mathbf{k} + \mathbf{Q}_k + \mathbf{q}, \tau)$, and $\Delta_{\mathbf{k}}$ is a $d$-wave gap. Here $|\mathbf{q}| \ll |\mathbf{k}_F|$ and $\mathbf{q}_k$ is a commensurate nesting vector antiparallel to the Fermi velocity at $\mathbf{k}$. Also we take $J < 0$ so that an AF transition takes place.

Before we discuss the AF critical point, we revisit results of the mean-field theory. To obtain a mean-field theory, it is sufficient to employ a mixed representation of the momentum to separate the Fermi surface label and the small relative momentum near the Fermi surface as follows:

$$S = S_0 + \int d^2x \ d\tau \left[ -\frac{1}{2J} N^2(x) \right.$$

$$- \sum_{\mathbf{p}} e^{-i\mathbf{Q}_\mathbf{p} \cdot \mathbf{N}(x)} \cdot \frac{1}{2} \psi^\dagger_{\alpha}(\mathbf{p}; x) \sum_{\beta} \sigma^\alpha_{\beta} \psi^\beta(\mathbf{p} + \mathbf{Q}_\mathbf{p}; x) \left. \right]$$

where

$$S_0 = T \sum_{\omega} \sum_{\mathbf{p}} \left\{ \psi^\dagger_{\alpha}(\mathbf{p}; q) [i\omega - \xi_{\mathbf{p}}(\mathbf{q})] \psi^\alpha(\mathbf{p}; q) + \Delta_{\mathbf{p}} \psi^\dagger(\mathbf{p}; q) \psi^\alpha(-\mathbf{p}; -\mathbf{q}) + \text{c.c.} \right\}. $$

Here we have separated the AF exchange interaction by introducing a staggered magnetization $\mathbf{N}$ via Hubbard-Stratonovich transformation. The momentum $\mathbf{p}$ labels points on the Fermi surface, and $\mathbf{q}$ is a small momentum deviation from the Fermi surface. $q = (\mathbf{q}, \omega)$ is a $(d+1)$-dimensional wave-vector and similarly, $x = (x, \tau)$. In this representation, the $d$-wave symmetry of the gap dictates that $\Delta_{\mathbf{p}} = \Delta_{-\mathbf{p}}$ and $\Delta_{\mathbf{p}} = -\Delta_{\mathbf{p} + \mathbf{Q}_\mathbf{p}}$. Taking $|\mathbf{N}| = N_z = \text{constant},$ we obtain, for instance, the quasiparticle Greens function $G(\mathbf{p}; q) = -(i\omega + \xi_{\mathbf{p}}(\mathbf{q}))/\omega^2 + \xi^2_{\mathbf{p}} + |\Delta_{\mathbf{p}}|^2 + N^2/4. $ As expected, the quasiparticle gains a gap of the form $\sqrt{|\Delta_{\mathbf{p}}|^2 + N^2/4}.$

From the following mean-field self-consistency condition,

$$\frac{N}{|J|} = \sum_{\mathbf{p}} \frac{1}{2} \left( \sigma^\alpha_{\beta} \langle \psi^\dagger_{\alpha}(\mathbf{p}; x) \psi^\beta(\mathbf{p} + \mathbf{Q}_\mathbf{p}; x) \right),$$

we obtain the relation

$$|N|/2 + \sqrt{\Delta^2_{\mathbf{p}} + N^2/4} = E_{\Lambda} e^{-1/|J|N_0},$$

where $E_{\Lambda}$ is an upper energy cutoff which is of order $E_{F}, N_0$ is the density of states at the Fermi surface, and $\Delta_0$ is the maximum gap. This suggests that due to the gap in the quasiparticle spectrum, the AF transition is inhibited to such a degree that a sufficiently strong exchange interaction is needed for a transition. In fact, we refer from Eq. (3) that the AF coupling $J$ needs to be at least of comparable strength to the superconducting pairing strength; on a circular Fermi surface, even stronger exchange interactions would be required. This is in contrast to the case of Fermi liquid on a nested Fermi surface where arbitrary strength of exchange interaction leads to an AF instability. Therefore, a weak-coupling fermionic renormalization group (RG) analysis is inadequate for this problem. Instead, we turn to the Ginzburg-Landau (GL) functional of the Néel order parameter below.

Now we come back to Eq. (3) which reduces to a spatially anisotropic massless Dirac fermionic action near the gap nodes. In terms of the small momentum deviation $\mathbf{q}$ from the Fermi wave-vector, the fermion Greens functions have poles at $\omega \approx \pm \sqrt{v_F^2 |q||x^2 + v_F^2 q^2}.$, where $v_F$ is the Fermi velocity, $v_\Delta$ is the slope of the gap at the node in the momentum space, and $q_{\parallel}$ ($q_{\perp}$) is the component of momentum parallel (perpendicular) to the Fermi velocity at the node. Although the bare theory does not have an exact Lorentz symmetry due to this anisotropy, we assume that even if we enforce Lorentz symmetry by hand, the quality of the quantum critical point is not crucially changed and take $v_F = v_\Delta = 1$ for simplicity.

To arrive at the GL functional of the order parameter, we integrate out the fermion degrees of freedom. For now we assume that this procedure is under control, although we will show below that at $T = 0$ it is beset with singularities in GL coefficients. We confine our discussion to an AF transition sufficiently far away from a superconductor-insulator transition, and retain only the Néel order parameter. After formally integrating out the fermionic fields,

$$S[\mathbf{N}] = \sum_n \int d^d x_1 \ldots d^d x_n \ d\tau_n \ Gamma(x_1, \ldots, x_n)$$

$$\times \mathbf{N}(x_n),$$

where $n$ is an even integer. The Fourier transform of $\Gamma_2$ is obtained from

$$\Gamma_2(\mathbf{q}, \nu) = -\frac{1}{2J} + \frac{1}{2} \int \frac{d\omega}{2\pi} \sum_{\mathbf{k}} \left[ G(\mathbf{k}, \omega) G(\mathbf{k} + \mathbf{Q}_k + \mathbf{q}, \omega + \nu) \right],$$

where $G$ is the diagonal component of the quasiparticle Greens function. Collecting the lowest powers of the momentum and frequency, we find that for $2 \leq d < 3,$ which is the range of dimensionality of our interest, the leading term is non-analytic in $|q|$:
\[ \Gamma_2 = t + c|q|^{d-1}, \]  

where \(|q| = \sqrt{q^2 + u^2}\) and \(c > 0\). Similarly, one can show that \(\Gamma_n \sim |q|^{d-n-1}\). Using the Gaussian approximation, \(\langle N \cdot N \rangle = \frac{1}{(t + c_2|q|^{d-1})}\). Taking \(t\) as the distance from the critical point, we obtain various critical exponents: \(\gamma = 1\), \(\nu = 1/(d-1)\), and \(\eta = 3 - d\). By including higher order GL expansions and introducing an \(O(3)\) symmetry-breaking term \(\mathbf{h} \cdot \mathbf{N}\), we can obtain the equation of state. In the presence of the staggered density \(\delta S/\delta N = 0\), therefore, \(\Gamma_n \sim N^{d-n+1}\) obtains, and the equation of state \(\langle \delta S/\delta N = 0 \rangle = tN + N^d \approx h\). From this, we obtain two more exponents: \(\beta = 1/(d-1)\) and \(\delta = d\).

Fixing the Gaussian term as marginal, we may estimate the scaling dimensions of higher GL expansions. By transforming \(q \rightarrow bq\) and \(N \rightarrow b^{-d}N\), we find that the \(n\)-th GL expansion in \(N\) scales as \(b^{d-n-1}\). This means that if we have a local GL theory, all high order expansions in \(N\) are irrelevant in the tree level. However, since the coefficient \(\Gamma_n\) scales as \(b^{d-n-1}\) due to the long-ranged interaction, all higher order terms gain marginal scaling. Therefore, there are infinitely many marginal operators in this theory, and the Gaussian approximation may break down. This is because of the singularities in \(\Gamma_n\) that occur as \(T \rightarrow 0\), which suggests that a more careful RG analysis is called for. The result of the \(c = 4 - (d+1)\) expansion in this model shows that there exists a non-trivial stable fixed point at the AF transition \(\mathcal{B}\). In this paper we use the large-\(n\) expansion method by introducing \(n\) fermion species to estimate the leading correction to the critical exponents and take \(n = 1\) at the end.

We come back to Eqs. (1) and (4), and introduce fictitious \(n\) fermion flavors which couple to the Néel order parameter symmetrically. We take the upper momentum cutoff \(\Lambda < \Delta_0\) and re-express the effective action in terms of the fermions coupled to the Néel field as follows

\[ S_{\text{eff}} = \sum_{j=1}^{n} S_0^j + \int d\omega \, d^dx \big[ N(q) \cdot N(-q) \, (t + q^2) \big] + g \sum_j e^{-iQ \cdot x} N(x) \cdot \frac{1}{2} \bar{\psi}^\dagger_{\alpha,j}(x) \, \sigma^\mu_{\alpha,\beta} \psi^\dagger_{\mu,j}(x), \]  

where each fermion species is labeled by the index \(j\). We have not included higher order local expansions in \(N\) since more significant non-local expansions will be perturbatively generated by the long-wavelength fermions. Here each \(S_0^j\) is of the same form as Eq. (1) except that the momentum and frequency are confined to within a sphere of radius \(\Lambda \ll \Delta_0\) so that the fermionic spectrum can be well-approximated by the Dirac spectrum.

Now we take the large-\(n\) limit and estimate the critical exponents by calculating the Néel propagator. Note that \(n\) is not the number of order parameter components but the number of fermion species. We find that this is a convenient choice since the singular GL coefficients in Eq. (5) are ultimately determined by the long-wavelength fermions and the coupling \(g\) in Eq. (10). In this way, we can systematically calculate \(g\)-independent critical exponents as expansions in \(1/n\) by the perturbation technique \(\mathcal{B}\). In Eq. (6), each vertex function \(\Gamma_n\) consists of one fermionic loop which has a factor of \(n\). This means that \(1/n\) expansion is equivalent to loop expansions in the Néel field \(-1/n\) takes the role of \(h\). In practice, it is more convenient to directly work with fermions rather than to integrate them out at the outset to perform loop expansions in the order parameter field. Figure 2 (a) shows the leading Néel propagator in the large-\(n\) limit, which is \(\langle N(q)N(-q) \rangle = [ng^2|q|/16 + t]^{-1}\) in \(d = 2\), and \(\sim |q|^{d-1} + t\) in general dimensions. Note that the leading non-analyticity is already obtained here. The critical exponents at the leading order agree with the Gaussian approximation of Eq. (6). In order to estimate the \(1/n\) correction to the critical exponents, we calculate the diagrams shown in Fig. 2 (b). Here we focus on two spatial dimensions, as it is difficult to carry out analytic calculations in general dimensions. Setting \(t = 0\), we can calculate the correction to \(\eta\) by finding the coefficient of the term \(|q| \ln |q|\) in the Néel self-energy correction. In \(d = 2\), since there is fermion self-energy correction \(\sim (1/n) \ln |k|\), we may expect a Néel self-energy correction of the form \((1/n) |q| \ln |q|\) on the dimensional ground. Explicit calculation shows that there is no such logarithmic correction from any of the three diagrams in Fig. 2 (b). Therefore, we obtain \(\eta = 1 + O(1/n^2)\). Setting a non-zero \(t > 0\), however, we may obtain the correction to \(\gamma\) by finding the coefficient of the self-energy correction of the form \(t \ln t\), and we find that \(\gamma \approx 1 + 0.78/n + O(1/n^2)\).

![Figure 2](image-url)

FIG. 2. (a) The thick wavy line denotes the leading order Néel propagator in the large-\(n\) limit, and the thin solid line is the bare fermion propagator. The dashed line is the bare AF exchange coupling and the bubble is the bare fermionic AF spin susceptibility. (b) Corrections to the Néel self-energy of order \(O(1/n)\).

The long-ranged interaction discussed above is dominant only in the \(T \rightarrow 0\) limit, but the finite-temperature crossover behavior \(\mathcal{B}\) is beyond the scope of discussion in this report. We merely comment on the classical finite-temperature transition for \(2 < d < 3\) where the finite-temperature Néel order is assumed to be stabi-
lized by weak interlayer coupling of cuprates, assuming that the nodal quasiparticles survive at non-zero temperatures. When the temperature is the largest energy scale of the problem, the non-local interaction of the Néel order parameter gives subleading power laws near the transition. As a result, the leading Gaussian GL expansion is of the form \( \int dq |q|^2 \mathcal{N}(q) \mathcal{N}(-q) \) where \( t = (T - T_c)/T_c \). This coincides with the usual classical GL functional, and therefore we find no distinctive critical behavior in this case.

As pointed out by Hertz \cite{Hertz1976}, AF transitions on nested Fermi surfaces and superconducting transitions in Fermi liquids are two other examples which suffer from the \( T \to 0 \) singularities in GL coefficients. In fact, in these two examples, zero-temperature GL expansions are more difficult because of \( \ln |q| \) singularity in the Gaussian term. This is related to the fact that the Fermi liquid ground state is always unstable in these cases.

We have shown that the existence of a d-wave gap in the quasiparticle spectrum leads to distinctive critical behavior at zero-temperature phase transitions, due to the effective long-ranged interaction of the order parameter. We showed that the nodal liquid phase is stable against an AF instability within a sizable window of AF exchange coupling and that there exists a non-trivial fixed point that the distance from the quantum critical point \( t \) can be controlled. In principle, \( t \) depends on the AF exchange interaction which in turn is controlled by doping. Estimates from two-magnon Raman scattering experiments on cuprates \cite{Balents1997} show that the effective AF super-exchange coupling \( J \) takes a value of \( \sim 125 \) meV for AF insulators and decreases as doping. Here we assume that the only effect of doping is to reduce the effective exchange coupling, and also ignore the possibility of a spin-density-wave ordering with incommensurate wavevectors \cite{Balents1997}. We expect a scaling form of thermodynamic quantities in the quantum critical regime such as the critical specific heat coefficient, \( \gamma_v = c_v/T \sim T^d - 1 F(\nu, v, \eta) / T \) in terms of a scaling function \( F(x) \). From the scaling relation, we find that \( \nu = \gamma_{2} / (2 - \eta) \approx 1 + 0.78 / n + O(1/n^2) \). This analysis may provide a check on the notion of the nodal liquid as the zero-temperature pseudogap phase of the underdoped cuprates. Also we notice that the d-wave like excitation is possibly ubiquitous even in undoped or underdoped insulating cuprates, as recently revealed by the angle-resolved photoemission spectroscopy on an insulating parent compound \( \text{Ca}_2\text{CuO}_2\text{Cl}_2 \) \cite{Millis1997}, and theories on nodal excitations merit further attention.

It would be also interesting to study the effect of nodal quasiparticles on the superconductor-insulator transition in the cuprates. At first glance, however, the coupling of the superconducting order parameter to nodal quasiparticles is suppressed by a d-wave angular factor of \( \cos 2\phi \) near \( \phi = \pi (2m + 1)/4 \) and we expect that it is subleading in the RG sense near the quantum phase transition of the \( 2 + 1 \) dimensional XY type.

The author would like to thank Alan Dorsey, Brad Marston, Pierre Ramond, Subir Sachdev, and Rob Wickham for helpful discussions, and Matthew Fisher for pointing out an error in an earlier manuscript. This work was supported by the National High Magnetic Field Laboratory and by NSF grant DMR 96-28926.