Theory of the Quantum Critical Fluctuations in Cuprate Superconductors

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The statistical mechanics of the time-reversal and inversion symmetry breaking order parameter, possibly observed in the pseudogap region of the phase diagram of the cuprates, can be represented by the Ashkin-Teller model. We add kinetic energy and dissipation to the model for a quantum generalization and show that the spectrum of the quantum-critical fluctuations is of the form postulated in 1989 to give the marginal Fermi-liquid properties. The model solved and the methods devised are likely to be of interest also to other quantum phase transitions.

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A mean-field solution of a microscopic model predicts that the *pseudogapped* region of the phase diagram of the cuprates (Region II in Fig. 1 of Ref. [1]) has a spontaneous current pattern depicted in Fig. 1(a) [2]. Such a state breaks time-reversal, inversion, and three of the four reflection symmetries of the square lattice while preserving translational symmetry. The observed magnetic diffraction in neutron scattering [1] as well as the dichroism observed in angle-resolved photoemission spectroscopy [3] with circularly polarized photons is consistent with such a state.

The transition temperature of this state varies continuously with hole density x and tends to 0 at $x = x_c$, the quantum-critical point. Anomalous normal state properties are observed in the funnel shaped region (Region I in Fig. 1 of Ref. [1]) emanating from the quantum critical point. They were shown to follow from a phenomenological spectrum [4]:

$$\mathrm{Im}\,\chi(\mathbf{q}, \omega, T) \propto \omega/T, \quad \text{for } \omega \ll T,$$
$$\propto \text{const}, \quad \text{for } T \ll \omega \ll \omega_c, \tag{1}$$

where ω_c is a cutoff, determinable from experiments. The corresponding real part of the fluctuations, $\mathrm{Re}\chi(\mathbf{q}, \omega, T) \propto \ln(\omega_c/\omega)$ for $\omega/T \gg 1$ and $\propto \ln(\omega_c/T)$ for $\omega/T \ll 1$. Since this spectrum has a singularity in the limit $(T, \omega) \to 0$, it specifies the fluctuations near a quantum-critical point [5]. For small $\mathbf{q}$, this spectrum is directly observed in Raman scattering [6]. The two unusual properties of Eq. (1), ω/T scaling [5] and no dependence (or a smooth dependence) on $\mathbf{q}$, are sufficient to generate a marginal Fermi liquid [4]. The observed anomalous properties are well explained by the marginal Fermi liquid and its predictions for the single-particle spectra have been verified in experiments.

The purpose of this work is to show that the quantum-critical spectrum of Eq. (1) is the spectrum of fluctuations of the order parameter which condense to give the observed order depicted in Fig. 1(a).

To do so, we consider a quantum generalization of the classical model whose solution gives such an order parameter. The four possible configurations in each unit-cell of Fig. 1(a) can be represented by four vectors with arrows representing time reversal and orientation representing the only plane of reflection symmetry, as shown in Fig. 1(b). A classical model with such a pair of Ising degrees of freedom is the Ashkin-Teller [7] model:

$$H = -\sum_{\langle i,j\rangle} J_2(\sigma_i\sigma_j + \tau_i\tau_j) + J_4(\sigma_i\tau_i\sigma_j\tau_j); \tag{2}$$

σ_i and τ_i are Ising spins. This model can be derived [8] from the microscopic model with which the symmetry breaking of Fig. 1(a) is derived [2].

The Ashkin-Teller model has a variety of phases depending on J_4/J_2 and T/J_2 [7,9,10]. Especially interesting to us is the region $-1 < J_4/J_2 < 0$ in which the ordered phase has ferromagnetic order in $\langle\sigma_i\rangle, \langle\tau_i\rangle$ as well as $\langle\sigma_i\tau_i\rangle$ just as in the order observed. Two more properties of this region are of special interest: on the critical line, the model is Gaussian (with stiffness depending on J_4/J_2) and the specific heat at the transition has no divergence. With the transformation $\cos(\theta_i) = (\sigma_i + \tau_i)/2$; $\sin(\theta_i) = (\sigma_i - \tau_i)/2$, the Ashkin-Teller model becomes

$$H = \sum_{i,jnn} 2J_2\cos(\theta_i - \theta_j) + J_4\cos 2(\theta_i - \theta_j) + h_4\cos 4\theta_i. \tag{3}$$

The restriction that $\theta_i = 0,\ \pi/2,\ \pi,\ 3\pi/2$ has been written in terms of a fourfold anisotropy term $\propto h_4$. Monte Carlo calculations show [11] that the classical phase diagram of model (2) and of (3) are the same. This is

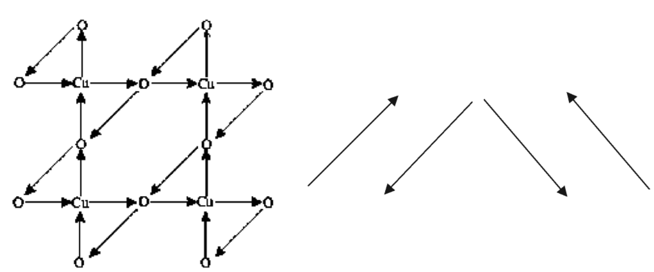

FIG. 1. Current pattern (a) and its abstraction (b).

consistent with the fact that h_4 is irrelevant above the critical point in the xy model; h_4, however, is relevant below the transition enforcing an Ising state [12].

For a quantum theory for the model, two additional features must be included: the kinetic energy of the θ variables and the dissipation. For the latter, we note that $(\theta_i - \theta_j)$ is proportional to the collective part of the current between sites i and j. This is coupled [2] linearly to the incoherent fermion current and decays into it providing the dissipation for the collective modes. The current correlations of fermions decay in time as $1/(\tau - \tau')^2$. This process is mathematically identical to that derived by Caldeira and Leggett [13] for decay of Josephson current into incoherent fermion current. Integrating over the fermion current leads to the Caldeira-Leggett dissipative term in the action parametrized by α

$$S_{\rm diss} = \int d\tau \int d\tau' \sum_{\langle ij\rangle} \frac{\alpha}{8\pi} \left(\frac{[\theta_{ij}(\tau) - \theta_{ij}(\tau')]}{(\tau - \tau')} \right)^2, \qquad (4)$$

where $\theta_{ij}(\tau) = \theta_i(\tau) - \theta_j(\tau)$.

For simplicity of presentation, we start with $J_4 = 0$. We will show that no essential modification arises at least for $|J_4|/J_2 < 1/2$, which is in the interesting regime. We will also take $h_4 = 0$ and show that in the fluctuation regime, which is our primary interest, a finite h_4 does not change the results. With these simplifications the quantum-mechanical action for the problem is

$$S = S_K + S_{\rm diss} + \int \sum_{\langle ij\rangle} d\tau 2J_2 \cos[\theta_i(\tau) - \theta_j(\tau)]. \qquad (5)$$

Here $S_K = \int d\tau \sum_i \frac{1}{E}(\frac{d\theta_i}{d\tau})^2$ is the kinetic energy of the θ field; the effective charging energy E serves as inertia.

We use the Villain representation of the periodic functions and introduce integer link variables $\mathbf{m}_i = m_{ix}\hat{x} + m_{iy}\hat{y}$ and discretize time in steps $\Delta\tau$ to get

$$S = \sum_{\langle \mu\nu\rangle} \sum_i \frac{1}{E\Delta\tau} (\theta_{i\mu} - \theta_{i\nu})^2 + S_{\rm diss} + \sum_{\langle ij\rangle} \sum_\mu 2J_2 \Delta\tau (\theta_{i\mu} - \theta_{j\mu} - 2\pi m_{ij})^2. \qquad (6)$$

After a Fourier transform and integration over the θ_{ln} variables, the action for the vector field $\mathbf{m}$ is obtained:

$$S = \frac{1}{L^2\beta} \sum_{ln} (2\pi)^2 J G(\mathbf{k}_l, \omega_n) \Big[J a^4 |\mathbf{k}_l \times \mathbf{m}_{ln}|^2 + \left(J_t + \frac{\alpha}{4\pi c} \frac{k_l^2}{|\omega_n|} \right) a^2 (\Delta\tau)^2 |\omega_n \mathbf{m}_{ln}|^2 \Big]. \qquad (7)$$

Here $\mathbf{k}_l$ are discretized momenta, $\mathbf{k}_l = (2\pi l_x/a)\hat{\mathbf{x}} + (2\pi l_y/a)\hat{\mathbf{y}}$, ω_n are the Matsubara frequencies, $\omega_n = 2\pi n/\beta$, and $J = 2J_2\Delta\tau/a$, $J_t = 1/Ea\Delta\tau$. The propagator $G(\mathbf{k}_l, \omega_n)$ is given by $G(\mathbf{k}_l, \omega_n) = (Jck_l^2 + J_t\omega_n^2/c + \alpha|\omega_n|k_l^2/4\pi)^{-1}$.

Quantum dynamics introduces sources and sinks in the vector field. Therefore, this action includes besides the vortices, (curl $\mathbf{m}$), the time derivatives of $\mathbf{m}$. Sources and sinks due to quantum dissipation suggest that the time derivative must include a field with a divergence. We define two *orthogonal* sources, $\rho_v(\mathbf{k}, \tau)$ and $\rho_w(\mathbf{k}, \tau)$ (in the continuum limit), through

$$\rho_v(\mathbf{k}, \tau) = [\mathbf{k} \times \mathbf{m}(\mathbf{k}, \tau)] \cdot \mathbf{z}, \qquad (8)$$

$$\rho_w(\mathbf{k}, \tau) = (1/c)\hat{\mathbf{k}} \cdot d\mathbf{m}(\mathbf{k}, \tau)/d\tau, \qquad (9)$$

where the velocity $c = a/\Delta\tau$. Using Eqs. (8) and (9), $\omega_n^2 |\mathbf{m}|^2 = \omega_n^2/k_l^2 |\rho_v|^2 + c^2|\rho_w|^2$. In the theory of the xy model, the charges ρ_v are sources of "vortices" where the $\mathbf{m}(\mathbf{r}, t)$ is transverse with a strength falling off as $1/r$. We have introduced ρ_w as the sources of the orthogonal longitudinal field [14]. From (9), it is seen that ρ_w's are events in time where the divergence of $\mathbf{m}(\mathbf{r}, t)$ changes. We will refer to such field configurations as "warps."

In terms of ρ_v, ρ_w, the action, in the continuum limit, neatly splits into three parts: $S = S_v + S_w + S'_w$

$$S_v = \frac{1}{L^2\beta} \sum_{ln} \frac{J}{ck_l^2} |\rho_v(\mathbf{k}_l, \omega_n)|^2,$$
$$S_w = \frac{1}{L^2\beta} \sum_{ln} \frac{\alpha}{4\pi|\omega|} |\rho_w(\mathbf{k}_l, \omega_n)|^2, \qquad (10)$$
$$S'_w = \frac{1}{L^2\beta} \sum_{ln} G(\mathbf{k}_l, \omega_n) \left(JJ_t - \frac{\alpha J_t |\omega_n|}{4\pi c} - \frac{\alpha^2 k_l^2}{16\pi^2} \right) \times |\rho_w(\mathbf{k}_l, \omega_n)|^2.$$

The interesting part about this decomposition [15] is that S_v is the Coulomb gas representation of the xy model with charges interacting logarithmically in space but locally in time and S_w is the Coulomb gas representation of the Kondo problem with charges interacting logarithmically in time but locally in space [16]. S'_w has nonsingular interactions and is unimportant compared to S_v and S_w [17]. Being orthogonal, the charges ρ_v and ρ_w are uncoupled; the action is a product of the action over configurations of ρ_v and of ρ_w. Any physical correlations are determined by correlations of both charges. Both the $\langle\rho_v\rho_v\rangle(\mathbf{k}, \omega)$ and the $\langle\rho_w\rho_w\rangle(\mathbf{k}, \omega)$ correlations are well understood. For any finite J, the field ρ_v is confined in the limit $T \to 0$; no free vortices exist. The phase transition can come about only due to free ρ_w's, due to a tuning of dissipation parameter α. We therefore first remind ourselves of the correlation function of the ρ_w's.

Let us introduce a core energy Δ for the ρ_w's just as is done to control the fugacity of ρ_v's, the vortices. Next consider how the renormalization of α and Δ proceeds. Including the core energy, the action S_w is

$$S_w = \sum_i \bigg[T \sum_n \frac{\alpha}{4\pi} \frac{1}{|\omega_n|} |\rho_{wi}(\omega_n)|^2 + \int d\tau \Delta |\rho_{wi}(\tau)|^2 \bigg]. \tag{11}$$

The renormalization group equations for Eq. (11) are well known [16,18]

$$\frac{d\tilde{\Delta}}{dl} = (1-\alpha)\tilde{\Delta}, \qquad \frac{d\alpha}{dl} = -\alpha\tilde{\Delta}^2, \tag{12}$$

where $\tilde{\Delta} = \Delta\tau_c$ and $\tau_c \approx (2J_2E)^{-1/2}$ is the short time cutoff. The critical point of interest is at $\alpha_c = 1$ [19], where $\tilde{\Delta}$ scales to 0; for $\alpha < 1$ the charges ρ_w freely proliferate as "screening" due to $\tilde{\Delta}$ becomes effective. $\alpha > 1$ represents the ordered or confined region in which the anisotropy field h_4 is strongly relevant. We are interested here only in the region $\alpha \leq 1$. Well in the quantum-critical region, the (singular part of the) propagator for ρ_w is

$$\langle \rho_w(\omega_n)\rho_w(-\omega_n)\rangle = (1/4\pi|\omega_n|\tau_c)^{-1}. \tag{13}$$

The crossover to the quantum-disordered or screened state is given for $T = 0$ when $\omega = \omega_x$ which is of the order of the inverse of the characteristic screening time, which may be estimated similarly to Kosterlitz's estimate [20] of the screening length in the xy problem:

$$\omega_x \approx \tau_c^{-1} \exp(-b/\sqrt{1-\alpha}), \tag{14}$$

where b is a numerical constant of $O(1)$. At finite temperatures and low frequencies, the crossover temperature T_x is of $O(\omega_x)$.

Finally, we come to the correlation function of interest, that of the order parameter, i.e., of the flux in the loops:

$$C_{i,j,\mu,\nu} = \langle e^{\imath\theta_{i\mu}} e^{-\imath\theta_{j\nu}} \rangle \equiv \frac{\int d[\theta] e^{-\bar{S}}}{\int d[\theta] e^{-S}}. \tag{15}$$

To compute this, we will employ a procedure similar to the one used by Jose *et al.* [12] for the $2d$ xy model. Consider a path from $i\mu$ to $j\nu$ and split it into two: $i\mu \rightarrow j\mu$ and $j\mu \rightarrow j\nu$. All paths should give the same answer so we have chosen the one most convenient. A vector field $\vec{\eta}_{i\mu}$ is defined which lives on the sites of the lattice and whose components are 1 if the path crosses site $i\mu$ and zero otherwise. To capture the second part of the path, we define a scalar field $\eta^w_{i\mu}$, which lives on the links in time and is nonzero only for paths on the link. Including the fields described above and integrating over the $\theta' s$, we get

$$\bar{S} = S_v + S_w + \frac{1}{L^2\beta}\sum_{ln}(2\pi)JG(\mathbf{k}_l, \omega_n) \times [(\omega_n\eta^{w\star}/2)(\imath\mathbf{k}_l\cdot\mathbf{m}_{ln}) + (\mathbf{k}_l\cdot\vec{\eta}^\star/2)(\imath\mathbf{k}_l\cdot\mathbf{m}_{ln}) + \text{c.c.} + |\omega_n\eta^w/2 + \mathbf{k}_l\cdot\vec{\eta}^\star/2|^2]. \tag{16}$$

The last term in the sum gives the spin wave contribution to the correlation function. Clearly the spin wave contribution is finite and this is indeed the standard result that spin wave fluctuations do not disorder the state in three dimensions. The second term in the sum can be written in terms of the linear coupling of $(\mathbf{k}\times\vec{\eta})$ to ρ_v's, the source of vortices. The vortices are confined for $T \rightarrow 0$ for a finite J and are therefore not interesting. The first term can be written in terms of a linear coupling between η^w's and ρ_w's. This is the interesting term because the divergence in frequency induced by the dissipation as α is tuned leads to a proliferation of ρ_w's and thus to disorder. Following the discussion after Eq. (10), the correlation function is a product over configurations of ρ_v's and ρ_w's which are independent. The singular part of the correlation function near the quantum-critical point is thus determined entirely by the dynamics of ρ_w's. The correlation function is $C(\mathbf{r}-\mathbf{r}', \tau-\tau') \propto \exp(-F)$,

$$F = -\frac{J^2c^2}{4}T\sum_n \int d\mathbf{k}\frac{k^2}{\omega_n^2}\langle\rho_w(\omega_n)\rho_w(-\omega_n)\rangle \times G^2(\mathbf{k},\omega_n)\{1-\cos[\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}') + \omega_n(\tau-\tau')]\}. \tag{17}$$

Deep in the quantum-critical regime the correlations function $\langle\rho_w(\omega_n)\rho_w(-\omega_n)\rangle$ is given by Eq. (13). The summand over n in F has a leading $1/|\omega|$ part. It is easy to see that for any finite $|\mathbf{r}-\mathbf{r}'|$ the sum over n is divergent. Thus, for any finite spatial separation, the correlation function $C(\mathbf{r}-\mathbf{r}', \tau)$ is identically zero for τ larger than the crossover scale τ_c. On the other hand, for $|\mathbf{r}-\mathbf{r}'| = 0$, the correlation function is given by $C(0,\tau-\tau') \propto \exp[-F(0,\tau-\tau')]$, where

$$F(0,\tau-\tau') = -2\pi T\sum_n \frac{1-\cos[\omega_n(\tau-\tau')]}{|\omega_n|} \times \log(|\omega_n|\tau_c). \tag{18}$$

Such correlation functions have been calculated in other contexts. In particular, using the calculation by Ghaemi *et al.* [21], the spectral function of the correlation is

$$\text{Im}\,\chi(\mathbf{q},\omega) = \bar{\tau}_c \tanh(\omega/2T), \qquad \omega \lesssim \tau_c^{-1}. \tag{19}$$

$\bar{\tau}_c$ is $O(\tau_c)$. The phenomenological spectrum of Eq. (1) is thereby derived with its cutoff and the crossover from ω and T specified.

We now summarize the calculations for the effect of the anisotropy field h_4. As in Ref. [12], we supplement the action of Eq. (10) by introducing a new field p_i

$$e^{h_4\cos(4\theta_i)} \approx \sum_{p_i} e^{\ln(y_4)p_i^2 + \imath 4 p_i\theta_i}, \tag{20}$$

where $y_4 = h_4/2$. Introducing the $\mathbf{m}$ fields as before and performing the θ integral leads to additional terms in the action which couple p_i linearly to $\rho_{w,i}$. This linear coupling can be eliminated with a renormalization of the coupling constant α to 2α. This does not change the critical behavior in the quantum-critical regime; the correlation remains of the form (19). For $\alpha > \alpha_c$, h_4 is relevant just as in the classical problem and enforces an Ising state.

The coupling J_4 is easier to treat. For $-0.5 < J_4/J_2 < 0$, the bare potential continues to have the absolute minima at $(\theta_i - \theta_j) = 0$. Therefore, the Villain representation of periodic functions can be made as above with an altered coefficient. This affects the cutoffs in the solution but not the form of the correlation function below the cutoffs. The theory is valid only in this range; for smaller J_4, an Ising transition to a different symmetry is expected as in the classical model.

To summarize, we have considered a statistical mechanical model which has the symmetries and the degeneracies of the observed phase in underdoped cuprates. The specific heat at the classical transition in this model is a smooth function of temperature as in experiments. We have generalized the model by including inertial as well as dissipative dynamics. On tuning the parameter α, which we take to be function of doping x, a quantum phase transition occurs, i.e., the pseudogap temperature goes to zero at $\alpha(x_c) = 1$. The quantum-critical fluctuations of the model are determined by the dynamics of point defects, the warps. These quantum fluctuations represent the transitions of the flux patterns of Fig. 1 among the four domains at various length and time scales. The ω/T scaling and spatial locality of the fluctuations, which were postulated to explain the experimental properties in the quantum-critical regime of the cuprates, have been derived. New results are the detailed form (19), including the value of the cutoff τ_c^{-1}.

More generally, our results are applicable also to the dissipative quantum xy model and hence relevant to critical properties of Josephson junction arrays in two dimensions. The Ashkin-Teller model is a staggered 8-vertex model. We expect that our method has application to quantum versions of 6- and 8-vertex models generally to which many physical problems of interest correspond.

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[15] In the absence of dissipation, one can define a two-dimensional charge, $\mathbf{J} = \imath c \omega \mathbf{m}$ and combine it with the scalar charge ρ_v to define a single three-dimensional *current* $\mathbf{j}$. The action is then (with properly scaled frequency and wave-vector variables) $\propto \sum_{\tilde{k},\tilde{\omega}} |\mathbf{j}(\tilde{\mathbf{k}}, \tilde{\omega})|^2/(\tilde{k}^2 + \tilde{\omega}^2)$. With a fugacity term added, this is a model of interacting vortex loops, which maps through a duality transformation to the $3d$ xy model; [see C. Dasgupta and B. I. Halperin, Phys. Rev. Lett. **47**, 1556 (1981)]. However, adding dissipation to the model leads with this choice of charges to a term $\propto \alpha|\mathbf{J}|^2/|\tilde{\omega}|$, which is more singular than the rest. Moreover, since the singularity due to dissipation explicitly breaks the equivalence of space and time, the continuity equation is lost; dissipation thus no longer permits a duality transformation. A different choice of variables with which to explore a dissipation induced transition is therefore called for. Our choice in (8) and (9) permits this.
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