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<td>doi://10.1103/PhysRevLett.101.027005</td>
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Nodal quasiparticles and the onset of spin density wave order in the cuprates

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(Dated: February 5, 2008)

We present a theory for the onset of spin density wave order in the superconducting ground state of the cuprates. We compute the scaling dimensions of allowed perturbations of a ‘relativistic’ fixed point with O(4)⊗O(3) symmetry, including those associated with the fermionic nodal Bogoliubov quasiparticles. Analyses of up to six loops show that all perturbations with square lattice symmetry are likely irrelevant. We demonstrate that the fermion spectral functions are primarily damped by the coupling to fluctuations of a composite field with Ising nematic order. We also discuss the influence of quenched disorder.

A large number of experiments have investigated the magnetic correlations in the cuprate superconductors [1]. There is good evidence for collinear spin density wave (SDW) correlations near the wavevectors

\[ \mathbf{K}_1 = \left( \frac{2\pi}{a}, \frac{1}{2} - \vartheta \right), \quad \mathbf{K}_2 = \left( \frac{2\pi}{a}, \frac{1}{2} \cdot \frac{1}{2} - \vartheta \right), \]

where \( a \) is the square lattice spacing and the incommensurate \( \vartheta \) varies with the hole doping concentration, especially in the La based compounds, this order is best formed near \( \delta = 1/8 \), where \( \vartheta \approx 1/8 \). This SDW order coexists with superconductivity (SC), and a theory [2] for the tuning of the transition between the SDW+SC and SC states by an applied magnetic field has been tested in a number of experiments [3,4,5,6,7]. In this paper, we will examine the interplay between the SDW order and the fermionic Bogoliubov quasiparticle excitations of the superconductor. Because of the \( d \)-wave nature of the Cooper pairs, these quasiparticles have the spectrum of massless Dirac particles whose energy vanishes at four wavevectors (the nodal points) in the Brillouin zone (±Q, ±Q); these nodal wavevectors bear no relation to the SDW ordering wavevectors \( \mathbf{K}_{1,2} \). Using a theory for the critical fluctuations of the SDW order developed in Refs. [2,8,9], we will show that the dominant coupling between nodal quasiparticles and the SDW order is to a composite Ising nematic order [10], associated with the choice of the SDW ordering between the \( \mathbf{K}_1 \) and \( \mathbf{K}_2 \) wavevectors. We emphasize that the unique selection of Ising nematic order here is not a phenomenological assumption, but a non-trivial consequence of the internal structure of the SDW fixed point of De Prato et al. [9]: indeed, this is the main point of this paper. Our theory predicts nodal quasiparticle spectral functions which have been measured in numerous photoemission and scanning tunnelling microscopy experiments. The importance of the Ising nematic order in damping nodal quasiparticles was noted recently by Kim et al. [11] in a different model [12], and we will compare our results to theirs.

Our theory is expressed in terms of the complex-valued order parameters \( \Phi_{1,i} \) and \( \Phi_{2,i} \), where \( i = x, y, z \) denotes spin components, which are related to the spin operator, \( S_1 \), at position \( \mathbf{r} \) and imaginary time \( \tau \) by

\[ S_i(\mathbf{r}, \tau) = \text{Re} \left[ e^{i \mathbf{K}_i \cdot \mathbf{r}} \Phi_{1,i}(\mathbf{r}, \tau) + e^{-i \mathbf{K}_i \cdot \mathbf{r}} \Phi_{2,i}(\mathbf{r}, \tau) \right]. \]

This parameterization implies the transformation properties of \( \Phi_{1,2} \), under the symmetry operations on the underlying square lattice Hamiltonian, which are summarized in Fig. 1. By writing down all terms invariant under these operations, and expanding in powers and gradients of \( \Phi_{1,2} \), we obtain the following quantum field theory for the fluctuations of the SDW order [2,8], with action \( \int d^2 \mathbf{r} \tau \mathcal{L}_\Phi \) and

\[
\mathcal{L}_\Phi = |\partial_r \Phi_1|^2 + v_1^2 |\partial_x \Phi_1|^2 + v_2^2 |\partial_y \Phi_1|^2 \\
+ |\partial_r \Phi_2|^2 + v_2^2 |\partial_x \Phi_2|^2 + v_1^2 |\partial_y \Phi_2|^2 + \tau (|\Phi_1|^2 + |\Phi_2|^2) \\
+ w_1 (|\Phi_1|^4 + |\Phi_2|^4) + w_2 (|\Phi_1|^2 + |\Phi_2|^2)^2 \\
+ w_3 |\Phi_1|^2 |\Phi_2|^2 + w_4 |\Phi_1 \cdot \Phi_2|^2 + w_5 |\Phi_1^* \cdot \Phi_2|^2, \tag{2}
\]

where \( v_1, v_2 \) are spin-wave velocities, \( r \) is the coupling which tunes the system across the transition to a state...
with SDW order, and $u_{1,2}$ and $w_{1,2,3}$ are the crucial quartic couplings which stabilize and select the SDW order. Linear spatial derivative terms such as $\Phi_i^\dagger \partial_i \Phi_1$ are also permitted, but can be absorbed by a redefinition of the incommensuration $\vartheta$. For some of the cuprates with $\delta \approx 1/8$, the ordering is commensurate with $\vartheta = 1/8$; in this case a lock-in term $\sim (\Phi_i^\dagger)^4 + (\Phi_2^\dagger)^4$ is allowed, but this eighth order term is clearly irrelevant near the critical point, and can be safely neglected in our considerations here.

The weight of the experimental evidence, reviewed e.g. in Ref. [1] is that the SDW order in the cuprates is collinear in spin space, and picks a definite spatial direction by a choice of condensing either $\Phi_1$ or $\Phi_2$. So a particular state has

$$\langle \Phi_{1i} \rangle = n_i e^{i \vartheta}, \quad \langle \Phi_{2i} \rangle = 0,$$

or an equivalent state with $1 \leftrightarrow 2$, with $n_i$ an arbitrary real vector and $e^{i \vartheta}$ a common complex phase for the components of $\Phi$. In mean field theory, such a state is the ground state of the theory $S_\Phi$ in a subset of the region of parameters satisfying $\tau < 0$, $w_1 > 0$, $w_1 + w_2 + w_3 > 0$, $w_2 < \min[0, w_1 - u_1, w_1 + w_2 + w_3 - u_1, (w_1 + w_2 - u_1)/2, (w_1 + w_3 - u_1)/2]$. Going beyond mean field theory, a detailed analysis of the transition into this SDW state under the Lagrangian $\mathcal{L}_\Phi$ was provided in Ref. [2]. It was found that such a transition was in the domain of attraction of a fixed point with $O(4) \otimes O(3)$ symmetry within two three-dimensional perturbative schemes: (i) the massive zero-momentum scheme (MZM) defined in the unbroken phase (to six loops), and (ii) the minimal subtraction scheme (MS) without expansion in $3 - d$ (d is the spatial dimension, and $d = 2$ was set after renormalization) defined in the massless critical theory (to five loops). High-order perturbative calculations indicate the stability of this point also in the SDW model $\mathcal{L}_\Phi$, i.e. the quartic perturbations present in $\mathcal{L}_\Phi$ turn out to be irrelevant at $O(4) \otimes O(3)$ fixed point. The values of the quartic couplings in the fixed-point Lagrangian $\mathcal{L}_\Phi^*$ obey $w_1^* = u_1^* - u_2^*$ and $w_2^* = w_2^* + u_3^*$, and the spin-wave velocities are equal $v_1^* = v_2^*$. The symmetry of the fixed point becomes explicit by introducing a 12-component real field $\varphi_{ai}$, with $a = 1 \ldots 4$, related to the SDW order

$$\Phi_{1i} = \varphi_{1i} + i \varphi_{2i}, \quad \Phi_{2i} = \varphi_{3i} + i \varphi_{4i};$$

now the $O(4)$ and $O(3)$ rotations act on the $a$ and $i$ indices respectively. The critical exponents associated with this fixed point are the correlation length exponent, $\nu = 0.9(2)$, and the anomalous dimension of the SDW order parameter, $\eta = 0.15(10)$.

We are now ready to turn to our new results on the coupling between the above SDW fluctuations and the excitations of the superconductor.

Density fluctuations of the superconducting condensate will couple to $|\Phi_1|^2 + |\Phi_2|^2$. For short-range repulsive interactions between the Cooper pairs, this coupling has scaling dimension $13(2 - 3\nu)/2 < 0$ and so is irrelevant. The long-range Coulomb interactions further suppress density fluctuations, and so we need not consider this coupling further.

Far more interesting, and subtle, are the couplings between $\Phi_{1,2}$ and the fermionic nodal quasiparticles. Let us denote the electron annihilation operator with momenta in the vicinity of the nodes as $(Q, \mathbf{Q})$, $(-Q, \mathbf{Q})$, $(-Q, -\mathbf{Q})$, and $(Q, -\mathbf{Q})$ by $f_{1a}$, $f_{2a}$, $f_{3a}$, and $f_{4a}$ respectively; here $a = \uparrow, \downarrow$ is an electron spin index. Next, we introduce the 4-component Nambu spinors

$$\Psi_{1a} = \left( \begin{array}{c} f_{1a} \\ \varepsilon_{\alpha\beta} f_{3\beta}^\dagger \end{array} \right), \quad \Psi_{2a} = \left( \begin{array}{c} f_{2a} \\ \varepsilon_{\alpha\beta} f_{4\beta}^\dagger \end{array} \right)$$

where $\varepsilon_{\alpha\beta} = -\varepsilon_{\beta\alpha}$ and $\varepsilon_{11} = 1$. We will use Pauli matrices $\tau^i$ which act on the Nambu particle-hole space, while $\sigma_{\alpha\beta}$ will act on spin space. In the vicinity of the nodal points, we can expand the standard Bogoliubov Hamiltonian of a $d$-wave BCS superconductor in term of gradients of $\Psi_{1,2}$, and obtain the low energy theory $S_\Phi = \int d^2 r d\tau \mathcal{L}_\Phi$ with

$$\mathcal{L}_\Phi = \Psi_1^\dagger \left( \partial_\tau - i \frac{v_\tau}{\sqrt{2}} (\partial_x + \partial_y) \tau^\dagger - i \frac{v_\Delta}{\sqrt{2}} (\partial_x + \partial_y) \tau^\dagger \right) \Psi_1 + \Psi_2^\dagger \left( \partial_\tau - i \frac{v_\tau}{\sqrt{2}} (\partial_x + \partial_y) \tau^\dagger - i \frac{v_\Delta}{\sqrt{2}} (\partial_x + \partial_y) \tau^\dagger \right) \Psi_2.$$  \hspace{1cm} (6)

Here $v_\tau$ and $v_\Delta$ are the fermionic velocities normal and parallel to the underlying Fermi surface. As was the case with $S_\Phi$, the transformations of the fermionic fields $\Psi_{1,2}$ are also crucial to our analysis, and these are summarized in Fig. 1.

We now write down the most general couplings between the SDW fields $\Phi_{1,2}$ and the Dirac fermion excitations $\Psi_{1,2}$ which are allowed by the symmetries in Fig. 1. The translational symmetries $T_{x,y}$ immediately rule out any terms linear in $\Phi$: the SDW fluctuations scatter the electrons by wavevectors $K_{1,2}$ and these do not, in general, connect the low energy excitations at any pair of nodal points. Moving on to terms quadratic in $\Phi$, which are generated by a virtual scattering process to a high energy intermediate fermion excitation (see also Ref. [14]), all the allowed terms are

$$\mathcal{L}_1 = \lambda_1 (|\Phi_1|^2 + |\Phi_2|^2) \left( \Psi_1^\dagger \tau^\dagger \Psi_1 + \Psi_2^\dagger \tau^\dagger \Psi_2 \right),$$

$$\mathcal{L}_2 = \lambda_2 (|\Phi_1|^2 - |\Phi_2|^2) \left( \Psi_1^\dagger \tau^\dagger \Psi_1 + \Psi_2^\dagger \tau^\dagger \Psi_2 \right),$$

$$\mathcal{L}_3 = \epsilon_{ijk} \left[ (\Phi_{1i}^* \Phi_{1k} + \Phi_{2i}^* \Phi_{2k}) - \lambda_3 (\Psi_1^\dagger \tau^\dagger \sigma^i \Psi_2 + \Psi_2^\dagger \tau^\dagger \sigma^i \Psi_1) \right. \right. \left. \left. + (\Phi_{1i}^* \Phi_{1k} - \Phi_{2i}^* \Phi_{2k}) \left( \lambda_4 \Psi_1^\dagger \tau^\dagger \sigma^i \Psi_1 - \lambda_4 \Psi_2^\dagger \tau^\dagger \sigma^i \Psi_2 \right) \right] \right].$$

Key to our remaining analysis are the scaling dimensions of the $\lambda$ couplings at the $O(4) \otimes O(3)$ fixed point $\mathcal{L}_\Phi$. 

discussed earlier, at which the fermions are decoupled from the SDW order. The free Dirac fermion theory $\mathcal{L}_\Psi$ is also invariant under the same scaling transformation as $\mathcal{L}_\Phi$, with $\dim[\Phi] = 1$, and this allows us to obtain the $\dim[A]$ from a knowledge of the dimensions of the associated composite operators of $\Phi$ under $\mathcal{L}_\Phi$. In particular, we perturb $\mathcal{L}_\Phi$ by the same quadratic $\Phi$ operators above but without the fermion terms, and subtract 2 from the scaling dimension of such a perturbation. So e.g. we consider the theory $\mathcal{L}_\Phi + \lambda_1 (|\Phi_1|^2 + |\Phi_2|^2)$ and obtain $\dim[\lambda_1] = \dim[\tilde{\lambda}_1] - 2$. We classify such perturbations under representations of $O(4) \otimes O(3)$, with $D_K$ indicating a dimension $D$ representation of $O(K)$. Then $\tilde{\lambda}_1$ corresponds to a $\mathbf{(1, 1, 3)}$ operator, $\tilde{\lambda}_2$ to $\mathbf{(9, 1, 1, 3)}$, and $\tilde{\lambda}_3$ to $\mathbf{(6, 1, 3, 3)}$.

The $\mathbf{(1, 1, 3)}$ operator tunes away from the transition by changing $r$, and so

$$\dim[\lambda_1] = 1/\nu - 2. \quad (8)$$

From the value of $\nu$ quoted earlier, we conclude that $\lambda_1$ is safely irrelevant.

The second coupling between $\Phi$ and the fermions involves the operator $\phi \equiv |\Phi_1|^2 - |\Phi_2|^2$, which is the Ising nematic order parameter $\mathbf{(1, 1, 1)}$. This measures fluctuations which break the orthorhombic symmetry, $C_{4v}$, of the square lattice to tetragonal symmetry, $C_{2v}$, by making a choice of the SDW order between the $\mathbf{K}_1$ and $\mathbf{K}_2$ wavevectors. This operator is a component of the $\mathbf{(9, 1, 1, 3)}$ operators, and to obtain its scaling dimension we computed and analyzed perturbative series within the MZM (to six loops) and $\overline{\text{MS}}$ (to five loops) expansion schemes. Details on the perturbative calculations and the series will be reported elsewhere. The comparison of the analyses within the MZM and $d = 3 \overline{\text{MS}}$ schemes represents a non trivial check of the results. In order to estimate the scaling dimension, we need to resum the series and then to evaluate them at the fixed point values of the quartic couplings. The resummation of the series is performed by using the so-called conformal mapping method, which exploits the knowledge of the large-order behavior of the expansions $\mathbf{16, 17}$. In this manner we obtained

$$\dim[\lambda_2] = \begin{cases} 
1.95(18) - 2 & \text{MZM} \\
1.90(27) - 2 & d = 3 \overline{\text{MS}}
\end{cases} \quad (9)$$

These results favor the irrelevance of $\lambda_2$ at the decoupled fixed point, although the precision of our results does not allow us to state this conclusively. In any case, it is clear that $\dim[\lambda_2]$ is nearly zero, indicating that $\lambda_2$ hardly flows under the renormalization group (RG).

Finally, the $\lambda_3, \lambda'_3$ couplings in Eq. (7) involve composite $\Phi$ operators (which are components of $\mathbf{(6, 1, 3, 3)}$), which measure spiral spin correlations, as is easily deduced from Eq. (1). By an analysis as above, we found

$$\dim[\lambda_3, \lambda'_3] = \begin{cases} 
1.16(8) - 2 & \text{MZM} \\
1.24(8) - 2 & d = 3 \overline{\text{MS}}
\end{cases}, \quad (10)$$

indicating that such perturbations are clearly irrelevant.

We have now established one of the main results of our paper: the only important coupling of the nodal fermions to the SDW order is $\lambda_3$, which couples the fermionic and SDW contributions to the Ising nematic order $\phi$.

Let us now compute of the influence of the SDW fluctuations on the fermionic spectral functions perturbatively in $\lambda_3$. At leading order, we use the propagator for $\phi$, implied by its scaling dimension in Eq. (9)

$$G_{\phi}(p, \omega) \sim \left[v^s p^2 + \omega^2\right]^{-1/2 - \dim[\lambda_2]}$$

where $p$ and $\omega$ are the momentum and imaginary frequency carried by $\phi$. To second order in $\lambda_3$, for the fermion Green’s function $G_{\Psi}$ we obtain the self energy

$$\Sigma_{\Psi}(q, \Omega) = \lambda_3^2 \int \frac{d^2p}{4\pi^2} \frac{d\omega}{2\pi} G_{\phi}(p, \omega) \tau^x G_{\Psi}(q - p, \Omega - \omega) \tau^x \quad (12)$$

From the finite temperature ($T$) generalization of Eq. (12), we obtain at the nodal point, the retarded, real frequency self energy $\text{Im} \Sigma_{\Psi}(0, 0) \sim T^{1 - \dim[\lambda_2]}$ in the quantum-critical region $\mathbf{12}$. This is the leading $T$ dependence for $\dim[\lambda_2] < 0$. For $\dim[\lambda_2] > 0$, the RG flow must be computed to higher order in $\lambda_2$, and if there is a fixed point with a non-zero $\lambda_2^*$, then $T$ is characteristic energy scale for quasiparticle damping. Given the near-marginality of $\lambda_2$ (Eq. (9)), it is valid to ignore its RG flow in experimental applications, and so we obtain a quasiparticle scattering rate which is practically linear in $T$. Similarly, at the nodal wavevectors, a nearly linear frequency dependence is found in the fermion self energy at $T = 0$. These are phenomenologically attractive features $\mathbf{18}$.

In describing the $q$ dependence of the fermion spectrum, we can use results from the computation by Kim et al. $\mathbf{11}$. They used a model $\mathbf{12}$ in which the $\phi$ field was the primary order parameter undergoing phase transition, and not a composite of the SDW order as in our theory above. In such a primary $\phi$ theory, the $\lambda_2$ coupling is strongly relevant at the decoupled fixed point $\mathbf{12}$ (in contrast to the nearly marginal $\lambda_2$ in our theory), and a RG analysis is necessary to find a fixed point at non-zero $\lambda_2$. No such fixed point was found in the $3 - d$ expansion of Ref. $\mathbf{12}$ for any number of fermion flavors, while Kim et al. $\mathbf{11}$ noted that a second order transition was present $d = 2$ in the limit of an infinite number of fermion flavors. Regardless of the status of this possible fixed point for the physical case, for our purposes here, we note that Kim et al.’s computation of the fermion spectrum differed from Eq. (12) only in their assumed form for $G_{\phi}$, with Eq. (11) replaced by $G_{\phi} \sim \left[\omega^2 + v^s p^2 + \omega^2 + v_{\lambda}^2 p^2\right]^{1/2} +$.
It is also present in our theory, as an order of fermion fluctuations to the propagator. Such contributions are also present in our theory, as an order $\lambda_2^2$ contribution to $G_\phi$ by $G_{\phi}^{-1} \rightarrow G_{\phi}^{-1} + \lambda_2^2 G_{\phi}^{-1}$, given that $\lambda_2$ is nearly marginal at the decoupled fixed point, it is reasonable that this correction, which is formally higher in $\lambda_2$, should be included in Eq. (12).

With $G_\phi$ renormalized with fermion loop contributions as above, our results for the fermion spectral function are reasonable that this correction, which is formally higher in $\lambda_2$, should be included in Eq. (12).

We can also use our results here for the scaling dimensions of the quadratic perturbations at the $O(4) \otimes O(4)$ fixed point to analyse the influence of quenched disorder. Unless magnetic impurities are explicitly introduced, the quenched disorder in the cuprates is spin rotation invariant, and we assume so in our discussion here. Such disorder can only couple to operators, $O_D$, which transforms as $D_{\alpha}$, the only allowed values are $D = 1, 9$, and the scaling dimension of the associated couplings were quoted in Eqs. (59). After an average over disorder in a replica analysis, the perturbation to $L_\phi$ can be written as

$$\gamma_D \sum_{\ell, m} \int d^2 x d\tau d\tau' O_D^\ell(x, \tau) O_D^{m}(x, \tau')$$

where $\ell, m$ are replica indices. A computation of scaling dimensions now shows that the maximum value of $\dim[\gamma_D]$ is for $D = 9$, and so the most relevant disorder-induced coupling is $\gamma_9$ with

$$\dim[\gamma_9] = 2 \dim[\lambda_2] + 2,$$

which is clearly strongly relevant. One of the components of $O_9$ is $\phi$, the Ising nematic order, while the remaining 8 components correspond to the complex charge density wave order parameters $\Phi_2^\ell, \Phi_2^m, \Phi_3, \Phi_3^*$ at the wavevectors $2K_1, 2K_2, K_1 + K_2, K_1 - K_2$, respectively. Quenched disorder will therefore induce these orders in glasses configurations, as was studied numerically in Refs. [15, 22].

This paper has shown that the well-established SDW order of the cuprate superconductor series [1, 4, 5, 6, 7] has precursor quantum fluctuations which can naturally explain key features [18, 19, 20, 21] of the spectrum of single electron excitations. We showed that an Ising nematic order, associated with fluctuations which reduce the square lattice symmetry to a rectangular symmetry [10], was uniquely selected as a composite of the SDW order which couples most efficiently to the low energy single-electron excitations.

We thank Erez Berg, Eduardo Fradkin, Eun-Ah Kim, Steven Kivelson, Michael Lawler, and Cenke Xu for useful discussions. This research was supported by NSF grant DMR-0537077.