Specific heat anomaly in the d-density wave state and emergence of incommensurate orbital antiferromagnetic order

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We study the effect of finite chemical potential on the d-density wave state that has been proposed to explain the pseudogap phenomena in underdoped cuprates. We find that the specific heat anomaly at the transition temperature, below which the d-density wave state forms, gets weaker when finite chemical potential is introduced. This provides a useful ground for the proper interpretation of the specific heat measurement in regard to the existence of the d-density wave state below the pseudogap temperature. Further increase of the chemical potential leads to an incommensurate orbital antiferromagnetic state before the system eventually turns into the normal state. This is an inhomogeneous state characterized by novel charge ordering and an analog of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state in superconductivity.

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a. Introduction One of the recent interesting proposals made in high temperature superconducting cuprates is that the so-called d-density wave state is responsible for the pseudogap phenomena.\cite{1, 2} The d-density wave state is a particle-hole paired state with a finite momentum $Q_0 = (\pi, \pi)$. The particle-hole pair wavefunction has a d-wave symmetry, $f(k) \propto \cos k_x - \cos k_y$, that occurs due to the formation of staggered currents circulating in the square lattice. Therefore, the d-density wave state breaks the translational and time reversal symmetries.\cite{3, 4}

Since the d-density wave state is an orbital antiferromagnetic state, there should be an elastic neutron scattering signal at the momentum $Q_0$. This is a direct consequence of the broken symmetry. It was argued that the recent neutron scattering experiment is consistent with the existence of the d-density wave state in underdoped cuprates\cite{5, 6}. On the other hand, there is no clear experimental evidence of the broken symmetry state in thermodynamic quantities, such as specific heat at $T^*$ where the pseudogap develops. It has been regarded that this is at odds with the proposal, because one may expect that there should be a clear specific heat jump due to the translational symmetry breaking. In fact, in the case of the half-filled band, the normalized specific heat jump for the d-density wave state is the same as that of the d-wave superconducting state within the mean field theory. This is simply because these states have the same form of the quasiparticle spectrum, $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$ when the chemical potential is zero ($\mu = 0$). Here $\Delta_k = \Delta_0 \cos (2\theta_k)$ is the d-wave gap in the d-density wave state or in the d-wave superconductor. The specific heat measurements\cite{4} show a clear evidence of the phase transition at $T_c$, while there is no anomaly reported at $T^*$.

This conclusion should be, however, reexamined when the system is away from half-filling. In the presence of the finite chemical potential, $\mu$, the quasiparticle spectrum is quite different for two cases. In the d-wave superconductor, the quasiparticle dispersion is given by $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}$, while in the d-density wave state it is given by $E_k = -\mu + \sqrt{\epsilon_k^2 + \Delta_k^2}$. The difference comes from the fact that one is a particle-particle paired state and the other is a particle-hole paired state.

In this paper, motivated by the above observations, we study the effect of the finite chemical potential on the incommensurate orbital antiferromagnetic state dubbed “d-density wave state”. Using a BCS-like Hamiltonian for the d-density wave state, we show that 1) the specific heat anomaly at the transition temperature, $T = T_d$, due to the d-density wave ordering gets weaker as the chemical potential increases. Therefore, when the chemical potential is appreciably large, it will be hard to determine the existence of the d-density wave state by measuring the specific heat. In view of the importance of the finite chemical potential, we ask whether there is a phase transition driven by the chemical potential. We find that 2) the stability of the d-density wave state gets weaker as the chemical potential increases, and beyond a critical value, an incommensurate orbital antiferromagnetic state occurs in a range of chemical potential. It is an inhomogeneous state characterized by charge ordering in contrast to the d-density wave state with uniform charge density and an analog of the FFLO state in superconductivity.\cite{8}

Certain choices of the incommensuration correspond to the stripe patterns of the charge ordering similar to those discussed in the context of the spin density wave in the cuprates.\cite{9}

b. Role of the chemical potential The d-density wave state is a particle-hole paired state where the band dispersion of the particles and holes satisfy $\epsilon_k = -\epsilon_{k+Q_0}$ with $Q_0 = (\pi, \pi)$. Within mean field approximation, the d-density wave state can be stable in an extended Hubbard model at half-filling, i.e., $\mu = 0$, where the particle-hole symmetry exists.\cite{10}

When the chemical potential becomes finite, $\mu \neq 0$, the number of particles is not equal to that of holes. Therefore, the chemical potential suppresses the tendency of paring and effectively acts as a pair breaker. In other words, the nesting condition gets weaker with finite chemical potential, so does the stability of the d-
density wave state. In fact, the chemical potential can be regarded as an analog of the Zeeman magnetic field in superconducting states, where the Zeeman field splits the up- and down-spin bands and acts as a pair breaker. We will show below that the gap equation of the d-density wave state with finite \( \mu \). Eq. [3] is the same as that of the d-wave superconducting state with a finite Zeeman field. [14, 13] Once we realize this simple analogy, it is clear that the specific heat anomaly will be reduced by introducing the chemical potential. This is because the Fermi surface is no longer a point, but there will be a hole pocket whose size depends on the magnitude of \( \mu \). There were similar studies in the spin density wave showing that the specific heat jump gets smaller when the nesting condition gets weaker. [12]

c. Specific heat anomaly in the d-density wave state

In order to compute the specific heat jump at the transition temperature, \( T_d \), we use the following BCS-like Hamiltonian.

\[
H - \mu N = \sum_{k,\sigma} (\epsilon_k - \mu) c_{k,\sigma}^d c_{k,\sigma}^\dagger + \sum_{k, k', Q, \sigma, \sigma'} g_{kk'Q} \epsilon_k^Q c_{k,\sigma}^d c_{k+Q,\sigma'}^d c_{k',\sigma'}^\dagger c_{k',\sigma'}^\dagger, \tag{1}
\]

where \( \epsilon_k \) is the band dispersion and satisfies \( \epsilon_k = -\epsilon_k + Q_0 \). \( g_{kk'Q} \) is the pairing potential that takes the following form when \( Q = Q_0 \).

\[
g_{kk'Q_0} = -g \cos (2\theta_k) \cos (2\theta_{k'}). \tag{2}
\]

The gap equation is obtained in the mean field approximation as follows.

\[
1 = \frac{g N(0)}{2} \int_0^\omega \frac{d\epsilon}{2\pi} \int_0^{2\pi} \frac{d\theta}{2\pi} \frac{\cos^2 2\theta}{\epsilon^2 + \Delta^2 \cos^2 2\theta} \times \left[ \tanh \left( \frac{E_k - \mu}{2T} \right) + \tanh \left( \frac{E_k + \mu}{2T} \right) \right], \tag{3}
\]

where \( E_k^2 = \epsilon_k^2 + \Delta^2 \cos^2 2\theta \) and we define \( \mu \) to be positive.

Here \( N(0) \) is the density of state at \( \epsilon = 0 \), and we have assumed that there is no singularity in \( N(0) \).

Using the standard procedure, one can obtain the following formula for the transition temperature \( T_d(\mu) \) at finite chemical potential.

\[
\ln \frac{T_{d0}}{T_d} = \text{Re} \Psi \left( \frac{1}{2} + \frac{i\mu}{2\pi T_d} \right) - \psi \left( \frac{1}{2} \right), \tag{4}
\]

where \( T_{d0} \) is the transition temperature when \( \mu = 0 \) and \( \psi(x) \) is the di-gamma function. As expected, \( T_d(\mu) \) decreases as the chemical potential increases.

Now let us evaluate the specific heat jump at \( T = T_d \). Since we are interested in the specific heat anomaly at \( T = T_d \), we expand the gap equation in \( \Delta(\mu, T)/\pi T \). Using the conventional method described in [14], the specific heat jump at \( T_d \) can be computed as

\[
C_{ddw}(T_d) - C_N(T_d) = \frac{16\pi^2 T_c}{3\text{Re} \Psi(3, 1/2 + i\mu/2\pi T_d)} \times \left[ 1 + \frac{\mu}{2\pi T_d} \text{Im} \zeta(2, 1/2 + i\mu/2\pi T_d) \right]^2, \tag{5}
\]

where \( \zeta(s, a) = \sum_{n=0}^\infty 1/(n + a)^s \). Here \( C_{ddw} \) and \( C_N \) represent specific heat of the d-density wave state and normal state respectively.

The specific heat coefficient \( \gamma_{ddw} = C_{ddw}/T \) at \( T = T_d \) is shown in Fig. 1 as a function of \( \mu/T_d \), where \( \gamma_N \) in the normal state is set to be unity (\( \gamma_N = 1 \)). As shown in Fig. 1, the specific heat anomaly, \( \delta \gamma_{ddw}/\gamma_N = (\gamma_{ddw} - \gamma_N)/\gamma_N \) gets smaller as \( \mu \) increases. Now let us compare the absolute value of the specific heat anomaly, \( \delta \gamma_{ddw}/\gamma_N \), with that of the d-wave superconducting state, \( \delta \gamma_{s/c}/\gamma_N = 0.9 \). In the case of the d-density wave state, when \( \mu = 0.6T_d \), \( \delta \gamma_{ddw}/\gamma_N = 0.26 \).

Thus, the specific heat jump associated with the d-density wave state can be quite small compared with that of the d-wave superconducting state when the chemical potential is finite. Notice that our results are obtained in the mean field theory and the anomaly can be even smaller once we take into account the fluctuation effects.

d. Phase transition

Provided that the chemical potential in the d-density wave state plays the same role as the Zeeman magnetic field in superconductors, let us first review the phase transition driven by a Zeeman field in superconductors. It is clear that sufficiently strong Zeeman field will eventually drive a phase transition into the normal state. The nature of the transition is determined by the competition between two energy scales; the condensation energy \( \frac{1}{2} N(0) \Delta^2 \) and the magnetic energy \( \chi H^2 \) where \( \chi \) is the spin susceptibility proportional to the density of state \( N(0) \). This competition leads to the phase transition between the BCS state and normal state at a critical Zeeman field \( H_c = \Delta/(\sqrt{2}\mu_B) \) (\( \mu_B \) is the Bohr magneton) for s-wave superconductors. On the other hand, it has been also known that, for a range of intermediate strength of the Zeeman field around \( H_c \), it is more favorable to pair up- and down-spin electrons across the spin-split Fermi surfaces and form an inhomogeneous superconducting state. This is called the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state. [13, 10] The phase
transition from the BCS superconducting state to the FFLO state is the first order transition for both s-wave and d-wave superconductors\cite{11,12,13}.

The d-density wave state with finite chemical potential should experience the same kind of phase transition due to the existence of two competing energy scales. The condensation energy favors the particle-hole paired state. As the chemical potential increases, however, the normal state is favored by $N(0)\mu^2$. Therefore, the qualitative phase diagram should be similar to those obtained in superconductivity\cite{11,12,13}. What is really interesting is that there is a window of chemical potential where a novel phase, an analog of the FFLO state, is favorable over the commensurate orbital antiferromagnetic and normal states. This phase is the incommensurate orbital antiferromagnetic state, where the particle-hole pairing occurs with a momentum $\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}$, where $|\mathbf{q}| \propto \mu$ at $T = 0$. Similar studies were undertaken in the context of the excitonic insulator and an inhomogeneous phase with the s-wave symmetry was identified.\cite{13}

e. Incommensurate orbital antiferromagnetic state

The incommensurate orbital antiferromagnetic order arises when a staggered current is circulating in the plane but its periodicity is incommensurate with the underlying square lattice.

![FIG. 2: (a) An example of the incommensurate orbital antiferromagnetic state with $\mathbf{q} = (0, \pi/3)$. The numbers represent the relative strength of each bond current. Since $q_x = 0$, the current is alternating with the same strength along the x-direction. (b) The charge modulation in real space for $\mathbf{q} = (0, \pi/3)$. The black and white circles represent the amplitudes of the charge modulation proportional to $\sin(\pi/3)$ and $\sin(-\pi/3)$ respectively. There is no charge modulation at the empty sites.](image)

Current modulation: It is straightforward to obtain the expectation value of the bond current in the incommensurate orbital antiferromagnetic state, $\langle J_{\mathbf{r}'\mathbf{r}} \rangle = i \langle c_{\mathbf{r}' \mathbf{r}}^\dagger c_{\mathbf{r} \mathbf{r}} \rangle$. Taking $\mathbf{r}' = \mathbf{r} + \hat{x}$ and $\mathbf{r}' = \mathbf{r} + \hat{y}$, the current modulation is obtained as

$$\langle J_{\mathbf{r},\mathbf{r}+\hat{x}} - J_{\mathbf{r},\mathbf{r}+\hat{y}} \rangle = i \sum_{\mathbf{k}} \langle c_{\mathbf{r}' \mathbf{k}+\mathbf{Q}_0+\mathbf{q}}^\dagger c_{\mathbf{r} \mathbf{r}} \rangle \times \{ [f(\mathbf{k}, \mathbf{q}) - ig(\mathbf{k}, \mathbf{q})] \cos[(\mathbf{Q}_0 + \mathbf{q}) \cdot \mathbf{r}] - [g(\mathbf{k}, \mathbf{q}) + if(\mathbf{k}, \mathbf{q})] \sin[(\mathbf{Q}_0 + \mathbf{q}) \cdot \mathbf{r}] + c.c. \}. \quad (6)$$

Here $f(\mathbf{k}, \mathbf{q})$ and $g(\mathbf{k}, \mathbf{q})$ are given by

$$f(\mathbf{k}, \mathbf{q}) = \cos k_x - \cos k_y$$
$$+ \cos (k_x + q_x) - \cos (k_y + q_y),$$
$$g(\mathbf{k}, \mathbf{q}) = \sin k_y - \sin k_x$$
$$+ \sin (k_x + q_x) - \sin (k_y + q_y). \quad (7)$$

The order parameter of a particle-hole paired state with the momentum $\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}$ is the simplest choice for the incommensurate orbital antiferromagnetic order.

$$\langle c_{\mathbf{k} \mathbf{r}' \mathbf{k}+\mathbf{Q}_0+\mathbf{q}} \rangle = \frac{1}{2} \Delta_{\mathbf{Q}_0+\mathbf{q}} f(\mathbf{k}, \mathbf{q}), \quad (8)$$

where $f(\mathbf{k}, \mathbf{q})$ is given by Eq. (6). This order parameter of the particle-hole pairing is an analog of the FFLO order parameter of the particle-particle pairing. It is also reduced to the order parameter of the d-density wave state when $\mathbf{Q} = \mathbf{Q}_0$.

The order parameter, Eq. (8), leads to the following current pattern in real space:

$$\langle J_{\mathbf{r},\mathbf{r}'} \rangle = (-1)^r \Delta_{\mathbf{Q}_0+\mathbf{q}}$$
$$\times \left[ \delta_{x',x+1} \delta_{y',y} \{ \cos(\mathbf{q} \cdot \mathbf{r}) + \cos(\mathbf{q} \cdot \mathbf{r} + q_x) \} \right.$$
$$+ \delta_{x',x-1} \delta_{y',y} \{ \cos(\mathbf{q} \cdot \mathbf{r}) + \cos(\mathbf{q} \cdot \mathbf{r} - q_x) \}$$
$$- \delta_{y',y+1} \delta_{x',x} \{ \cos(\mathbf{q} \cdot \mathbf{r}) + \cos(\mathbf{q} \cdot \mathbf{r} + q_y) \}$$
$$- \delta_{y',y-1} \delta_{x',x} \{ \cos(\mathbf{q} \cdot \mathbf{r}) + \cos(\mathbf{q} \cdot \mathbf{r} - q_y) \} \]. \quad (9)$$

One example of the incommensurate staggered current patterns is shown in Fig. 2 (a), where $\mathbf{q} = (0, \pi/3)$. Different choices of the ordering vector $\mathbf{Q}$ lead to different patterns of the incommensurate staggered currents. For $\mathbf{q} = (0, \pi/3)$, the current density has the modulation with the period $[2a, 3a]$ in the x- and y-directions, where $a$ is the lattice constant. Notice that there exists a set of the vanishing bond currents, $J_{\mathbf{r},\mathbf{r}+\mathbf{q}} = 0$, that are aligned along the x-direction. This “bond-centered” stripe-like structure leads to the charge modulation (computed in the next section) that has the same periodicity as that of the current, as shown in Fig. 2 (b).

On the other hand, when $\mathbf{q} = (0, \pi/4)$, a set of the vanishing bond currents in the y-direction, $J_{\mathbf{r},\mathbf{r}+\hat{y}} = 0$, exists. This corresponds to the “site-centered” stripe-like structure along the y-direction in the current pattern. As a result, the periodicity of the current is $[2a, 8a]$, while that of the charge density is $[2a, 4a]$. That is, the periodicity of the current along the y-direction is twice larger than that of the charge.

Charge ordering in the incommensurate orbital antiferromagnetic state: The staggered current pattern in the d-density wave state gives no charge modulation due to $\sum_{\mathbf{k} \in RBZ} \cos(k_x - k_y) = 0$, where RBZ
stands for the reduced Brillouin zone. This property distinguishes the d-density wave state from the ordinary charge density wave state.

In the incommensurate orbital antiferromagnetic state, we find that there exists a charge modulation. As an example, let us compute the charge density when the staggered current pattern is given by Fig. 2 (a), where \( q = (0, \pi/3) \). The local charge density can be obtained from

\[
\langle \psi^\dagger (\mathbf{r}) \psi (\mathbf{r}) \rangle = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} (c^\dagger_{\mathbf{k}'} c_{\mathbf{k}}) \exp [i (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]
\]

\[= n_0 + \Delta q_{\mathbf{k}_0} \sin \left( |\mathbf{Q}_0 + \mathbf{q}| \cdot \mathbf{r} \right), \tag{10}\]

where

\[
h(q_y) = \sum_{\mathbf{k} \in RBZ} \left[ 2 \cos k_x - \cos k_y - \cos (k_y + q_y) \right] \tag{11}\]

The resulting charge modulation is shown in Fig. 2 (b). Notice that the stripe patterns of the charge ordering occur for \( q = (0, \pm q_y) \) and \( q = (\pm q_x, 0) \). The amplitude of the charge modulation depends on the value of \( q_y \) via \( h(q_y) \) (for example, \( h(\pi/5) = -0.42 \)) and it vanishes at \( q_y = 0 \), which confirms the absence of a charge modulation in the d-density wave state. A similar, but different, relation between the charge density wave and the spin density wave was discussed in Refs. [9] and [19].

The charge ordering patterns depend on the nature of the incommensuration of the current density and can be observed by X-ray scattering. Some of the possible charge ordering patterns have stripe structures similar to, but different from, those discussed in the context of the spin density wave in the cuprates.

A checker-board pattern of the charge ordering can also occur if \( q = (\pm |q_x|, \pm |q_y|) \). The checker-board pattern gets distorted as the asymmetry between \( q_x \) and \( q_y \) increases.

### f. Discussion and Conclusion

We show, at the mean-field level, that the specific heat jump at the transition temperature of the d-density wave order gets weaker when the chemical potential is finite. As a result, it becomes more difficult to determine the existence of the d-density wave state as the system is away from half-filling. The relevance of our results to the cuprates depends on the doping dependence of the chemical potential, which is currently not well understood. There is an indication in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) that the chemical potential may be pinned in the underdoped regime. In this case, our result of the weak specific heat anomaly does not apply. Our results are more relevant when the chemical potential moves sensitively as the doping concentration changes, which seems to happen near the optimally doped regime. Further increase of the chemical potential leads to a phase transition into the incommensurate orbital antiferromagnetic state, where a novel charge ordering occurs. The charge ordering patterns depend on the nature of the incommensuration of the current density and can be observed by X-ray scattering. Some of the possible charge ordering patterns have stripe structures similar to, but different from, those discussed in the context of the spin density wave in the cuprates.

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