Intimate relations between electronic nematic, d-density wave and d-wave superconducting states

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Abstract
This paper consists of two important theoretical observations on the interplay between $l = 2$ condensates; d-density wave (ddw), electronic nematic and d-wave superconducting states. (1) There is $SO(4)$ invariance at a transition between the nematic and d-wave superconducting states. The nematic and d-wave pairing operators can be rotated into each other by pseudospin $SU(2)$ generators, which are s-wave pairing and electron density operators. The difference between the current work and the previous $O(4)$ symmetry at a transition between the ddw and d-wave superconducting states (Nayak 2000 *Phys. Rev.* B **62** R6135) is presented. (2) The nematic and ddw operators transform into each other under a unitary transformation. Thus, when a Hamiltonian is invariant under such a transformation, the two states are exactly degenerate. The competition between the nematic and ddw states in the presence of a degeneracy breaking term is discussed.

1. Introduction

Motivated by the discovery of exotic ordered states in strongly correlated materials, the interplay between different order parameters has been of great interest. In particular, competition and/or cooperation of the d-wave superconducting state and other nearby ordered states in high temperature cuprates have been subjects of intensive theoretical research activities. A few examples of nearby ordered states proposed in high temperature cuprates include the Néel antiferromagnet [2, 3], the ddw state (also called the staggered flux phase) [4–6] and the electronic nematic phase [7–11].

Among these, the antiferromagnetic state is an s-wave particle–hole condensate, while the ddw, electronic nematic and d-wave superconducting states share a common d-wave feature; the d-wave superconducting state is formed by a condensation of particle–particle pairs of $l = 2$ relative angular momentum, while the ddw and electronic nematic states are formed by condensations of particle–hole pairs of $l = 2$ relative angular momentum, but at different wavevectors.

In this paper, we study whether there are intimate relations between these $l = 2$ condensates, which will shed light on our understanding of the competition and/or cooperation between them. The d-wave superconducting, ddw and electronic nematic states are represented by their order parameters which

capture the characteristic broken symmetries of each state. The well-known d-wave superconducting order parameter is written as

$$\langle \Delta_{\text{d-sc}}^{+} \rangle = -\frac{1}{\sqrt{2}} \sum_{\mathbf{k}} \mathrm{d}(\mathbf{k}) \langle c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} \rangle. \tag{1}$$

On the other hand, the ddw and electronic nematic order parameters are given by

$$\langle \Delta_{\text{ddw}} \rangle = \frac{i}{2} \sum_{\mathbf{k}\sigma} \mathrm{d}(\mathbf{k}) \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{Q}\sigma} \rangle,$$
$$\langle \Delta_{\text{nem}} \rangle = \frac{1}{2} \sum_{\mathbf{k}\sigma} \mathrm{d}(\mathbf{k}) \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle, \tag{2}$$

where $\mathrm{d}(\mathbf{k}) = \cos(k_x) - \cos(k_y)$, σ represents up- and down-spin, and $\mathbf{Q} = (\pi, \pi)$. We set a, the lattice constant of a two-dimensional square lattice, to be unity. Since the ddw order parameter is a complex value defined at the wavevector $\mathbf{Q}$, it breaks translational, time-reversal and $\pi/2$-rotational symmetries, while the nematic state breaks only $\pi/2$-rotational symmetry.

It was shown that there is $O(4)$ invariance at a transition between the d-wave superconducting and ddw states [1, 12]. Below we show that there is $SO(4)$ invariance at a transition

between the nematic state and the d-wave superconductor, where the pseudospin $SU(2)$ generators are s-wave pairing and density operators; the spin $SU(2)$ and pseudospin $SU(2)$ forms $SO(4)$. We discuss the difference between our finding and the previous $O(4)$ symmetry at a transition between the ddw and d-wave superconducting states. We then present a relation between the nematic and ddw states, and its competition between them.

2. Pseudospin $SU(2)$ generators

To understand the relation between the nematic and d-wave superconducting states, let us first review a similar relation found between the ddw and the d-wave superconductor, where the pseudospin generators are η pairing operators. The pseudospin η operators was first discussed by Yang in the Hubbard model [13]. η^+, $\eta^- = (\eta^+)^\dagger$ and η_z are defined as follows:

$$\eta^+ = \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{Q}\downarrow}^\dagger,$$
$$\eta_z = \sum_{\mathbf{k}} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} + c_{\mathbf{k}+\mathbf{Q}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{Q}\downarrow} - 1 \right). \tag{3}$$

Note that these operators form an $SU(2)$ algebra. It was shown that the η-pairing state is an eigenstate of the Hubbard Hamiltonian. It is interesting to note that the η-pairing state is a finite center-of-mass momentum pairing state (FFLO) of s-wave superconductors with momentum $\mathbf{Q} = (\pi, \pi)$. It was later proved that the η-pairing state with a finite Zeeman field can be mapped to the Nagaoka ferromagnetic state with a finite doping by a particle–hole transformation, which simultaneously maps the negative-U Hubbard model to the positive-U Hubbard model, respectively [14]. It was also shown that the on-site s-wave pairing operator and charge density wave operator can be rotated into each other by the pseudospin $SU(2)$ generators, which is summarized by the following relation [15]:

$$[\eta^+, \rho_{\mathbf{Q}}] = \sqrt{2}\tilde{\Delta}_{\mathrm{ssc}}^+, \tag{4}$$

where $\rho_{\mathbf{Q}} = \frac{1}{2}\sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q}\sigma}$, $\tilde{\Delta}_{\mathrm{ssc}}^+ = -\frac{1}{\sqrt{2}}\sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$, and $\tilde{\Delta}_{\mathrm{ssc}}^- = -(\tilde{\Delta}_{\mathrm{ssc}}^+)^\dagger$.

Following Yang, the pseudospin $SU(2)$ symmetry was adapted to a critical point between the d-wave superconductor and the ddw state [1][3]. The generators, $i\eta^+$, $i\eta^-$, η_z, were defined to have the same forms of η. However, there is a difference: the factor of i in $\eta^\pm$ was introduced due to the factor i in the ddw operator. The rotation between the ddw and d-wave superconducting operators can be captured by the following commutation relation:

$$[i\eta^+, \Delta_{\mathrm{ddw}}] = \sqrt{2}\Delta_{\mathrm{d-sc}}^+, \tag{5}$$

where $\Delta_{\mathrm{ddw}} = \frac{i}{2}\sum_{\mathbf{k}\sigma} d(\mathbf{k}) c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{k}\sigma}$, $\Delta_{\mathrm{d-sc}}^+ = -\frac{1}{\sqrt{2}}\sum_{\mathbf{k}} d(\mathbf{k}) c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$ and $\Delta_{\mathrm{d-sc}}^- = -(\Delta_{\mathrm{d-sc}}^+)^\dagger$. $O(4)$ invariance at a transition between the ddw and d-wave superconducting state was further discussed in [1].

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[3] Since the ddw state breaks time-reversal symmetry, the symmetry at a transition between the ddw and d-wave superconducting state is $SU(2) \times SU(2) \times Z_2$.

3. Rotation between the nematic and d-wave superconducting operators

It is straightforward to find a similar relation between the nematic and d-wave pairing operators, where the pseudospin $SU(2)$ generators are

$$L_+ \equiv \Delta_{\mathrm{s-sc}}^+ = \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger,$$
$$L_- \equiv \Delta_{\mathrm{s-sc}}^- = (\Delta_{\mathrm{s-sc}}^+)^\dagger, \tag{6}$$
$$L_0 \equiv \Delta_z = \frac{1}{2}\sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - N,$$

where N is the total number of lattice sites. Note that the operators $\Delta_{\mathrm{d-sc}}^+ (m = 1)$, $\Delta_{\mathrm{d-sc}}^- (m = -1)$ and $\Delta_{\mathrm{nem}} (m = 0)$ form an irreducible tensor of rank $l = 1$ under the $SU(2)$ algebra, as follows:

$$[L_\pm, \Delta_m] = \sqrt{l(l+1) - m(m \pm 1)}\Delta_{m\pm 1},$$
$$[L_0, \Delta_m] = m\Delta_m, \tag{7}$$

where $l = 1$. Therefore, the nematic and d-wave superconducting operators can be rotated into each other by the pseudospin generators:

$$[\Delta_{\mathrm{s-sc}}^+, \Delta_{\mathrm{nem}}] = \sqrt{2}\Delta_{\mathrm{d-sc}}^+. \tag{8}$$

The above equation implies that there is $SO(4)$ invariance at a transition between the nematic and d-wave superconducting (nematic-dsc) states. However, a small symmetry breaking term can be present, which will favor one state over the other. For example, it is possible that potential terms such as $-g(\Delta_{\mathrm{nem}}^2 - \Delta_{\mathrm{d-sc}}^2)$ can be present, which favors the nematic phase (the d-wave superconductor) for $g > 0$ ($g < 0$). Then, a different symmetry breaking term such as a finite chemical potential can lead to a transition from the nematic state to the d-wave superconducting state, so there is $SO(4)$ symmetry at a bi-critical point.

Similar scenarios were proposed in the previous study of the ddw and d-wave superconducting (ddw–dsc) transition, as well as in $SO(5)$ theory of antiferromagnetic and d-wave superconducting states. However, there is a crucial difference between the ddw–dsc and nematic-dsc transitions. In the case of the $O(4)$ symmetry at a transition between the ddw and d-wave superconducting state, the chemical potential is a symmetry breaking term. Since the chemical potential couples to one of the $SU(2)$ generators ($\propto \mu\eta_z$), a finite chemical potential favors the d-wave superconducting state over the ddw state. Therefore, if an effective interaction is $O(4)$ invariant, the system equally favors the ddw and d-wave superconducting states at the half-filling with a tight-binding dispersion. On the other hand, if an effective interaction favors the ddw state at the half-filling, there is a first-order transition from the ddw state to the d-wave superconducting state at a finite chemical potential, which is like a spin-flop transition. Note that the nearest-neighbor hopping term is $O(4)$-invariant. In other words, the nearest-neighbor hopping term commutes with the η pairing operator which results from $\epsilon_{\mathbf{k}} = -\epsilon_{\mathbf{k}+\mathbf{Q}}$, where $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$.

The nearest-neighbor hopping term has a quite different effect on the nematic and d-wave superconducting transition. Since the pseudospin generator is an s-wave pairing operator, the nearest-neighbor hopping term is a symmetry breaking term, in addition to the chemical potential term. The nearest-neighbor hopping term can be written as

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}^{\alpha\sigma\dagger} \tau_{3\alpha}^{\beta} \psi_{\beta\sigma\mathbf{k}}, \tag{9}$$

where $\psi_{\mathbf{k}}$ is the vector field with four components, $\alpha(\beta)$ represents pseudospin index, τ is a Pauli matrix for pseudospin and σ denotes spin index. Since the electron field forms a doublet under the pseudospin $SU(2)$ in addition to the spin $SU(2)$, $\psi_{\mathbf{k}}$ is defined as

$$\psi_{\mathbf{k}} = \left(c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c_{-\mathbf{k}\downarrow}^{\dagger}, c_{-\mathbf{k}\uparrow}^{\dagger} \right). \tag{10}$$

Therefore, when an interaction equally favors the nematic and d-wave superconducting state, the d-wave superconducting state wins over the nematic due to the presence of a nearest-neighbor kinetic term even at $\mu = 0$. An introduction of the chemical potential further favors the d-wave superconducting state, because again it couples to the Δ_z operator. Therefore, the realization of the nematic state in a realistic system requires a potential term which strongly favors the nematic state over the d-wave superconducting state in order to compensate for the effect of a nearest-neighbor hopping term. The coexistence of nematic and d-wave superconducting phases has been found by a mean-field theory in [16], where a strong nematic-favoring interaction was used. This is consistent with our finding that the nearest-neighbor hopping term is a pseudospin symmetry breaking term, and a strong nematic interaction is required to compensate for its effect.

4. Unitary transformation between the nematic and the ddw operators

Now one may ask about a relation between two different rotations: equations (7) and (5). We will show below that these two equations transform from one to the other by a unitary transformation. Therefore, if a Hamiltonian is invariant under such a transformation, two states (nematic and ddw) are exactly degenerate.

We consider the following unitary transformation:

$$U^{\dagger} c_l^{\dagger} U = e^{i(-1)^l \frac{\pi}{4}} c_l^{\dagger}, \tag{11}$$

where l denotes a lattice site. $U = e^{i\frac{\pi}{4}(N_A - N_B)}$ where N_A and N_B are the total number operators for sublattice A and B sites. Under the above transformation, it is straightforward to show that the ddw and nematic state can be smoothly rotated:

$$U^{\dagger} \Delta_{\text{ddw}} U = \Delta_{\text{nem}}. \tag{12}$$

What is the significance of the above relation between the operators? The importance of the relation is that, if and only if a Hamiltonian of interest is invariant under the transformation, i.e. $U^{\dagger} H U = H$, then

$$\langle \phi_1 | H | \phi_1 \rangle = \langle \phi_2 | H | \phi_2 \rangle$$
$$\langle \phi_1 | \Delta_{\text{ddw}} | \phi_1 \rangle = \langle \phi_2 | \Delta_{\text{nem}} | \phi_2 \rangle, \tag{13}$$
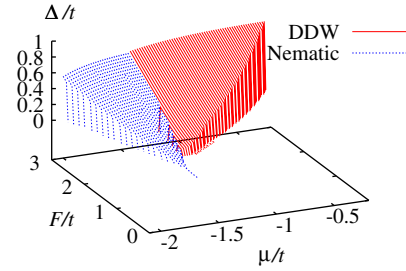

Figure 1. The ddw and nematic order parameters as a function of chemical potential μ and the effective interaction F. We set $t = 1$, $t' = -0.4t$, and $t'' = 0$. The red and blue regions are the ddw and nematic phases, respectively.

(This figure is in colour only in the electronic version)

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are smoothly connected by a rotation, $U|\phi_1\rangle = |\phi_2\rangle$, and exactly degenerate. Therefore, the ddw and nematic states are exactly degenerate. What breaks this degeneracy?

Since the unitary transformation involves the sublattices of A and B, any types of density–density or spin–spin interactions do not break the degeneracy. However, the kinetic term does. The most important and relevant term which breaks the degeneracy is the nearest-neighbor hopping term which is not invariant under this transformation[4]. Therefore, one of the states always wins over the other due to the presence of a non-zero nearest-neighbor hopping integral in realistic systems. While the next-nearest (t') and next-next-nearest (t'') hopping terms, and chemical potential, are invariant under the unitary transformation, the effect of t on selecting a state can be changed in the presence of these terms. The energetic difference between the ddw and nematic states is presented in figure 1 using mean-field theory for a given set of hopping parameters and an interaction F which equally favors the nematic and ddw states. Here we set $t = 1$, $t' = -0.4t$ and $t'' = 0$, and show how the state is stabilized as a function of the chemical potential μ and the effective interaction F.

As is shown, the ddw state is favorable at relatively low doping, while the nematic state wins at higher doping. The origin of the phase transition is related to a change in the density of states, since the ddw state is favorable near doping with the nesting $\epsilon_{\mathbf{k}} = -\epsilon_{\mathbf{k+Q}}$, while the nematic state is favorable near doping with a van Hove singularity. A reasonable amount of t' moves the nematic state to higher doping by shifting a van Hove singularity, which is a way to avoid the competition with the ddw state. The two phases are separated by the first-order phase transition; this occurs around $\mu = -1.4$ which corresponds to the hole doping of 0.2 and is almost independent of the strength of the effective interaction F.

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[4] At a limit of $t \to 0$, the ddw order parameter is ill defined, since the ddw order parameter is defined via a current on each link between the nearest-neighbor bonds. Therefore, the ddw order parameter cannot represent translational and time-reversal symmetries, and it is nothing but a different gauge choice of the nematic state.

5. Summary and discussion

Finite angular momentum condensates have been studied to understand various exotic phases in strongly correlated systems. In particular, condensates of particle–particle or particle–hole pairs of $l = 2$ relative angular momentum have been proposed in the context of high T_c cuprates. We studied the relations between different $l = 2$ condensates: the d-wave superconducting, ddw and electronic nematic states proposed as relevant phases of underdoped cuprates.

We showed that there is $SO(4)$ invariance at a transition between the electronic nematic and d-wave superconducting state. The pseudospin $SU(2)$ generators that rotate the nematic to d-wave pairing operators are s-wave pairing and electron density operators. The important difference between a similar $O(4)$ invariance at a transition between the ddw and d-wave superconducting state transition is that the nearest-neighbor hopping term is a symmetry breaking term, which in turn always favors the d-wave superconducting state over the nematic state even at $\mu = 0$. A finite chemical potential further favors the d-wave superconducting state.

We also found that the electronic nematic operator and the ddw operator transform into each other under a unitary transformation. Therefore, if Hamiltonians are invariant under the unitary transformation, the ddw and nematic states are exactly degenerate. The most important and relevant term which breaks the degeneracy is the nearest-neighbor hopping integral. Since the nearest-neighbor hopping is finite in realistic materials of our interest, one of the two states is always energetically lower than the other. While the chemical potential term is invariant under the unitary transformation, the role of t on its energetic selection changes as one changes μ. We found that the ddw state is stabilized over the nematic at lower chemical potential, while the nematic wins over the ddw state for higher chemical potential within a mean-field approximation, when the interactions equally favor these two states.

A further study on the competition between the nematic and d-wave superconducting states may lead us to understand a series of anisotropic scattering patterns observed in $YBa_2Cu_3O_{7-\delta}$ [17–21]. The competition between the ddw, nematic and d-wave superconducting states beyond the mean-field theory is also an important issue, which we will address in the near future [22].

References

[1] Nayak C 2000 *Phys. Rev. B* **62** R6135
[2] Demler E, Hanke W and Zhang S C 2004 *Rev. Mod. Phys.* **76** 909 and references therein
[3] Chubukov A, Pines D and Schmalian J 2003 *Review Chapter in The Physics of Superconductors* ed K H Bennemann and J B Ketterson (New York: Springer) pp 450–90 and references therein
[4] Chakravarty S, Laughlin R B, Morr D K and Nayak C 2002 *Phys. Rev. B* **64** 094503
[5] Affleck I and Brad Marston J 1988 *Phys. Rev. B* **37** 3774
[6] Lee P A 2007 *Rep. Prog. Phys.* ('key issue' essay)
Lee P A 2007 *Preprint* 0708.2115 references therein
[7] Kee H Y, Kim E and Chung C H 2003 *Phys. Rev. B* **68** 245109
Khavkine I, Chung C H, Oganesyan V and Kee H Y 2004 *Phys. Rev. B* **70** 184521
[8] Yamase H and Kohno H 2000 *J. Phys. Soc. Japan* **69** 2151
[9] Halboth C J and Metzner W 2000 *Phys. Rev. Lett.* **85** 5162
[10] Oganesyan V, Kivelson S and Fradkin E 2001 *Phys. Rev. B* **64** 195109
[11] Kivelson S A, Fradkin E, Oganesyan V, Bindloss I P, Tranquada J M, Kapitulnik A and Howald C 2003 *Rev. Mod. Phys.* **75** 1201 and references therein
[12] Nayak C 2000 *Phys. Rev. B* **62** 4880
[13] Yang C N 1989 *Phys. Rev. Lett.* **63** 2144
[14] Singh R R P and Scalettar R T 1991 *Phys. Rev. Lett.* **66** 3203
Kee H-Y and Zhang S 1998 unpublished
[15] Zhang S 1990 *Phys. Rev. Lett.* **65** 120
[16] Yamase H and Matzner W 2007 *Phys. Rev. B* **75** 155117
[17] Hinkov V, Bourges P, Pailhes S, Sidis Y, Ivanov A, Frost C D, Perring T G, Lin C T, Chen D P and Keimer B 2007 *Nat. Phys.* **3** 780
[18] Hinkov V, Haug D, Fauque B, Bourges P, Sidis Y, Ivanov A, Bernhard D, Lin C T and Keimer B 2008 *Science* **319** 597
[19] Stock C, Buyers W J L, Yamani Z, Broholm C L, Chung J-H, Tun Z, Liang R, Bonn D, Hardy W N and Birgeneau R J 2006 *Phys. Rev. B* **73** 100504(R)
[20] Kao Y-J and Kee H-Y 2005 *Phys. Rev. B* **72** 24502
[21] Yamase H and Metzner W 2006 *Phys. Rev. B* **73** 214517
[22] Doh H and Kee H-Y 2008 unpublished