Field induced $d_{x^2-y^2} + id_{xy}$ state in $d$-density-wave metals

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We argue that the $d_{xy}$ component of the order parameter can be generated to form the $d_{x^2-y^2} + id_{xy}$-density wave state by the external magnetic field. The driving force for this transition is the coupling of the magnetic field with the orbital magnetism. The fully gapped particle spectrum and the magnetically active collective mode of the condensate are discussed as a possible signature of the $d + id'$ density wave state.

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Recently, Chakravarty et al. [1] proposed to model the pseudogap (PG) of underdoped high-$T_c$ cuprates in the formation of a new order —$d$-density wave (DDW) state, which breaks the parity and time-reversal symmetry, and the invariance of translation by one lattice constant and rotation by $\pi/2$. The scenario is supported by the experiments showing that the PG and the superconducting gap coexist distinctly below $T_c$. Although the debate about the mechanism for the PG is far from settled, it is suggestive that the typical characteristics of the PG as observed in many experiments, including photoemission [2], tunneling [3], muon spin relaxation [4], can be explained by the DDW model. More recently, the detection of the DDW ordering using impurity resonance has been proposed [5].

We are going to argue here that, in addition to the dominant $d_{x^2-y^2}$ ($d$) component of the DDW order parameter, a subdominant $d_{xy}$ ($d'$) component can be generated by the magnetic field. We find that i) the presence of the additional gap component $d'$ will lead to the fully gapped quasiparticle spectrum; ii) the inherently two component order parameter $d + id'$ of the ddw phase in the field will exhibit collective mode that can be excited in an out-of-plane ac magnetic field. Both of these features can be used to distinguish between ddw scenario and alternatives. We discuss experimental consequences below. The existence of the field induced $d + id'$ superconducting state in high-$T_c$ cuprates has recently been intensively studied.

The existence of the field induced $d + id'$ superconducting state in high-$T_c$ cuprates has recently been intensively studied. It was first proposed by Laughlin [6] and Ramakrishnan [7], to explain the kink behavior observed in the thermal transport experiment [8], that the magnetic field can drive the original $d$-wave ordering into the $d + id'$ state. In the original proposal, the generation of the $d'$ component was thought to be through the first-order bulk phase transition, but the important role of the vortices for the anomaly was also pointed out by other authors [1] [9] [10]. Later on it was argued [12] that even when the magnetic field is near the upper critical field, the $d$-wave state can be “distorted” by the external field, leading to a bulk $d + id'$-wave state with the intrinsic orbital moment. There is a significant distinction between the $d$-wave superconducting (DSC) state and the DDW state: The magnetic induction in the superconducting state is inhomogeneous. In the DSC state, the electromagnetic $U(1)$ gauge invariance is broken so in an external magnetic field, the system is in either the Meissner state (type-I superconductors), where the magnetic flux is expelled from its bulk region, or nucleating an array of vortices (type-II superconductors). The DDW state does not break the gauge invariance and has no analog of the Meissner effect or the Abrikosov vortices. It is then expected that magnetic field inside a sample in the DDW state is homogeneous. In view of this distinction, we argue that there should be an instability of the $d$-density wave state into the $d + id'$-density wave state even in the presence of a weak magnetic field.

As in the DSC state, there also exists low-lying quasiparticle states around the nodes of the $d$-density wave energy gap. At these nodes, the low-lying quasiparticles have vanishingly small energy gap and they are most sensitive to an external electromagnetic perturbation, which opens the possibility of the generation of the second component of the order parameter, orthogonal to the initial $d$-density wave state. Second component of the order parameter can be of $s$-wave or $d'$-wave orbital symmetry. Although, the $s$-wave component may be induced due to the scattering at surfaces or interfaces, the $d'$-wave order parameter is likely to be generated in the bulk sample when an external magnetic field is applied. The physical origin of this instability is the bulk orbital magnetic moment $\langle M_z \rangle$ in the $d + id'$ state. When an external magnetic field $H$ is applied perpendicular to the plane of the two-dimensional (2D) system under consideration (namely, $H \parallel \hat{z}$), the resulting coupling of the magnetic induction $B$ with the orbital magnetic moment, $-\langle M_z \rangle B$, lowers the system free energy. As mentioned above, since in the DDW state there is no screening effect on the magnetic field, the magnetic induction $B$ is homogeneous throughout the system and is close to the external magnetic field $H$. In the absence of the magnetic field, the pure $d$-density wave state can be regarded as the equal admixture of the orbital angular moment
\[ L_z = \pm 2 \text{ pairs:} \]
\[ W_0(\Theta) = iW_0 \cos(2\Theta) = \frac{iW_0}{2} \left[ \exp(2i\Theta) + \exp(-2i\Theta) \right]. \]  
(1)

Here we have made an approximation to the order parameter \( W_0(k) \propto \langle c_{k+\mathbf{Q},\sigma}^\dagger c_{k,\sigma} \rangle \propto W_0(\cos k_x a - \cos k_y a) \) by confining the wave vector \( k \) near the Fermi surface and defined \( \Theta \) as the 2D azimuthal angle of the Fermi momentum, where \( c_{k,\sigma} \) annhilates an electron of spin \( \sigma \) at \( k \), \( W_0 \) is the magnitude of the pure \( d \)-wave component. In the presence of an external magnetic field, the \( L_z \) is still call the resulting DDW state as having the \( d \)-wave component. In particular, the coupling of the magnetic field (parallel to the orbital angular momentum) can be explicitly written as:
\[ \tilde{W}_0 \propto (1 + \eta B) \exp(2i\Theta) + (1 - \eta B) \exp(-2i\Theta) \]
\[ = iW_0(\Theta) + iBW_1(\Theta), \]  
(2)
where \( B = H \) and \( W_1 \approx \eta \sin(2\Theta) \). Unlike the DSC, the pure \( d \)-density wave order parameter is imaginary while the field generated \( d' \)-wave component is real. We will still call the resulting DDW state as having the \( d + id' \) symmetry because the relative phase between the two components is still \( \pi/2 \) in the equilibrium.

To support the above physical intuitive, we provide a microscopic analysis in the following. The \( d \)-density wave ordering comes from the formation of the particle-hole pairs caused by the electron interactions. The collective motion of these pairs can be represented by the center-of-mass coordinates, while the relative motion by the relative coordinate. The structure of the pair wave-function is determined by the relative motion of two paired particles. In the tight-binding model, both the \( d \)-wave term and the coupling term between the magnetic field with the electron orbital angular momentum (i.e., the orbital Zeeman coupling) are associated with the bi-linear operator \( c_{k,\sigma}^\dagger c_{k,\sigma} \). Therefore, in the presence of magnetic field, both of these two terms should be assigned, together with the kinetic energy term, a phase factor \( \exp\left( \frac{ig}{\hbar c} \int_{\mathbf{R}^2} A \cdot dl \right) \) to ensure the gauge invariance of the system Hamiltonian, where \( \Phi_0 = \hbar c/e \) and \( A \) is the vector potential. This fact indicates that the DDW order parameter is not influenced by the gauge phase factor, and allows us to treat the orbital Zeeman coupling effect on the DDW order parameter independently. Explicitly, the coupling of the magnetic field (parallel to \( z \) direction) with the orbital angular momentum can be written as:
\[ H_B = -i\mu_B B \sum_{i,\delta,\sigma} \langle c_{i,\delta,\sigma}^\dagger (r_x \times \delta)_z c_{i,\delta,\sigma} \rangle \]
Here \( \delta = (\pm a, 0) \) or \( (0, \pm a) \) is the unit vector along the \( x \) or \( y \) axis, \( a \) is the lattice constant, \( r \) is the lattice vectors, \( \mu_B \) is the Bohr magneton, \( g = 2m_e a^2/\hbar^2 \) with \( t \) the nearest-neighbor hopping integral [the energy unit used thereafter], \( m_e \) the effective mass of electrons and \( \hbar \) the Planck’s constant. In the momentum space, the system Hamiltonian can be written as:
\[ H = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} [W_k c_{k,\sigma}^\dagger c_{k+\mathbf{Q},\sigma} + H.c.] \]
\[ -ig\mu_B B \sum_{k,\sigma} c_{k,\sigma}^\dagger \langle \sin k\alpha \times \partial_{k\alpha} \rangle c_{k,\sigma}. \]  
(3)

Here \( \xi_k = -2[\cos k_x a + \cos k_y a] - \mu \) with \( \mu \) the chemical potential is the single particle energy measured relative to the Fermi energy. The DDW order parameter is given by \( W_k = iW_0(\Theta) + W_1(\Theta) \), where \( \phi_0(k) = \cos k_x a - \cos k_y a \) and \( \phi_1(k) = \sin k_x a \sin k_y a \). The amplitude of the \( d \)- and \( d' \)-wave components \( W_{0,1} \) are determined self-consistently:
\[ W_0 = \frac{iW_0}{2N} \sum_k \langle c_{k+\mathbf{Q},\sigma}^\dagger c_{k,\sigma} \rangle \phi_0(k), \]  
(4)
and
\[ W_1 = -\frac{2W_1}{N} \sum_k \langle c_{k+\mathbf{Q},\sigma}^\dagger c_{k,\sigma} \rangle \phi_1(k), \]  
(5)
where \( W_{0,1} \) are, respectively, the \( d \)- and \( d' \)-channel interaction, \( N \) is the number of 2D lattice sites. That the \( d \)-wave component is imaginary is due to the equivalence of \( Q = (\pi, \pi) \) and \( -Q \) enforced by the underlying band structure. The notation \( \sin(k_x a)\partial_{k_y a} - \sin(k_y a)\partial_{k_x a} \) represents \( \phi_0(k) \). We define \( \phi_0(k + Q) = -\phi_0(k) \) and \( \phi_1(k + Q) = \phi_1(k) \). In view of the fact that the DDW state breaks the translational symmetry with lattice constant but conserves that by \( \sqrt{2a} \) along the diagonals of the square lattice, it is convenient to have the Brillouin zone, by introducing two kinds of electron operators \( c_{k,\sigma} \) and \( c_{k+\mathbf{Q},\sigma} \). The pairing of the particles and holes must cause correlations in their relative motions. According to the structure of the Hamiltonian and the self-consistency conditions for the DDW order parameter, we can introduce the following Green’s functions to describe the correlation:
\[ \mathcal{G}_{11}(k, k'; \tau) = -\langle T_\tau [c_{k,\sigma}(\tau)c_{k',\sigma}^\dagger(0)] \rangle, \]  
(6a)
\[ \mathcal{G}_{12}(k, k'; \tau) = -\langle T_\tau [c_{k,\sigma}(\tau)c_{k',\sigma}^\dagger(0)] \rangle, \]  
(6b)
\[ \mathcal{G}_{21}(k, k'; \tau) = -\langle T_\tau [c_{k,\sigma}(\tau)c_{k'+\mathbf{Q},\sigma}^\dagger(0)] \rangle, \]  
(6c)
\[ \mathcal{G}_{22}(k, k'; \tau) = -\langle T_\tau [c_{k+\mathbf{Q},\sigma}(\tau)c_{k'+\mathbf{Q},\sigma}^\dagger(0)] \rangle, \]  
(6d)
where the factor \( T_\tau \) is a \( \tau \)-ordering operator as usual, \( c_{k,\sigma}(\tau) = e^{iH_\tau} c_{k,\sigma} e^{-iH_\tau} \) is the operator in the Heisenberg representation. Given the Hamiltonian Eq. (3), with aid of the equation of motion for the field operator \( c_{k,\sigma}(\tau) \) and \( c_{k,\sigma}^\dagger(\tau) \), and by performing a Fourier transform with respect to \( \tau \),
\[ \mathcal{G}(k, k'; \omega_n) = k_B T \sum_{\omega_n} \mathcal{G}(k, k'; i\omega_n) e^{-i\omega_n \tau} \]  
(7)
with \( \omega_n = (2n + 1)\pi k_B T \), we establish a closed set of the self-consistent equations for \( G(k, k'; \omega_n) \), e.g.:

\[
\delta_{kk'} = (i\omega_n - \xi_k + i\gamma_B B \sin(k + Q)a \cdot \partial_{(k+Q)\omega_n}) \\
\times G_{22}(k, k'; \omega_n) - 2(W_k + W_{k+Q})G_{21}(k, k'; \omega_n),
\]

(8a)

and

\[
0 = (i\omega_n - \xi_k + i\gamma_B B \sin(ka \cdot \partial_{ka})_z) G_{21}(k, k'; \omega_n) \\
- 2(W_k + W_{k+Q})G_{22}(k, k'; \omega_n).
\]

(8b)

To the approximation up to the first order in the orbital-magnetic field coupling, we obtain

\[
G_{21}(k, k'; \omega_n) = \frac{(W_k + W_{k+Q})\delta_{kk'}}{D(k; \omega_n)},
\]

(9)

and

\[
\delta G_{21}(k, k'; \omega_n) = -\frac{i\gamma_B B (\omega_n - \xi_k + Q)}{D(k; \omega_n)} \\
\times \sin(ka \cdot \partial_{ka}) G_{21}(k, k'; \omega_n).
\]

(10)

where \( D(k; \omega_n) = (i\omega_n - E_{k,1})(i\omega_n - E_{k,2}) \) with \( E_{k,1,2} = \pm \sqrt{\xi_k^2 + \lvert W_k + W_{k+Q} \rvert^2 - \mu} \). We take the ansatz that \( V_0 \) is bigger than \( V_1 \) such that in the absence of the magnetic field, the \( d' \)-wave ordering is pure and no secondary phase transition for the appearance of the \( d' \) ordering occurs. Therefore, the DDW gap appearing in the \( G^0 \), \( W_k = iW_0 \varphi_0(k) \). The momentum dependence of \( \varphi_0(k) \) leads to \( \sin(ka \cdot \partial_{ka}) \varphi_0(k) = 2 \varphi_1(k) \).

Substitution of Eq. (11) into Eq. (9) yields:

\[
W_1 = -\frac{4V_1}{N} \sum_{k \in R BZ} \text{Re} [\delta G_{21}(k, k; \tau = 0)] \varphi_2(k) \\
= \eta BW_0,
\]

(11)

where

\[
\eta = -\frac{16\gamma_B V_k k_B T}{N} \sum_{k \in R BZ} \sum_{\omega_n} \frac{\xi_k \varphi_2^2(k)}{D^2(k; \omega_n)}
\approx \frac{16\gamma_B N(0)V_1}{E_F},
\]

(12)

where \( N(0) \) is the density of states at the Fermi energy \( E_F \). By taking the Fermi wave length of a few lattice constant \( a \) \((\sim 4A)\) and \( N(0)|V_1| \sim 0.3 \), it is estimated \( |W_1/W_0| \approx 10^{-2} \) at \( B = 10T \), which makes the amplitude of the induced component \( |W_1| \) to be on the order of a few Kelvin. Eq. (11) shows microscopically that the magnetic field can drive the pure \( d' \)-wave state into the \( d + id' \) state. This analysis also indicates that the \( d + is \)-density wave state could not be generated by the applied magnetic field, which is significantly different from the situations at the sample surfaces or interfaces.

Equation (11) suggests that the phenomenological Ginzburg-Landau (GL) free energy functional must contain the linear coupling between the original \( d \)-density wave order parameter and the field-induced \( d' \)-density wave order parameter, \( f_{\text{int}} = (1/2)(iW_0)W_1^* B + c.c. \). Consequently, we can write down the system GL functional of the form:

\[
\mathcal{F} = \int d^2r \left[ \frac{\alpha_1}{2} \left| W_1(r) \right|^2 + \frac{\alpha_2}{2} \left| W_0(r) \right|^2 \right] \\
+ K_0 |\nabla(iW_0(r))|^2 + \frac{K_1}{2} |\nabla W_1(r)|^2 + \frac{\alpha_1}{2} \left| W_1(r) \right|^2 \\
+ f_{\text{int}}(r),
\]

(13)

where the first two terms describe the instability of the pure \( d \)-density wave state, with \( T_0^d \) being the transition temperature in the absence of magnetic field. The last two terms represent the energy shift of the \( d' \)-wave state as a result of the field-induced \( d' \)-wave order parameter, where \( \alpha_1 \) is positive. Notice that, unlike the superconducting order parameter, the gradient operator on the DDW order parameter is not shifted by the vector potential because the DDW pairs do not carry charge. It follows from Eq. (13) that, as far as the \( d' \)-wave component is concerned, the coupling to the magnetic field term \( i[\partial_{\alpha} \varphi_0] \) is linear, while the stiffness term \( i[\partial_{\alpha} \varphi_0] \) is quadratic. Therefore, at least at the weak field so that \( W_1 \) is small, the linear term is dominant. Therefore, the system gains energy by having a nonzero equilibrium value of \( W_1 \). By treating \( W_1 \) and \( W_0 \) as independent variables, the GL functional \( \mathcal{F} \) is minimized by enforcing \( \nabla \mathcal{F} = \frac{\partial \mathcal{F}}{\partial W_1} = 0, \frac{\partial \mathcal{F}}{\partial W_0} = 0 \), which leads to

\[
W_1 = \eta \frac{B}{\alpha_1} W_0.
\]

(14)

Upon substituting the above result into Eq. (13), we find the energy gained by the system with the induced \( d' \)-density wave component: \( \delta \mathcal{F} = -\int d^2r \eta^2 \left| W_0 \right|^2 B^2 / 2\alpha_1 \). Therefore, the transition temperature which is now field dependent, and is renormalized by the magnetic field as: \( T_c(B) = T_0^d + \delta T_c(B) \), where \( \delta T_c(B) = \eta^2 B^2 / 2\alpha_1 \). It then follows that coupling of the magnetic field with the orbital angular momentum shifts the instability of the \( d \)-density wave ordering to the high temperature as schematically shown in the \( (T, B) \) phase diagram. Here we note that, since the particle-hole pairing takes place with the equal spin, the coupling between the magnetic field and the electron spin (i.e., the spin Zeeman coupling) will not depress the induction of \( d' \) component in the DDW metal. We do not address here the effect of very strong field that could ultimately suppress the DDW state.

Up to now our analysis of the induction of the secondary \( d' \) component has been focused on the equilib-
perimental observation of the existence of the induced component. We now turn to the exper-
mence of the relative phase \( \phi = \phi_1 - \phi_0 \), which is governed by [14]:
\[
\frac{\partial^2 \phi}{\partial t^2} = -\rho^{-1} \frac{\delta F}{\delta \phi},
\]
where \( \rho^{-1} \approx N(0) \). With Eq. (13), we find
\[
\frac{\partial^2 \phi}{\partial t^2} = -\rho^{-1} \eta B |W_0||W_1| \cos \phi - s^2 \nabla^2 \phi,
\]
which leads to the clapping mode with dispersion \( \omega^2(B, k) = \omega_0^2(B) + s^2 k^2 \) with \( \omega_0^2(B) = \eta B^2 |W_0|^2 / \rho \) and \( s^2 = |W_0|^2 (K_0 + \eta^2 B^2 K_1) / 4\rho \). This mode represents the oscillation of the relative phase between the \( d \) and \( d' \) components of the DDW order parameter, and is tunable by the magnetic field.

We thus have proved that (a) the applied magnetic field can generate the \( d_{xy} \) order parameter in the \( d \)-density wave metal, whose amplitude is linearly proportional to the field strength, and (b) the transition into the \( d + id' \)-density wave state occurs at a higher transition temperature, and (c) there exists a new clapping mode corresponding to the oscillation of the relative phase between the two components. We now turn to the experimental observation of the existence of the induced \( d' \) component. Angle resolved photoemission spectroscopy (ARPES) can be used to directly detect the existence of the induced \( d' \) component by measuring the low-lying excitations at the nodal directions, where, near the half filling, the dominant \( d \)-density wave gap closed at the Fermi surface while \( d' \)-density wave gap reaches the maximum. Figure 2 displays the low-temperatures ARPES signal \( f(k, \omega) = f(\omega) A(k, \omega) \) at \( k = (\frac{\pi}{2}, \frac{\pi}{2}) \) for various values of the induced \( d' \)-wave component \( W_1 \). Here is the Fermi distribution function \( f(\omega) = 1 / [\exp(\omega/k_B T) + 1] \) and the spectral function \( A(k, \omega) = 2[\delta(\omega - E_{k,1}) + \delta(\omega + E_{k,2})] \).

As is shown, the spectral peak is shifted with the magnitude of \( W_1 \), which is in turn linearly proportional to the magnetic field. As another consequence, in the presence of \( W_1 \), the quasiparticle spectrum is fully gapped. Therefore, if the magnetic field is applied perpendicularly to the 2D DDW metal, the electronic specific heat at low temperatures would be exponentially decaying.

To conclude, we show that the \( d \)-density wave state has an instability into the \( d + id' \) ordering in the presence of the magnetic field. The field induced \( d' \)-wave component is proportional to the field strength. The mechanism for the induction of the \( d' \) component is purely the coupling between the magnetic field and the orbital angular momentum.

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Because the pre-existing of the $d_{x^2−y^2}$-wave order parameter, the transition temperature for the appearance of the $d_{xy}$-component can be readily suppressed to be negative for $V_1 < V_0$, it is unnecessary for $V_1$ to have a different sign than $V_0$.

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