Quantitative Test of SO(5) Symmetry in the Vortex State of Nd$_{1.85}$Ce$_{0.15}$CuO$_4$

Han-Dong Chen
Department of Applied Physics, McCullough building, Stanford University, Stanford, CA 94305

Congjun Wu and Shou-Cheng Zhang
Department of Physics, McCullough building, Stanford University, Stanford, CA 94305

By numerically solving models with competing superconducting and antiferromagnetic orders, we study the magnetic field dependence of the antiferromagnetic moment in both the weak and strong field regimes. Through a comparison with the neutron scattering results of Kang and Matsura et al. on Nd$_{1.85}$Ce$_{0.15}$CuO$_4$, we conclude that this system is close to a SO(5) symmetric critical point. We also make a quantitative prediction on increasing the upper critical field $B_{c2}$ and the superconducting transition temperature $T_c$ by applying an in-plane magnetic field.

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A central question in the field of high $T_c$ superconductivity concerns the nature of the competing state and its quantum phase transition to the superconducting (SC) state\cite{1, 2}. The SO(5) theory\cite{3} considers the antiferromagnetic (AF) state to be the dominant competing state, and describes its competition with the SC state in terms of an unified theory with approximate SO(5) symmetry. This theory predicts that the competing AF order reveals itself in the SC vortex core\cite{3, 4}. This prediction has now been verified experimentally in a number of different compounds and by a variety of different experimental techniques\cite{5, 6, 7, 8, 9, 10, 11, 12, 13, 14}. Experimental and theoretical progress on the AF vortex state, and describes its competition with the SC state\cite{1, 2}. The quantum phase transition to the superconducting (SC) state is reviewed in recent articles\cite{1, 2}. While the experimental observation of enhanced AF correlation in the vortex state is encouraging, the limitation of low magnetic field could not convincingly establish the AF state as the competing order. Only recently, it became possible to probe the magnetic structure of the AF vortex core with magnetic fields comparable to the upper critical field $B_{c2}$. Kang et al. \cite{5} and Matsura et al. \cite{6} performed neutron scattering experiment on the electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4-\delta}$ (NCCO) crystal under a magnetic field of 16T, beyond the upper critical field $B_{c2} = 6.2T$ of this material. The experiment finds a field induced AF scattering at the commensurate wave vector $(\pi, \pi, 0)$, where the AF moment scales approximately linearly up to $B_{c2}$. The AF moment decreases with increasing field beyond $B_{c2}$. The experiment also finds field induced scattering at the $(\pi, 0, 0)$ position. Scattering at this position has a different field dependence at high field, and may not be intrinsically related to the $(\pi, \pi, 0)$ scattering. We shall not discuss this scattering position further in this paper.

The wealth of the experimental data on this system provides an opportunity to quantitatively test theoretical models. In this work, we use the Landau-Ginzburg model of competing AF and SC order, including the Zeeman term. By quantitatively fitting the parameters to the experimentally measured field dependence of the AF moment, we could determine how close this system is to a SO(5) symmetric point. We show that the departure from the SO(5) symmetric parameters in general leads to departure from the linear dependence of the AF moment on the magnetic field, in the high field regime. Therefore, the experimentally observed linear dependence up to $B_{c2}$ directly implies that Nd$_{1.85}$Ce$_{0.15}$CuO$_4$ is close to a SO(5) symmetric point. The magnetic field has a dual effect on the AF moment. On one hand, it creates AF moment in the vortex core, on the other hand, it reduces the AF moment by canting the spins uniformly towards field direction. This explains the reduction of the AF moment when the magnetic field exceeds $B_{c2}$. We also show that the SC coherence length is self-consistently determined by the interaction of the SC and AF order parameters, therefore, $B_{c2}$ is reduced in this system from its bare value. From this observation we predict that the value of $B_{c2}$ would be enhanced, if the AF order is suppressed by an in-plane magnetic field. The same reasoning lead to an enhancement of $T_c$ in a system where AF and SC coexist uniformly.

A minimal GL free energy that describes the competition of AF and SC orders under magnetic field takes the form

$$\mathcal{F} = \mathcal{F}_\psi + \mathcal{F}_m + \mathcal{F}_{int} + \kappa^2 b^2$$

with

$$\mathcal{F}_\psi = \rho_1 |(\nabla - i 2\pi \mathbf{A}) \psi|^2 + r_1 |\psi|^2 + \frac{\mu_1}{2} |\psi|^4$$

$$\mathcal{F}_m = \rho_2 |\nabla \mathbf{m}|^2 + r_2 |\mathbf{m}|^2 + \frac{\mu_2}{2} |\mathbf{m}|^4 + \chi \mathbf{b} \cdot |\mathbf{m}||\mathbf{m}|^2$$

$$\mathcal{F}_{int} = u_{12} |\psi|^2 |\mathbf{m}|^2.$$  

Here, we express the free energy and the order parameters in dimensionless form. $\mathcal{F}_\psi$ is the standard GL free energy of the SC order parameter $\psi$. $\mathcal{F}_m$ is the free energy of the AF order parameter $\mathbf{m}$. $\mathbf{A}$ is the vector...
potential and $\mathbf{b} = (\nabla \times \mathbf{A}) \times a^2$ is the dimensionless magnetic field measured in units of $\phi_0/a^2$, where $\phi_0 = \hbar c/2e$ is the London flux quantum and $a$ is the lattice constant. $\mathbf{m}_z$ is the component of the AF moment perpendicular to the magnetic field. $\kappa$ is the GL parameter. $\mu_B$ is the Bohr magneton. The $\chi$ term describes the Zeeman coupling of the AF moment with the external magnetic field. The interaction term $u_{12}$ is the key term describing the interaction between the AF and the SC order parameters. When $u_{12}^2 > u_{2}u_{1}$, there is a direct first order transition between the AF and the SC state. On the other hand, when $u_{12}^2 < u_{2}u_{1}$, the system undergoes two second order phase transitions, with an intermediate phase where AF and SC coexist uniformly. In the special case of $u_{12}^2 = u_{2}u_{1}$, the potential can be scaled into a $SO(5)$ symmetric form at the quantum critical point where $r_2/\sqrt{u_2} = r_1/\sqrt{u_1}$, and the AF and SC orders can be freely rotated into each other. Therefore, the relationship among the three quartic coefficients provides a crucial test on the $SO(5)$ symmetry of the model.

On the other hand, by tuning the doping and the chemical potential, the quadratic coefficients can always be tuned to reach the quantum critical points. By quantitatively fitting the neutron scattering data in the vortex state of $Nd_{1.85}Ce_{0.15}CuO_4$, we can determine the value $u_{12}/\sqrt{u_2u_1}$, and consequently the nature of the quantum phase transition between AF and SC.

We use the relaxation method [16, 17] to find the numerical solution that minimizes the GL free energy $F$. We assume the system is an extreme type-II superconductor, $\kappa \gg 1$, so that the magnetic field is uniformly distributed over the sample. We choose the symmetrical gauge so that the vector potential $\mathbf{A}$ reads

$$\mathbf{A} = \frac{\mathbf{r} \times \mathbf{b}}{2}. \quad (3)$$

The boundary conditions are then given by

$$\psi(\mathbf{r} + L_x \hat{x}) = \psi(\mathbf{r}) e^{-i2\pi A_z L_x/a} \quad (4a)$$
$$\psi(\mathbf{r} + L_y \hat{y}) = \psi(\mathbf{r}) e^{-i2\pi A_y L_y/a} \quad (4b)$$
$$m(\mathbf{r} + L_x \hat{x}) = m(\mathbf{r}) \quad (4c)$$
$$m(\mathbf{r} + L_y \hat{y}) = m(\mathbf{r}). \quad (4d)$$

Here, $L_x$ and $L_y$ are the width and height of the magnetic unit cell that satisfy the condition $(b_2 \phi_0/a^2)L_xL_y = \phi_0$. $A_x$ and $A_y$ are the components of the vector potential $\mathbf{A}$ in the $ab$-plane. With the free energy $F$ and the boundary conditions (3a–3d), we choose $\psi$, $\psi^*$ and $m$ as independent variables. The relaxation iteration equations read

$$\psi^{(n+1)} = \psi^{(n)} - \delta_1 \frac{\partial F}{\partial \psi^*}^{(n)} \quad (5a)$$
$$m^{(n+1)} = m^{(n)} - \delta_2 \frac{\partial F}{\partial m}^{(n)}, \quad (5b)$$

where $\delta_1$ and $\delta_2$ are small positive numbers adjusted to optimize the convergence and $n$ denotes the generation of the iteration. Starting from a proper initial state, this relaxation procedure quickly reaches convergence. We then repeat the relaxation procedure for different sizes of magnetic unit cell, or equivalently for different magnetic fields, to obtain the field dependence of the AF moment.

When $u_{12} = 0$, the two order parameters decouple. The bare SC coherence length is given by $\xi_0 = \rho_1/|r_1|$, and the bare upper critical field is given by $B_0 = \phi_0/2\pi\xi_0^2$. However, when $u_{12} > 0$, the magnetic field induces AF moment in the vortex core regions, which renormalizes the coherence length and the upper critical field to $\xi > \xi_0$ and $B_{c2} < B_0$. These values are self-consistently determined by solving the coupled GL equations in the vortex state. Fig.1 shows the field dependence of the AF moment, for different values of $u_{12}$. We see that this value directly determines the curvature of the field dependence curve. For strong repulsion, $u_{12}^2 > u_{2}u_{1}$, the AF moment increases slowly at low field since the AF moment is strongly suppressed by the SC order in the bulk. At high field close to $B_{c2}$, the AF moment increases steeply since most of the SC order are destroyed. Therefore, the field dependence of the AF moment has a positive curvature in this regime. In contrast, when $u_{12}^2 < u_{2}u_{1}$, the field dependence is reversed. The AF moment increases steeply for low field, and levels off at high field, leading to a negative curvature. In the $SO(5)$ symmetric case where $u_{12}^2 = u_{2}u_{1}$, the AF moment scales linearly with $B$ up to $B_{c2}$.

The linear dependence was first predicted by Arovas et al. [4] in the low field regime, based on the argument that the AF moment scales with the number of vortices, which is linearly proportional to the field. Here we have shown that this linear dependence generally does not hold for fields close to $B_{c2}$, unless the system is $SO(5)$ sym-
metric. Demler et al. [13] showed that the circulating currents around the vortices lead to a logarithmic correction of the form \( B \ln(B_{c2}/B) \). Their result is derived in the weak field regime \( B < B_{c2} \). This behavior leads to an infinite slope at \( B = 0 \). The experimentally measured field dependence shown in Fig. 3e of reference [3] does not have this feature. Zhang et al. [10] studied the similar problem, in the \( B < B_{c2} \) regime, mostly for the parameters where \( u_2^2 < u_1 u_2 \), and found the field dependence of the induced magnetic moment to have a negative curvature. This result is consistent with ours in the same parameter regime.

For field higher than \( B_{c2} \), the SC order is completely suppressed. Among those terms in Eq. (4), only the AF term \( \mathcal{F}_{\alpha} \) and the magnetic field energy term survive. The problem becomes uniform and can be solved analytically to yield

\[
m_B(B) = \sqrt{|r_2|/u_2 \sqrt{1 - B^2/B_s^2}} \tag{6}
\]

where

\[
B_s = \sqrt{|r_2|/\phi_0/a^2} \tag{7}
\]

is the critical field where the AF moment disappears.

In Fig. 2, we plot the fit of the experimental results of Matsuuara et al. [4, 21]. Both the intrinsic AF moment of NCCO and extrinsic FM moment of \( Nd_2O_3 \) impurity phase contribute to the \((\pi, \pi, 0)\) peak measured in \( HK0 \) zone [corresponding to field in \((0, 0, 1)\) direction] [21]. However, the extrinsic contribution of the \( Nd_2O_3 \) impurity phase can be easily subtracted. Due to the cubic symmetry of \( Nd_2O_3 \) crystal, we can subtract the integrated intensity of \((0, 0, 4.4\pi)\) peak measured in \( HHL \) zone, which arises exclusively from \( Nd_2O_3 \), from the normalized integrated intensity of \((\pi, \pi, 0)\) measured in \( HK0 \) zone, to obtain the intrinsic NCCO contribution of the AF moment [22]. We then take the square root of the integrated intensity to obtain the moment. We obtain a reasonably well fit of the field dependence of AF moment. For the field below \( B_{c2} \), our theory predicts that the FM moment per vortex scales linearly with the field. It follows that the total FM moment scales quadratically since the number of vortices is proportional to the field. The experiment observed a linear relation. We believe the quadratic relation between FM moment and field is overwhelmed by the contribution of \( Nd \), moment which is linearly polarized by the field.

The quantitative fit to the field dependence of the AF moment determines \( u_{12}/\sqrt{u_2 u_1} = 0.95 \). Therefore, the quartic terms are approximately \( SO(5) \) symmetric. The quadratic terms \( r_1 = -1 \) and \( r_2 = -0.85 \) deviate more from the \( SO(5) \) symmetric value. This is to be expected, since the system is close to optimal doping where the SC state is the stable ground state. Since \( r_1 \) depends on the chemical potential, it can always be tune to \( r_2 \) at the quantum phase transition point where both quadratic and quartic terms are approximately \( SO(5) \) symmetric.

The experimental result of the field dependence of AF moment beyond \( B_{c2} \) can be fitted very well by the simple formula Eq. (6) with a critical field \( B_s \sim 20.5T \). Energetically, this critical field is determined by the competition between the Zeeman energy and the condensation energy of the AF moment. From the fact that the observed AF moment at \( B_{c2} \) is about \( m = 0.05\mu_B \) per site, we estimate that the Zeeman energy at \( B_s \) is about \( B_s m \approx 0.05meV \). It follows that the AF coupling \( J_{AF} \) is about \( 20meV \), if the AF condensation energy can be written as \( E_{AF} = J_{AF}m^2 \).

The detailed agreement between our model and the experiment obtained above allows us to make a striking quantitative prediction. As we mentioned previously, the upper critical field \( B_{c2} \) is strongly reduced by the repulsion between AF and SC. Using the parameters obtained above, we estimate the bare value of the SC coherence value to be \( \xi_0^2 = \rho_1/|r_1| \), and the bare upper critical field is given by \( B_0 = \phi_0/|r_1|/2\pi\rho_1 \approx 23T \). If the AF order could be suppressed without disturbing the SC order, the SC order would be enhanced. Consequently, the upper critical field \( B_{c2} \) would increase too. Our idea is to apply a Zeeman field in the \( ab \)-plane. The Zeeman field suppress the AF moment through the canting term \( \chi \). After including the Zeeman field, the total field is

\[
b = b_2 \hat{z} + b_1 \hat{x} \tag{8}
\]

The dimensionless upper critical field \( b_{c2} \) is then given by the solution of the coupled equations:

\[
\sqrt{b_{c2}^2 - b_1^2} = |r_1|/u_{12} \mu_0 \sqrt{2\pi\rho_1/a^2} \tag{9a}
\]
m^2 = \max \left[ \frac{|r_2| - \chi b_{c2}^2}{u_2}, 0 \right]. \quad (9b)

The first equation gives the $z$-component of $b_{c2}$ as a function of $m$ while the second one gives the AF moment $m$ at $b_{c2}$. For small small $b_{||}$, the increase of the $z$-component of $b_{c2}$ is quadratic in $b_{||}$

$$\frac{b_{c2}^z(b_{||}) - b_{c2}^z(0)}{b_{c2}^z(0)} = \frac{\chi u_{12} b_{c2}^2 + O(b_{||}^3)}{u_2 |r_1| - u_{12} |r_2| - \chi u_{12} (b_{c2}^z(0))^2} \quad (10)$$

where $b_{c2}^z(0)$ is the upper critical field if $b_{||} = 0$, given by the solution of self-consistent equation

$$b_{c2}^z(0) = \frac{u_2 |r_1| - u_{12} |r_2| + \chi u_{12} (b_{c2}^z(0))^2}{2\pi u_2 r_1 / a^2}. \quad (11)$$

This effect can be used to quantitatively measure the competition between the AF and the SC order parameters. Fig. 3 plots the $z$-component of the upper critical field for NCCO system studied in previous paragraphs, as a function of the canting angle $\theta = \tan^{-1}(b_{c2}^z/b_{c2})$. It is interesting to note that a canting of $27^\circ$ increases the $B_{c2}$ by about 30%. In the above estimate we neglected the effect of the $ab$ plane field on the SC. If this effect is taken into account, the actual increase of $B_{c2}$ would be smaller.

Similarly, for a system with uniformly co-existing AF order and SC order at zero field, the suppression of the AF ordering due to the Zeeman field in the $ab$ plane would increase the transition temperature $T_c$, according to this formula:

$$\frac{T_c(b_{||}) - T_c(0)}{T_c(0)} = \frac{\chi u_{12} b_{c2}^2}{u_2 |r_1| - u_{12} |r_2|}. \quad (12)$$

Here, we assume $r_2(T) = r_2(1 - T/T_N^0), r_1(T) = r_1(1 - T/T_c^0)$ with $T_N > T_c^0$. We also assume that the Zeeman field $b_{||}$ is small enough so that the AF moment $m$ is nonzero at $T_c$. Again, the enhancement scales quadratically with the Zeeman field.

In summary, we have studied the competition of AF and SC orders in High-Tc superconductors by solving the GL free energy. We showed that the curvature of the AF moment versus B field plot directly determines the departure from the $SO(5)$ condition in the quartic terms of the GL functional. Reasonable agreement with the recent neutron scattering experiment on $Nd_{1.35}Ce_{0.15}CuO_4$ shows that this system is close to a $SO(5)$ symmetric quantum critical point. New experiments are predicted to increase $B_{c2}$ and $T_c$ by applying an in-plane magnetic field. The GL model with competing AF and SC order parameters can be derived from the projected $SO(5)$ model on the lattice [23], which can in turn be derived from the microscopic $t$-$J$ model by a contractor-renormalization-group algorithm [24]. The quantitative agreement between these approximately $SO(5)$ symmetric models and the experiment shows a promising direction towards a full microscopic theory of high Tc superconductivity.

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