

Quantitative Test of SO(5) Symmetry in the Vortex State of Nd_{1.85}Ce_{0.15}CuO₄

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(Received 21 May 2003; published 10 March 2004)

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 *et al.* and Matsuura *et al.* on Nd_{1.85}Ce_{0.15}CuO₄, 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.

DOI: 10.1103/PhysRevLett.92.107002

PACS numbers: 74.20.De, 74.25.Ha, 74.25.Op

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 [1,2]. The SO(5) theory [3] considers the antiferromagnetic (AF) state to be the dominant competing state, and describes its competition with the SC state in terms of a unified theory with approximate SO(5) symmetry. This theory predicts that the competing AF order reveals itself in the SC vortex core [3,4]. This prediction has now been verified experimentally in a number of different compounds and by a variety of different experimental techniques [5–14]. Experimental and theoretical progress on the AF vortex lattice is reviewed in recent articles [1,2].

While the experimental observation of enhanced AF correlation in the vortex state is encouraging, the limitation of the 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.* [5] and Matsuura *et al.* [6] performed neutron scattering experiments on the electron-doped Nd_{2-x}Ce_xCuO_{4-δ} (NCCO) crystal under a magnetic field of 16 T, beyond the upper critical field $B_{c2} = 6.2$ T 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 Letter.

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 (GL) 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}CuO₄ is close to a SO(5) symmetric point. The magnetic field has a dual effect on the AF moment. On one hand, it creates an AF moment in the vortex core; on the other hand, it reduces the AF moment by canting the spins uniformly towards the 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 leads 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

$$\mathcal{F} = \mathcal{F}_\psi + \mathcal{F}_m + \mathcal{F}_{\text{int}} + \kappa^2 b^2, \quad (1)$$

with

$$\mathcal{F}_\psi = \rho_1 |(\nabla - i2\pi\mathbf{A})\psi|^2 + r_1 |\psi|^2 + \frac{u_1}{2} |\psi|^4, \quad (2a)$$

$$\mathcal{F}_m = \rho_2 |\nabla\mathbf{m}|^2 + r_2 |\mathbf{m}|^2 + \frac{u_2}{2} |\mathbf{m}|^4 + \chi b^2 |\mathbf{m}_\perp|^2, \quad (2b)$$

$$\mathcal{F}_{\text{int}} = u_{12} |\psi|^2 |\mathbf{m}|^2. \quad (2c)$$

Here, we express the free energy and the order parameters in dimensionless form. \mathcal{F}_ψ is the standard GL free energy of the SC order parameter ψ ; \mathcal{F}_m is the free energy of the

AF order parameter \mathbf{m} [15]. \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 ϕ_0/a^2 , where $\phi_0 = hc/2e$ is the London flux quantum and a is the lattice constant. \mathbf{m}_\perp is the component of the AF moment perpendicular to the magnetic field. κ is the GL parameter. μ_B is the Bohr magneton. The χ 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 $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$, we can determine the value $u_{12}/\sqrt{u_2 u_1}$, 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 (1). 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

$$\psi(\mathbf{r} + L_x \hat{\mathbf{x}}) = \psi(\mathbf{r}) e^{-i2\pi A_x L_x/a}, \quad (4a)$$

$$\psi(\mathbf{r} + L_y \hat{\mathbf{y}}) = \psi(\mathbf{r}) e^{-i2\pi A_y L_y/a}, \quad (4b)$$

$$m(\mathbf{r} + L_x \hat{\mathbf{x}}) = m(\mathbf{r}), \quad (4c)$$

$$m(\mathbf{r} + L_y \hat{\mathbf{y}}) = m(\mathbf{r}). \quad (4d)$$

Here, L_x and L_y are the width and height of the magnetic unit cell that satisfy the condition $(b_z \phi_0/a^2)L_x L_y = \phi_0$. A_x and A_y are the components of the vector potential \mathbf{A} in the ab plane. With the free energy (1) and the boundary conditions (4a)–(4d), we choose ψ , ψ^* , and m as independent variables. The relaxation iteration equations read

$$\psi^{(n+1)} = \psi^{(n)} - \delta_1 \left. \frac{\partial \mathcal{F}}{\partial \psi^*} \right|^{(n)}, \quad (5a)$$

$$m^{(n+1)} = m^{(n)} - \delta_2 \left. \frac{\partial \mathcal{F}}{\partial m} \right|^{(n)}, \quad (5b)$$

where δ_1 and δ_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 $\xi_0^2 = \rho_1/|r_1|$, 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 an 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. Figure 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 is 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) symmetric. Demler *et al.* [18] showed that the circulating currents around the vortices lead to a logarithmic correction

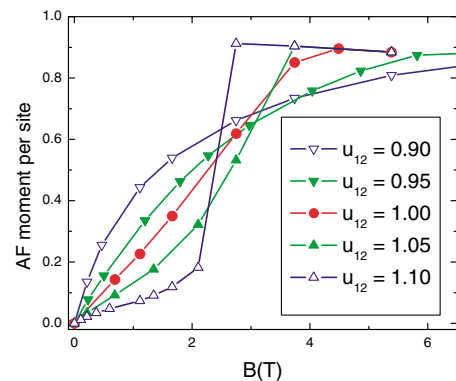


FIG. 1 (color online). The plot of field dependence of AF moment for different parameters. The other parameters are $\rho_1 = \rho_2 = a^2$, $r_1 = -1$, $r_2 = -0.85$, $u_1 = u_2 = 1$, and $\chi = 42.4$. Here, the parameters are chosen such that the maximum SC order is 1 and the SC coherence length at zero field equals the lattice constant a of our discrete model.

of the form $B \ln(B_{c2}/B)$. Their result is derived in the weak field regime $B \ll B_{c2}$. This behavior leads to an infinite slope at $B = 0$. The experimentally measured field dependence shown in Fig. 3e of Ref. [5] does not have this feature. Zhang *et al.* [19] studied the similar problem, in the $B < B_{c2}$ regime, mostly for the parameters where $u_{12}^2 < u_1 u_2$, 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 a field higher than B_{c2} , the SC order is completely suppressed. Among those terms in Eq. (1), only the AF term \mathcal{F}_m and the magnetic field energy term survive. The problem becomes uniform and can be solved analytically to yield

$$m(B) = \sqrt{|r_2|/u_2} \sqrt{1 - B^2/B_s^2}, \quad (6)$$

where

$$B_s = \sqrt{|r_2|/\chi} \phi_0/a^2, \quad (7)$$

is the critical field where the AF moment disappears.

In Fig. 2, we plot the fit of the experimental results of Matsuura *et al.* [6,20]. Both the intrinsic AF moment of NCCO and the extrinsic FM moment of the Nd_2O_3 impurity phase contribute to the $(\pi, \pi, 0)$ peak measured in the $HK0$ zone [corresponding to field in the $(0, 0, 1)$ direction] [21]. However, the extrinsic contribution of the Nd_2O_3 impurity phase can be easily subtracted. Because of the cubic symmetry of the Nd_2O_3 crystal, we can subtract the integrated intensity of the $(0, 0, 4.4\pi)$ peak measured in the HHL zone, which arises exclusively from Nd_2O_3 , from the normalized integrated intensity

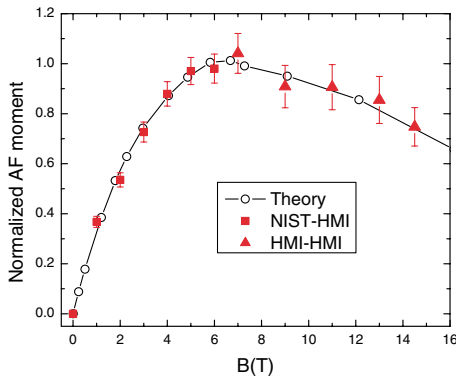


FIG. 2 (color online). The field dependence of the AF moment. The solid squares are obtained by subtracting the intensity of $(0, 0, 4.4\pi)$ measured at Hahn-Meitner-Institute (HMI) [20] from the intensity of $(\pi, \pi, 0)$ measured at National Institute of Standards and Technology [6]. The solid triangles are obtained subtracting the intensity of $(0, 0, 4.4\pi)$ measured at HMI [20] from the intensity of $(\pi, \pi, 0)$ measured at HMI [6]. The parameters used in obtaining the theoretical curve are $\rho_1 = \rho_2 = a^2$, $r_1 = -1$, $r_2 = -0.85$, $u_1 = u_2 = 1$, $u_{12} = 0.95$, and $\chi = 42.4$.

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 the FM moment and the field is overwhelmed by the contribution of the 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 tuned 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 $B_s \sim 20.5$ T. 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 [5], we estimate that the Zeeman energy at B_s is about $B_s m \approx 0.05$ meV. It follows that the AF coupling J_{AF} is about 20 meV, 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 $B_0 = \phi_0|r_1|/2\pi\rho_1 \approx 23$ T. 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 also. Our idea is to apply a Zeeman field in the ab plane. The Zeeman field suppresses the AF moment through the canting term χ . After including the Zeeman field, the total field is

$$\mathbf{b} = b_z \hat{\mathbf{z}} + b_{\parallel} \hat{\mathbf{x}}. \quad (8)$$

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

$$\sqrt{b_{c2}^2 - b_{\parallel}^2} = \frac{|r_1| - u_{12} m^2}{2\pi\rho_1/a^2}, \quad (9a)$$

$$m^2 = \max\left[\frac{|r_2| - \chi b_{c2}^2}{u_2}, 0\right]. \quad (9b)$$

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 b_{\parallel} , the increase of the z component of b_{c2} is quadratic in b_{\parallel} :

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

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

$$b_{c2}^z(0) = \frac{u_2|r_1| - u_{12}|r_2| + \chi u_{12}[b_{c2}^z(0)]^2}{2\pi u_2 \rho_1 / a^2}. \quad (11)$$

This effect can be used to quantitatively measure the competition between the AF and the SC order parameters. Figure 3 plots the z component of the upper critical field for the NCCO system studied in previous paragraphs, as a function of the canting angle $\theta = \tan^{-1}(b_{c2}^z/b_{\parallel})$. It is interesting to note that a canting of 27° increases the B_{c2}^z 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}^z would be smaller.

Similarly, for a system with *uniformly* coexisting 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 itself, according to this formula:

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

Here, we assume $r_2(T) = r_2(1 - T/T_N^0)$, $r_1(T) = r_1(1 - T/T_c^0)$ with $T_N^0 > T_c^0$. We also assume that the Zeeman field b_{\parallel} 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- T_c superconductors by solving the GL free energy. We showed that the curvature of the AF moment versus the 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 $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ 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

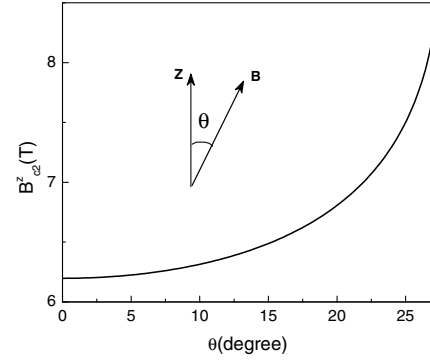


FIG. 3. The angle dependence of the z component of the upper critical field, given by the solution to coupled Eqs. (9a) and (9b). The parameters are the same as those used in fitting of the experimental data in Fig. 2.

promising direction towards a full microscopic theory of high- T_c superconductivity.

We would like to acknowledge useful discussions with Dr. M. R. Beasley, B. A. Bernevig, Dr. P. C. Dai, Dr. E. Demler, Dr. J. P. Hu, Dr. H. J. Kang, L. Lu, P. Mang, Dr. J. Zaanen, and G. Zeltzer. This work was performed on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC03-76SF00515 and the National Science Foundation under Grant No. DMR-9814289. H. D. C. and C. J. W. are also supported by Stanford SGF.

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