

## Superconducting Vortex with Antiferromagnetic Core

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We show that a superconducting vortex in underdoped high  $T_c$  superconductors could have an antiferromagnetic core. This type of vortex configuration arises as a topological solution in the recently constructed SO(5) nonlinear  $\sigma$  model and in Landau-Ginzburg theory with competing antiferromagnetic and superconducting order parameters. Experimental detection of this type of vortex by muon spin resonance and neutron scattering is proposed. [S0031-9007(97)04250-6]

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One of the most striking properties of high  $T_c$  superconductivity is the close proximity between the antiferromagnetic (AF) and the superconducting (SC) phases. While there are a number of theories [1] linking the microscopic origin of high  $T_c$  SC to antiferromagnetic correlations, it is natural to ask if the close proximity between these two phases could have any macroscopic manifestations. Recently, a unified theory [2] of AF and  $d$ -wave SC in the cuprates has been constructed based on an SO(5) symmetry. In this theory, the AF and the  $d$ -wave SC order parameters are unified into a five dimensional vector  $(n_1, n_2, n_3, n_4, n_5)$  called a superspin. The AF order parameters  $\vec{m}$  correspond to the  $(n_2, n_3, n_4)$  components, while the real and imaginary parts of the SC order parameter  $\psi$  correspond to the  $(n_1, n_5)$  components. It was shown that the chemical potential induces a first order superspin-flop transition where the superspin abruptly changes direction from AF to SC.

The SO(5) theory predicts a spin triplet of pseudo Goldstone bosons associated with the spontaneous breaking of SO(5) symmetry in the SC phase [2,3]; these can be identified with the recently observed resonant neutron scattering peaks in superconducting YBCO [4]. Physically, these modes correspond to Gaussian fluctuations of the superspin. However, it was noted [2] that the SO(5) theory also admits a special class of topological solutions called meron configurations. In this configuration, the superspin lies inside the SC plane far away from the origin, and the SC phase winds around the origin by  $2\pi$ . As the origin is approached from the radial direction, the superspin lifts up from the SC plane into the AF sphere in order to minimize the energy cost of winding the SC phase. The result is a SC vortex with an AF core [5].

The existence of SC vortices with AF cores leads to nontrivial macroscopic consequences which we shall explore in this paper. We first present detailed analytic and numerical solutions of the SO(5) vortex. We also study a more general Landau-Ginzburg (LG) theory obtained from the SO(5) theory by relaxing the constraint

on the magnitude of the superspin. This theory describes AF and SC order parameters in competition with each other. We show that even if the SC state wins in the bulk, under appropriate conditions a nonvanishing AF component can occur inside a SC vortex core. The nature of the condition leads us to conclude that a SC vortex with an AF core should only be realized in underdoped high  $T_c$  superconductors, not in the overdoped ones. We believe that the nature of the vortex core has nontrivial implications for the physics of high  $T_c$  superconductors in a high magnetic field. In recent experiments, Boebinger *et al.* [6] find that insulating and normal phases appear upon destruction of SC by a high magnetic field in underdoped and overdoped materials, respectively. This observation could be related to the insulating/normal vortex core in underdoped/overdoped materials which is found in this work. We also suggest possible neutron and muon spin resonance ( $\mu$ SR) experiments to probe the AF components of the vortex core.

The SO(5) theory has been constructed in its general form to allow for anisotropy in the AF and SC couplings [2,7]. However, in the underdoped regime close to the AF-SC transition, most forms of anisotropies are irrelevant [7]. In this work, we first study the isotropic limit of coupling constants, and allow only a quadratic symmetry breaking term. In this limit of the SO(5) theory, the free energy density takes the form [8]

$$\mathcal{F} = \frac{1}{2} \rho \left| \left( \vec{\nabla} + \frac{ie^*}{\hbar c} \vec{A} \right) \psi \right|^2 - \frac{1}{2} \chi (2\mu)^2 |\psi|^2 + \frac{1}{2} \rho |\vec{\nabla} \vec{m}|^2 - \frac{1}{2} g \vec{m}^2 + \frac{1}{8\pi} (\vec{\nabla} \times \vec{A})^2, \quad (1)$$

where  $\psi = n_1 + in_5$  and  $\vec{m} = n_2 \hat{x} + n_3 \hat{y} + n_4 \hat{z}$  are the SC ( $\psi$ ) and AF ( $\vec{m}$ ) order parameters. Because of the constraint  $\psi^* \psi + \vec{m}^2 = 1$ , the two are coupled. When  $\tilde{g} \equiv g - 4\mu^2 \chi \equiv 4\chi(\mu_c^2 - \mu^2)$  is negative, the bulk phase is superconducting;  $\tilde{g} > 0$  prefers the antiferromagnet. Assuming a constant direction for the Néel field, we

have  $\vec{m} = \sqrt{1 - |\psi|^2} \hat{m}$ , and the equations for  $\psi$  are

$$-\left(\vec{\nabla} + \frac{ie^*}{\hbar c} \vec{A}\right)^2 \psi - \xi^{-2} \psi + \frac{\vec{\nabla}^2 \sqrt{1 - |\psi|^2}}{\sqrt{1 - |\psi|^2}} \psi = 0, \quad (2)$$

$$\lambda_L^2 \vec{\nabla} \times \vec{\nabla} \times \vec{A} + |\psi|^2 \vec{A} + \frac{\hbar c}{e^*} \frac{1}{2i} (\bar{\psi} \vec{\nabla} \psi - \psi \vec{\nabla} \bar{\psi}) = 0,$$

where  $\xi \equiv \sqrt{\rho/(-\tilde{g})}$  is the coherence length;  $\tilde{g} < 0$  in the superconducting phase. As in the more familiar Ginzburg-Landau theory of SC vortices, there are two length scales in the problem.

*Vortex solutions.*—In searching for vortex solutions, it is convenient to work in polar coordinates  $(r, \phi)$  and to rescale distance,  $r \equiv \xi s$ , and vector potential,  $\vec{A}(\vec{r}) \equiv (\phi_L/2\pi\xi^2) s^{-1} \alpha(2) \hat{\phi}$ , where  $\phi_L = \hbar c/e^*$  is the London flux quantum. The magnetic field is then  $B(r) = (\phi_L/2\pi\xi^2) b(s)$  with  $b(s) = s^{-1} d\alpha/ds$ . We demand  $\alpha(0) = 0$  and  $\alpha(\infty) = m$ , the number of flux quanta through the plane. With  $\psi = f(r) \exp(im\phi)$ , then

$$0 = \frac{d^2 f}{ds^2} + \frac{1}{s} \frac{df}{ds} + \frac{f}{1-f^2} \left(\frac{df}{ds}\right)^2 + \left[1 - \left(\frac{\alpha-m}{s}\right)^2\right] (1-f^2) f, \quad (3)$$

$$0 = \frac{d^2 \alpha}{ds^2} - \frac{1}{s} \frac{d\alpha}{ds} - \frac{(\alpha-m)}{\kappa^2} f^2,$$

where  $\kappa \equiv \lambda_L/\xi$  is the Ginzburg-Landau parameter. We solve these equations by the shooting method, using the asymptotic solutions  $f(s \rightarrow 0) \sim C_1 s^m$ ,  $\alpha(s \rightarrow 0) \sim C_2 s^2$ ,  $f(s \rightarrow \infty) \sim 1 - C_3 \exp(-2s)$ ,  $\alpha(s \rightarrow \infty) \sim m - C_4 \exp(-2\sqrt{s}/\kappa)$ , where  $C_1, \dots, C_4$  are constants. The SC order parameter and magnetic field distribution near the vortex core is shown in Fig. 1 for different values of  $\kappa$ . In the SO(5) theory, the AF order parameter is simply given by  $\sqrt{1 - \Psi^2}$ . As in conventional vortex solutions, the SC order parameter is well approximated by a tanh. The vortex line energy has also been calculated and gives a value of  $\kappa_{\text{crit}}$ , separating type I and type II behavior, in good agreement with the value predicted from  $H_{c2}$  for this model,  $\kappa_{\text{crit}} = 1$  [9].

*Domain walls.*—The Gibbs free energy density is  $\mathcal{G} = \mathcal{F} - \frac{1}{4\pi} \vec{B} \cdot \vec{H}$ . In the bulk, the SC state is characterized by  $|\psi| = 1$ ,  $\vec{B} = 0$ , and a free energy density of  $\mathcal{G}_{\text{SC}} = \frac{1}{2} \tilde{g} = -\rho/2\xi^2$ . The AF state has  $|\psi| = 0$ ,  $\vec{B} = \vec{H}$ , and  $\mathcal{G}_{\text{AF}} = -\vec{H}^2/8\pi$ . Setting  $\mathcal{G}_{\text{SC}} = \mathcal{G}_{\text{AF}}$  gives the thermodynamic critical field  $H_c$ :  $H_c = \sqrt{4\pi\rho}/\xi = \phi_L/2\pi\xi\lambda_L$ . We now consider a domain wall separating a bulk AF ( $x \rightarrow -\infty$ ) from a bulk SC ( $x \rightarrow +\infty$ ) and compute the energy of the domain wall relative to that of either bulk state. We write  $x = \xi s$  and  $\vec{A} = (\hbar c/e^* \xi) a(s) \hat{y}$  to obtain the Ginzburg-Landau equations

$$0 = \frac{\partial^2 f}{\partial s^2} + (1 - a^2) f (1 - f^2) + \frac{f}{1 - f^2} \left(\frac{\partial f}{\partial s}\right)^2, \quad (4)$$

$$0 = \frac{\partial^2 a}{\partial s^2} - \frac{1}{\kappa^2} a f^2,$$

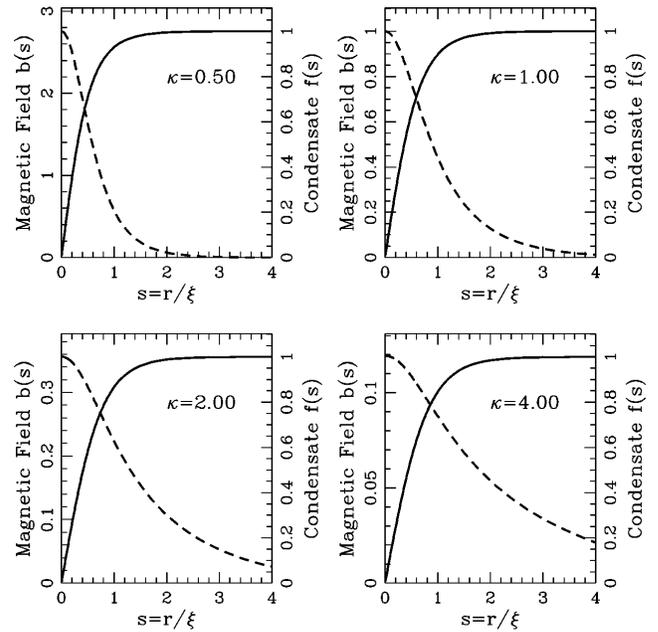


FIG. 1. Vortex profiles for a series of different values of  $\kappa$ . The dashed lines show the magnetic field distribution and the solid lines show the SC order parameter. The AF order parameter is related to the SC order parameter by the SO(5) constraint.

with asymptotic solutions  $f(s \rightarrow -\infty) \sim C_1 \exp(-s^2/2\kappa)$ ,  $a(s \rightarrow -\infty) \sim s/\kappa + C_2$ ,  $f(s \rightarrow \infty) \sim 1 - C_3 \exp(-2s)$ , and  $a(s \rightarrow \infty) \sim C_4 \exp(-s/\kappa)$ . We again solve by the shooting method, and the results are shown in Fig. 2 for various values of  $\kappa$ .

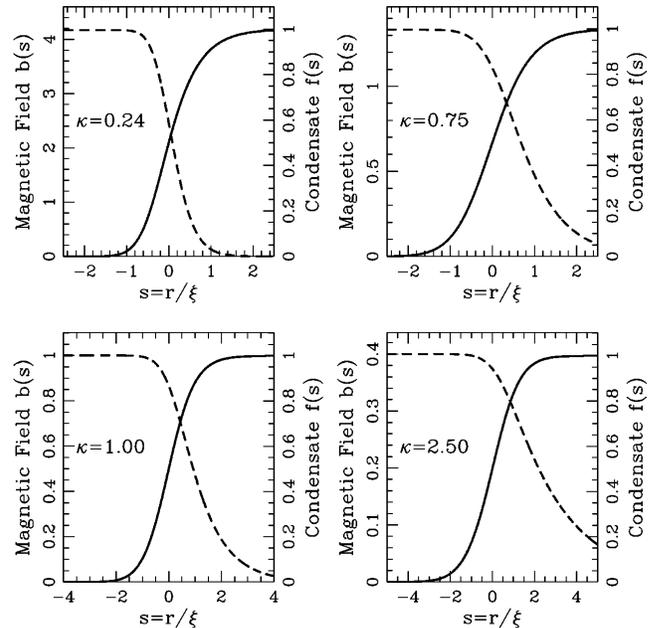


FIG. 2. Domain wall profiles for a series of different values of  $\kappa$ . The dashed lines show the magnetic field distribution, and the solid lines show the SC order parameter.

The domain wall free energy per unit length is

$$\sigma = \frac{\rho}{2\xi} \int_{-\infty}^{\infty} ds \left\{ \left( \kappa \frac{\partial a}{\partial s} - 1 \right)^2 - \left( \frac{f}{1-f^2} \frac{\partial f}{\partial s} \right)^2 \right\}. \quad (5)$$

Note that the integrand of Eq. (5) is a difference of two positive quantities. When  $\sigma > 0$  the domain wall energy is positive. This is type I behavior. When  $\sigma < 0$  the domain wall energy is negative, and we have type II behavior.  $\sigma = 0$  corresponds to  $\kappa_{\text{crit}} = 0.30$ , which differs from that determined by  $H_{c2}$  or the vortex line energy because of the gradients which appear in the fourth order terms due to the SO(5) constraint [9].

In the above calculations, the SO(5) constraint forces the vortex core to be antiferromagnetic. A normal core is describable within a soft superspin model. To explore the competition between AF and normal cores, we write  $\psi = n \cos \theta e^{i\phi}$  and  $\vec{m} = n \sin \theta \hat{m}$  with  $\phi = \tan^{-1}(y/x)$ . We further assume that  $\hat{m}$  is constant, and we work in the extreme type-II limit where the magnetic field is ignored. The free energy density is then

$$\mathcal{F} = \frac{1}{2}\rho[(\vec{\nabla}n)^2 + n^2(\vec{\nabla}\theta)^2 + \frac{1}{r^2}n^2\cos^2\theta] + \frac{1}{2}an^2 + \frac{1}{4}\tilde{g}(\cos 2\theta - 1)n^2 + \frac{1}{4}bn^4, \quad (6)$$

where  $a(T) = a'(T - T_c)$  in the vicinity of  $T_c$ . We now consider two trial vortex profiles: (i)  $n(r) = n_0 \tanh(r/\xi)$ ,  $\theta(r) = 0$  (normal core), and (ii)  $n(r) = n_0$ ,  $\theta(r) = \frac{\pi}{2} \exp(-r/\ell)$  (antiferromagnetic core). Here,  $\xi$  and  $\ell$  are variational parameters, while  $n_0 = \sqrt{(-a)/b}$  is the superspin magnitude far from the vortex core. We find  $\xi^2 = 3.385\rho/(-a)$  and  $\ell^2 = 0.9865\rho/(-\tilde{g})$ . The difference in free energy per unit length is then  $F_{\text{AF}} - F_{\text{normal}} \equiv \pi\rho n_0^2 [X(\lambda) - X_c]$ , where  $\lambda = 1.852\sqrt{\tilde{g}/a}$ ,  $X_c = 0.3214$ , and

$$X(\lambda) = \int_0^{\infty} \frac{du}{u} [\tanh^2 u - \cos^2(\frac{\pi}{2} e^{-\lambda u})]. \quad (7)$$

We find that the AF core is preferred for  $\lambda < 0.5683$ , i.e.,  $\tilde{g}/a < 0.0941$ .

The consequence of this analysis is that there is a line in the  $(T, \mu)$  plane separating regions with antiferromagnetic and normal cores. We find AF cores stable for  $4\chi(\mu^2 - \mu_c^2) < 0.0941(T_c - T)$ , hence, AF cores should be observable in underdoped materials at low temperatures. Increasing doping or temperature will eventually result in normal cores.

The general form of the free energy density when SO(5) has been broken down to  $O(2)_{\text{SC}} \times O(3)_{\text{AF}}$  is

$$\mathcal{F} = \frac{1}{2}\rho_\psi |\vec{\nabla}\psi|^2 + \frac{1}{2}\rho_m^\dagger |\vec{\nabla}\vec{m}|^2 + \frac{1}{2}\alpha |\vec{m}|^2 + \frac{1}{2}\beta |\psi|^2 + \frac{1}{2}u |\vec{m}|^4 + w |\vec{m}|^2 |\psi|^2 + \frac{1}{2}v |\psi|^4, \quad (8)$$

where we again work in the extreme type-II limit. We take  $\beta < 0$  and  $u, v, w > 0$ . Bulk SC is stable if  $\alpha/\beta < w/v$ ; this also precludes a mixed  $(|\psi|, m \neq 0)$  phase. If  $\alpha < 0$  and  $\alpha/\beta > u/w$  we must impose  $\beta^2/v > \alpha^2/u$  for global SC stability. We write  $\psi(\vec{r}) = \sqrt{|\beta|/2v} f(s) e^{i\phi}$  with  $s \equiv (|\beta|/\rho_\psi)^{1/2} r$ ;  $f$  is given by

the solution to

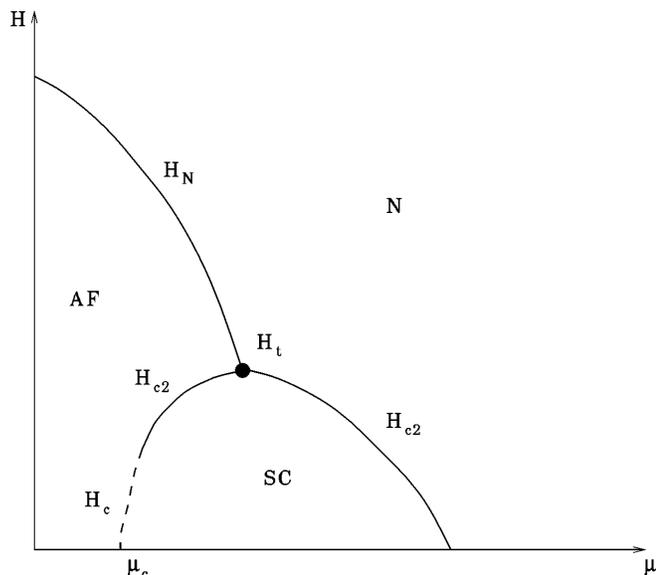
$$\frac{d^2 f}{ds^2} + \frac{1}{s} \frac{df}{ds} + \left(1 - \frac{1}{s^2}\right) f - f^3 = 0, \quad (9)$$

subject to  $f(0) = 0$  and  $f(\infty) = 1$ . The linearized equation for  $m(s)$  is then

$$-\frac{\rho_m}{\rho_\psi} \left( \frac{d^2 m}{ds^2} + \frac{1}{s} \frac{dm}{ds} \right) + \frac{w}{v} f^2(s) m = \frac{\alpha}{\beta} m. \quad (10)$$

This defines an eigenvalue problem, perhaps conveniently considered as a radially symmetric Schrödinger equation for a particle of mass  $M = \hbar^2 \rho_\psi / 2\rho_m$  in an attractive potential  $V(s) = -(w/v)[1 - f^2(s)]$ ; the energy eigenvalue is  $E = (\alpha/\beta - w/v)$ . Bound states, for which  $m(\infty) = 0$ , satisfy  $E < 0$ , in agreement with the aforementioned conditions. Antiferromagnetic cores will exist for  $E > -Y$ , where  $-Y$  is the lowest bound state energy; clearly  $Y(\rho_\psi/\rho_m, w/v)$  is an increasing function of  $w/v$  which vanishes when  $w/v = 0$ . Thus, we arrive at the condition  $w/v - Y(\rho_\psi/\rho_m, w/v) < \alpha/\beta < w/v$ . To compare with our earlier variational calculation, set  $\alpha/\beta = 1 - \tilde{g}/a$  and  $\rho_\psi/\rho_m = w/v = 1$ .

The SC vortex with an AF core has important consequences for the high magnetic field physics in underdoped high  $T_c$  superconductors. Within SO(5) theory, both the thermodynamic critical field  $H_c = \phi_L/2\pi\xi\lambda_L$  and the upper critical field  $H_{c2} = \phi_L/2\pi\xi^2$  describe phase transitions between SC and AF phases at fixed chemical potential  $\mu$  [10]. A schematic zero temperature phase diagram in the  $(H, \mu)$  plane is shown in Fig. 3. Applying a uniform magnetic field to the AF causes the Neel vector to flop into the plane perpendicular to the applied field, while the total magnetization vector is aligned in the field direction. The bulk AF-to-normal transition occurs at a critical field  $H_N = \alpha J/\hbar\mu_B$  (about 50 tesla if  $\alpha = 1$ ), where  $J$  is the AF exchange constant and  $\alpha$  is a dimensionless constant. Since doping (increasing  $\mu$ ) significantly weakens  $J$ , we expect  $H_N$  to decrease with increasing  $\mu$ . On the overdoped SC side, we also expect  $H_{c2}$  to decrease with increasing doping because of the loss in pairing energy. Surprisingly, on the underdoped side, the SO(5) theory gives  $H_{c2} = 4\chi\phi_L(\mu^2 - \mu_c^2)/2\pi\rho$  which increases with  $\mu$ . These three critical lines meet at a common tricritical point  $H_t$ . Several important features are to be noted about our proposed phase diagram. First of all, if we assume that the London penetration depth  $\lambda_L$  remains finite at  $\mu_c$ , then  $H_c$  will exceed  $H_{c2}$  sufficiently close to  $\mu_c$ , since  $\xi^{-2}$  behaves as  $\mu^2 - \mu_c^2$ . Therefore, the SC-to-AF transition will change from second order to first order in the vicinity of  $\mu_c$ , where these two phases are separated by the thermodynamic field  $H_c \propto \sqrt{\mu - \mu_c}$ . Second, all our discussions are carried out for a short ranged model at fixed  $\mu$ ; Coulomb interactions may lead to a significant modification of the phase diagram. However, we believe the most salient feature of our phase diagram, namely, the transition from a SC state to an

FIG. 3. Schematic  $T = 0$  phase diagram.

insulating state with applied field, will still remain valid in the underdoped regime.

Next we consider possible experimental methods for observing AF vortex cores. The AF vortex core size is on the order of the SC coherence length (four to five lattice constants). The density of vortices is proportional to the field. The local electron magnetic dipolar fields in the cores are hundreds of gauss, as they are in the pure AF [11], but because these AF regions are at best one dimensional (along the field direction), the local fields may not be static, except perhaps at low temperatures. The correlations along these small AF tubes depend on the weak interlayer exchange. Spin correlations between AF cores of neighboring vortices will be even weaker, and hence the AF order may not be coherent from one vortex to the next. This will show up in the neutron diffraction pattern. For neutron scattering, one expects to see peaks around  $(\pi, \pi)$  with a width of  $(\text{core size})^{-1}$ . If the spins are not static, this scattering will be quasielastic. The total intensity can be obtained by integrating over low frequencies. If the AF order were coherent from one vortex to the next, the periodicity of the vortex lattice would lead to superlattice diffraction peaks split by  $(\text{intervortex spacing})^{-1}$ . In any case, the integrated intensity of the broad peak at  $(\pi, \pi)$  will scale with field. For transverse field  $\mu\text{SR}$ , if the AF fields are static on the time scale of the muon precession frequency, it may be possible to observe the staggered local electron dipole field directly. The reason is that the field distribution from the center of a normal vortex core appears as a step at the high field end of the  $\mu\text{SR}$  spectrum. For AF cores, the dipolar field at the muon site will have a longitudinal component (along the  $c$  axis), of order 100 G [11], even if the electron spins lie in the  $a$ - $b$  plane. This longitudinal field at the muon site or sites will have

random sign and hence generate double or multiple steps in the absence of other broadening mechanisms. In a longitudinal field experiment, the fluctuating transverse fields due to the AF vortex cores could give rise to a substantial amount of relaxation. The magnitude of the relaxation depends on the amount of spectral density of transverse spin fluctuations at the Larmor frequency of the muon. The temperature dependence of this relaxation is a probe of the spin fluctuations within the vortex cores.

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- [1] N. E. Bickers, D. J. Scalapino, and S. R. White, *Phys. Rev. Lett.* **62**, 961 (1989); J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, *Phys. Rev. B* **39**, 11 663 (1989); D. Pines, *Physica (Amsterdam)* **235C**, 113 (1994).
- [2] S.-C. Zhang, *Science* **275**, 1089 (1997).
- [3] E. Demler and S.-C. Zhang, *Phys. Rev. Lett.* **75**, 4126 (1995).
- [4] J. Rossat-Mignod *et al.*, *Physica (Amsterdam)* **185C**, 86 (1991); H. Mook *et al.*, *Phys. Rev. Lett.* **70**, 3490 (1993); H. F. Fong *et al.*, *Phys. Rev. Lett.* **75**, 316 (1995); P. Dai *et al.*, *Phys. Rev. Lett.* **77**, 5425 (1996); H. F. Fong *et al.*, *Phys. Rev. Lett.* **78**, 713 (1997).
- [5] A related phenomenon occurs in  $^3\text{He}$ , where vortices may have ferromagnetic cores. See, e.g., G. E. Volovik, *Exotic Properties of Superfluid  $^3\text{He}$*  (World Scientific, Singapore, 1992).
- [6] G. S. Boebinger *et al.*, *Phys. Rev. Lett.* **77**, 5417 (1996); Y. Ando, G. S. Boebinger, A. Passner, T. Kimura, and K. Kishio, *Phys. Rev. Lett.* **75**, 4662 (1995).
- [7] C. P. Burgess and C. A. Lutken, Report No. cond-mat/9611070.
- [8] We ignore the Zeeman coupling, given by  $\mathcal{H}_{\text{Zeeman}} = -\frac{1}{2}\chi(\gamma B)^2(m_1^2 + m_2^2)$ .
- [9] D. P. Arovas, A. J. Berlinsky, C. Kallin, and S.-C. Zhang (unpublished).
- [10] In the cuprates, the chemical potential,  $\mu$ , reflects the equilibrium between the  $\text{CuO}_2$  planes and the intervening charge reservoir layers. For  $T = H = 0$ , the critical value  $\mu_c$  corresponds to a range of hole densities,  $0 < n_h < n_c$ , in which AF and SC phases coexist, presumably with some kind of striped microstructure. For  $\mu > \mu_c$  the SC phase is homogeneous. We assume that, for  $H > 0$ , the chemical potential of the combined SC, vortex core, charge reservoir system varies weakly with  $H$  and hence that  $H$  and  $\mu$  may be treated approximately as independent variables.
- [11] J. H. Brewer *et al.*, *Physica (Amsterdam)* **162-164C**, 157-158 (1989).