PHYSICAL REVIEW A **73**, 041603(R) (2006)

Ground-state description of a single vortex in an atomic Fermi gas: From BCS to Bose–Einstein condensation

Chih-Chun Chien, Yan He, Qijin Chen, and K. Levin
James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637, USA
(Received 24 October 2005; published 11 April 2006)

We use Bogoliubov-de Gennes (BdG) theory to describe a vortex in a neutral fermionic gas, for an attractive interaction that can be arbitrarily tuned to exhibit a crossover from BCS to Bose–Einstein condensation (BEC). We adopt the BCS–Leggett mean-field ground state for which a BdG approach is microscopically justified, and for which a Gross–Pitaevskii description emerges in the BEC limit. The local density of fermionic states is used to provide insight into the particle density depletion from BCS to BEC. We relate this depletion to the presence of unoccupied discrete states at the core center, as well as to a suppression of negative energy continuum states.

DOI: 10.1103/PhysRevA.73.041603 PACS number(s): 03.75.Hh, 03.75.Ss, 74.20.−z

One of the most exciting developments in atomic and condensed matter physics has been the mounting evidence in support of superfluidity in trapped fermionic systems [1–4]. In these systems, the presence of a Feshbach resonance provides a means of tuning the attractive pairing interaction with applied magnetic field. In this way the system undergoes a continuous evolution from BCS to Bose-Einstein condensed (BEC) superfluidity.

A conclusive demonstration of the superfluid phase has been the experimental observation of vortices [5]. Particularly interesting from a theoretical viewpoint is the way vortices evolve from BCS to BEC. This evolution is associated not just with a decrease in vortex size but with a complete rearrangement of the fermionic states which make up the core. As a result, there is a continuous evolution of the particle density within a vortex, thereby affecting the visibility of vortices in experiment. In this paper we discuss the behavior of a (single) vortex as the system crosses from BCS to BEC. Our work is based on the simplest BCS-like ground state first introduced by Leggett [6] and Eagles [7] to treat BCS-BEC crossover. With this choice of ground state inhomogeneity effects are readily incorporated as in generalized Bogoliubov-de Gennes (BdG) theory. Here we demonstrate analytically that the BdG strong coupling description of the $T=0$ vortex state coincides with the usual Gross-Pitaevskii (GP) treatment of vortices in bosonic superfluids. A fermionic theory based on BdG is, thus, very inclusive, and within this approach one expects a smooth evolution of vortices from the BCS to BEC limit as the statistics effectively change from fermionic to bosonic.

Previous studies of vortices in these fermionic superfluids addressed the BCS limit at $T=0$ [8] and $T\approx T_c$ [9]. There is also work [10] on the $T=0$ strict unitary case where a BdG approach was used with Hartree-Fock contributions included. In the present work, by contrast, we discuss the entire crossover regime and, importantly, present a detailed analysis of the energy and spatial structure within the core and how it evolves from BCS to BEC. A very different path integral approach was introduced in Ref. [11] to address vortices with BCS-BEC crossover, but here the authors note that density depletion effects appear to be unphysically large in the BCS regime. Our analytical approach builds heavily on previous work [12], which showed a general connection between GP theory and BdG. From this one can conclude that a generalized BCS theory [6] treats the bosonic degrees of freedom at the same level as GP theory. Different ground states can be contemplated (with incomplete condensation, say) but they will not be compatible with BdG theory. In a similar way, once $T\neq 0$ one has to incorporate noncondensed pairs and associated pseudogap physics [13], which are not present in a finite temperature BdG theory.

The general self-consistent BdG equations [14] are

$$\begin{pmatrix} h-\mu & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h^*+\mu \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n\begin{pmatrix} u_n \\ v_n \end{pmatrix}, \tag{1}$$

where $h=-(1/2m)\nabla^2+V_{ext}(\mathbf{r})$, $\Delta(\mathbf{r})$ is the $T=0$ gap function, which is importantly the same as the $T=0$ order parameter. $V_{ext}(\mathbf{r})$ is the external potential associated with the trap, and we choose $\hbar=1$. Because we will focus here on a single vortex, the effects of the trap potential are unimportant for the present purposes. There is a general symmetry of the BdG equations so that they are satisfied under the replacement $u_n\rightarrow v_n^*$, $v_n\rightarrow -u_n^*$, $E_n\rightarrow -E_n$. E_n corresponds to the quasiparticle dispersion and we restrict our discussion to $E_n\geqslant 0$ only. Here the fermionic chemical potential μ must be appropriately adjusted, as the attractive coupling constant is varied.

The quantities u_n and v_n are functions of $\mathbf{r}$ and define the amplitudes of the unoccupied and occupied pair states, respectively, in the ground-state wave function. They satisfy $\int d\mathbf{r}(|u_n|^2+|v_n|^2)=1$ for all energy levels n. The total number of particles is given by $n(\mathbf{r})=2\Sigma_n|v_n(\mathbf{r})|^2$. Not only do u_n, v_n, and E_n relate to ground-state properties, these quantities also appear in the $T=0$ spectrum for single fermionic excitations. We characterize this excitation spectrum via the local density of states (LDOS), $N(E,\mathbf{r})$, given by $2\Sigma_n[|u_n|^2\delta(E-E_n)+|v_n|^2\delta(E+E_n)]$. The total of the occupied and unoccupied states, $\int_{-\infty}^{\infty}N(E,\mathbf{r})dE$, is $\mathbf{r}$ independent. The local particle density, $n(\mathbf{r})$, is then given by integrating $N(E,\mathbf{r})$ over $E<0$, so that negative energies correspond to occupied states at $T=0$.

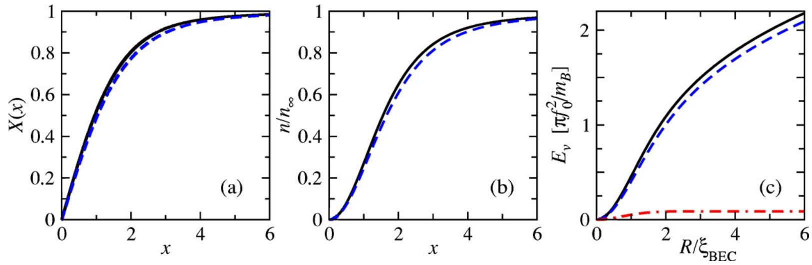

FIG. 1. (Color online) (a) Numerical solution of GP equation in the BEC limit with ($g_3'=0.1$, dashed lines) and without (solid lines) the three-body g_3 term; (b) the corresponding normalized particle density $n(x)/n_\infty$ as a function of x; and (c) the zero-temperature vortex energy cost E_v as a function of R/ξ_{BEC}. In (c), the difference is shown as the red dot-dashed curve. Here $n_\infty \equiv n(\infty)$.

For the most part, BdG approaches require detailed numerical solution [8,15–17], so it is particularly useful to have analytical tools. These tools were provided in Ref. [12] for the deep-BEC limit. Using a similar Green's-function formalism, combined with that of Ref. [15], one finds that the zero-temperature energy

$$E_0[\Psi] = \int d\mathbf{r}\left\{\frac{1}{2m_B}|\nabla\Psi(\mathbf{r})|^2 + 2V_{ext}(\mathbf{r})|\Psi(\mathbf{r})|^2 + \frac{1}{2}U_0|\Psi(\mathbf{r})|^4 - \mu_B|\Psi(\mathbf{r})|^2\right\}. \quad (2)$$

In this deep-BEC regime μ is negative and necessarily, $\Delta \ll |\mu|$. Here we have identified the condensate wave function $\Psi(\mathbf{r})$ as $\sqrt{m^2a/8\pi}\Delta(\mathbf{r})$; $U_0=4\pi a_B/m_B$, and $m_B=2m$ and $a_B=2a$ are the mass and the scattering length of the composite bosons.

Importantly, this expression has the same form as the $T=0$ energy of a gas of weakly interacting bosons [18] associated with GP theory. It should be noted that here this GP theory is written in terms of the grand canonical representation where the bosonic chemical potential (rather than the number of particles N) is held fixed. Minimizing the zero-temperature energy E_0 (via $\delta E_0/\delta\Psi^*=0$), leads to the well-known GP equation: $-(1/2m_B)\nabla^2\Psi(\mathbf{r})+2V_{ext}(\mathbf{r})+U_0|\Psi(\mathbf{r})|^2\Psi(\mathbf{r})=\mu_B\Psi(\mathbf{r})$.

We emphasize that this BdG analysis has, in effect, derived GP theory from a fermionic starting point. A Hartree contribution for the composite bosons is found here of the form $U_0|\Psi|^2\Psi \to U_0 n_B\Psi$ (where n_B is the density of bosons). This is, of course, unrelated to the Hartree term of the original fermions, which is absent in Eq. (1), as is consistent with the usual BCS-Leggett mean-field theory [6]. Indeed, the presence of a Hartree term in the BdG equations will destroy the simple analytic arguments presented here. The inclusion of Hartree terms [8] in the vortex problem has been accounted for in the literature, at weak [8] and strict unitary coupling [10], but they do not appear to lead to important differences.

The next order contribution to the zero-temperature energy E_0 in powers of Δ yields $\int d\mathbf{r} d_0(\mathbf{r})|\Delta(\mathbf{r})|^6$ with $d_0(\mathbf{r}) \simeq -5m^5a^7/256\pi$. This will contribute a term $g_3|\Psi(\mathbf{r})|^4\Psi(\mathbf{r})$ with $g_3=-15\pi^2a_B^4/4m_B$ in the GP equation; it introduces the appropriate analog in Eq. (2) as well. This three-body correction to the usual GP equation (g_3) [12] represents an effective attraction. In the composite-boson system, it provides a first-step correction of the deep-BEC limit en route to the fermionic or BCS end point.

In the presence of a single vortex, the wave function can be written as $\Psi(\mathbf{r})=f(r)e^{-i\theta}$. We introduce the BEC correlation length ξ_{BEC} in the strong-pairing limit as $(2m_B\xi_{BEC}^2)^{-1}=\mu_B=U_0f_0^2$, with $f_0\equiv f(r\to\infty)$. We rescale $r=\xi_{BEC}x$ and $f(r)=f_0X(x)$ and apply standard boundary conditions [18,19]. The results for $\Psi(\mathbf{r})$ in these units are plotted as the solid lines in Fig. 1. As shown in Fig. 1(a) (and consistent with earlier results in the literature [18,19]), the wave function rises smoothly from zero at the center of the core to its full magnitude at infinity on a length scale of ξ_{BEC}. In this deep-BEC limit of the BdG equations, the wave function is smooth, as a consequence of the absence of Andreev-like bound states [20] (i.e., states having $E_n<\Delta_\infty$). Here Δ_∞ is the value of gap function in the bulk, away from the core. This means that Friedel-like oscillations and the abrupt rise in the pair potential with small r (seen in the BCS regime [16]) are missing here.

The next order contribution in our composite-boson system is via the g_3 term in the GP equation and the corresponding term in the zero-temperature energy E_0. The effects of this addition, which reflect the underlying fermionic character, are plotted as dashed lines in Fig. 1 for (rescaled) $g_3'=-g_3f_0^2/U_0=0.1$. This g_3 contribution represents an attractive interaction, and, as shown in the figure, leads to a slight increase in the core size.

One can similarly compute the particle density $n_B(r)$ associated with composite bosons, which is simply related to the wave function as $n_B(r)=|\Psi(\mathbf{r})|^2=n(r)/2$, where n is the density of fermions. The density $n(x)$ is plotted in Fig. 1(b), normalized at the bulk value $n_\infty\equiv n(\infty)$, as a function of x. As expected, the particle density is strictly zero at the core center in the deep-BEC limit, where there is complete depletion.

The energy cost of a single vortex can also be calculated from Eq. (2) and the result is plotted in Fig. 1(c). The energy cost per unit length is given by

$$E_v = \left(\frac{\pi f_0^2}{m_B}\right)\int_0^{R/\xi_{BEC}}\left[\left(\frac{d\mathrm{X}}{dx}\right)^2 + \frac{\mathrm{X}^2}{x^2} + \frac{1}{2}(\mathrm{X}^2-1)^2\right]x dx,$$

where R is a cutoff needed to regularize the calculation of the vortex core energy. In Fig. 1(c) the solid line indicates E_v as a function of R/ξ_{BEC}. The shape of the curve for sufficiently large $R/\xi_{BEC}>2$ can be fitted to the usual functional form $E_v \propto \ln(D_G R/\xi_{BEC})$, where $D_G=1.48$. The dashed line in Fig. 1(c) presents results for E_v in the presence of the three-body term, where we take $g_3'=0.1$. This correction (red dot-dashed curve) lowers the vortex energy, as shown in the figure, and it approaches an asymptote as $R/\xi_{BEC}\to\infty$.

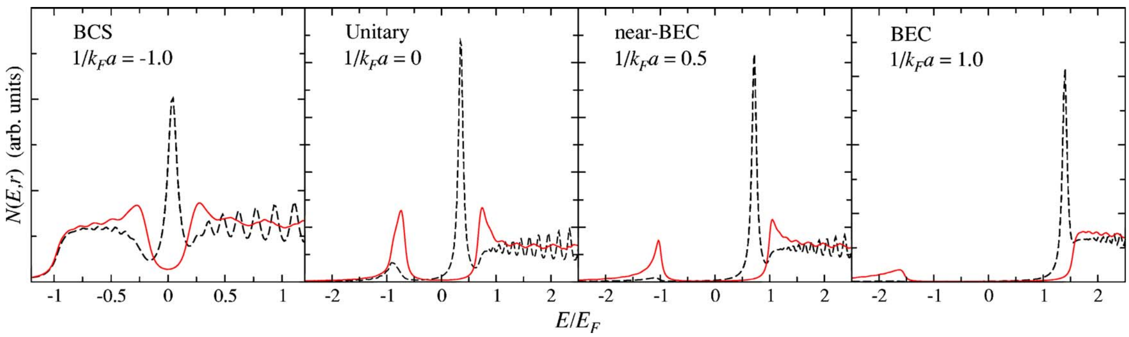

FIG. 2. (Color online) Local fermionic density of states $N(E,r)$ as function of E for the BCS ($1/k_Fa=-1$), unitary, near-BEC ($1/k_Fa=0.5$), and BEC ($1/k_Fa=1$) cases, at the center $r=0$ (black dashed curves) and radius $r=25/k_F$ (red solid curves) of the vortex core. The bulk value of the gap Δ_∞ is 0.21, 0.68, 1.01, $1.3E_F$, respectively. In the BEC case, $\mu\approx-0.8E_F$. Here $E_F=\hbar^2k_F^2/2m$ is the noninteracting Fermi energy at the trap center.

To understand the details of the core structure we turn now to numerical solutions, building on the above GP analysis in the deep-BEC regime, which provided a good check on our numerical algorithms. Here the physical coupling strength is controlled by the parameter $1/k_Fa$, where k_F is the noninteracting Fermi wave vector at the trap center. We have verified that changes in our high cutoff energy and coupling constant V do not affect the numerical results. Our numerical method is very similar to that in Ref. [21]. The chemical potential μ is approximated by the homogeneous solution, since the vortex core occupies only a small portion of the entire system.

We begin with a study of the local (fermionic) density of states, $N(E,r)$, which, when integrated over *negative energy* gives rise to the particle density distribution $n(r)$ inside the core. We ignore, for numerical simplicity, dependencies of the wave functions on the cylindrical variable z, since these do not lead to qualitative effects. Because the LDOS is a fundamentally fermionic quantity, this information is lost from the analytical analysis we presented earlier that leads to a Gross-Pitaevskii transcription of the BEC limit. We finally note that there is considerable interest in the literature in the behavior of the LDOS for high-T_c [22] as well as low-T_c superconductors [16], since this quantity is accessible through scanning tunneling microscopy.

Figure 2 represents a central figure of this paper which consolidates our observations about the ground state as well. Here we plot the LDOS inside the core, as a function of energy E for $r=0$ and in the bulk regime, $r=25/k_F$. A small spectral broadening for all energy levels E_n was introduced to regularize the numerics. The four panels correspond to the BCS ($1/k_Fa=-1$), unitary, near-BEC ($1/k_Fa=0.5$), and BEC ($1/k_Fa=1$) cases, respectively. The latter is not yet in the deep-BEC discussed analytically.

The figure shows a clear systematic evolution in which a discrete energy state (i.e., separated from the continuum) at the core center ($r=0$, with angular momentum $l=0$) evolves continuously from a peak at $E\approx 0$ in the BCS limit (where it corresponds to an Andreev-like bound state with $E_n<\Delta_\infty$) to the unitary case (where $E_n\approx\Delta_\infty/2$). Finally, in the BEC limit this discrete state gives rise to the peak at large positive energy shown in Fig. 2. The energy of the discrete state is large and positive in this latter regime (of order $\sqrt{\mu^2+\Delta_\infty^2}\approx|\mu|$), so that $E_n\geqslant|\mu|$ in the strong coupling limit. Physically, this means that fermionic excitations only exist in the core when the energy is sufficiently high so that the pairs are broken. It can be seen from Fig. 2, that in all cases at sufficiently large distances from the core center the fermionic density of states assumes the bulk value.

We turn now to the continuum contribution. Except for a small numerical broadening effect, both the bulk and core center continuum states experience an excitation gap, which is relatively smaller for the $r=0$ states. Away from the BCS regime, the corresponding weight of these continuum states with $E<0$ is relatively weak, falling off as E decreases. This reflects the behavior of the coherence factor $|v_n|^2$. By contrast for $E>0$, one can see from Fig. 2 that the continuum contribution varies as $\sqrt{E}$ at large E. At the core center, as compared with the bulk, there is thus a transfer of spectral weight from negative to positive energies.

We now focus on the density depletion and how it is reflected in the LDOS plotted in Fig. 2, first within the fermionic regime where $\mu>0$ (first three panels). We may use the sum rule on the LDOS, to observe that a bound state effectively removes spectral weight from the continuum contribution at both positive and negative energies. This can be seen from Fig. 2, when the bulk and $r=0$ contributions are compared. By removing spectral weight at $E<0$, *an unoccupied bound state thereby leads to a density depletion within the core*. In addition to this bound-state-derived depletion effect, the transfer of continuum spectral weight from negative to positive energy further adds to the depletion at the core center. Parenthetically, it should also be noted that there is a negative energy (and, therefore, occupied) contribution at $-E_n$ from the reflection of the discrete state. However, its weight, v_n^2, can be shown to be essentially zero, except in the BCS regime.

In the BCS case, where the gap is very small and $\mu=E_F$, the bound state (and its reflection) have energy $\pm E_n\approx 0$. In this limit, there is particle-hole symmetry so that both bound states, contributing equally to $n(r)$, are each half occupied. As a result, there is no particle density depletion in the extreme BCS limit. For the unitary case, by contrast, the depletion is considerable as a consequence of the transfer of continuum spectral weight from negative to positive energy and of the fact that the discrete state now appears at a positive

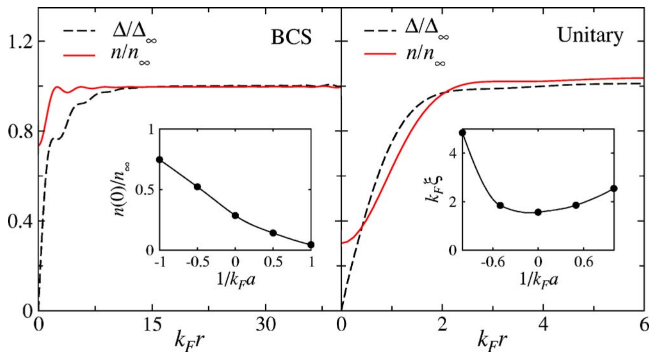

FIG. 3. (Color online) Gap function Δ (black dashed curves) and particle density n (red solid curves) as a function of r for BCS ($1/k_Fa = -1$) and unitary cases. All quantities are normalized by their bulk values. The insets to the left and right panels show detailed behavior of the depletion and vortex core size.

energy and is thus unoccupied. In the BEC limit, the depletion is close to complete. The local density of states yields results for $n(r)$, which are necessarily consistent with the GP-based approach derived earlier for the (albeit, deep) BEC regime.

In Fig. 3 we plot the position-dependent order parameter $\Delta(r)$ along with the particle density distribution $n(r)$ for the unitary and BCS ($1/k_Fa = -1$) cases shown in the previous figure. The two insets show the smooth evolution of the core center particle density and vortex core size (ξ) as deduced from the position r at which $\Delta(r)$ reaches 0.9 of its bulk value. Both insets represent plots as a function of $1/k_Fa$. We have found that the core size as obtained, alternatively, following Ref. [16] (from the maximum in the current density) leads to very similar, slightly nonmonotonic results within factors of order unity. The BCS-like case in Fig. 3 still has a reasonably large bulk gap, so that the bound-state energy is slightly positive, and, therefore, there is a non-negligible depletion at the core. This is in contrast to arbitrarily weak coupling, where the depletion vanishes. In agreement with Refs. [16] and [8], we find the small r oscillations in the BCS regime derive from the presence of the bound state and have been found here to be independent of system size.

Despite the fact that there are inadequacies of the mean-field approach associated with an overestimate of the inter-boson scattering length [23], the depletion in the present unitary case is surprisingly similar to that obtained earlier in Refs. [24] and [10]. In each case, the depletion was attributed differently to a Hartree-Fock correction [25] or closed-channel bosons [24]. Here, we interpret this depletion in terms of the local density of fermionic states as plotted in Fig. 2. It derives from a combined effect of an unoccupied discrete state, as well as a suppression of the negative energy continuum contribution to $n(r)$.

Note added

After submission of this paper, a paper appeared with similar calculations which attributed more significance to the high-energy core discrete state in the BEC limit (observable in our LDOS plot) than we do here [26].

We thank N. Nygaard for many helpful communications. This work was supported by NSF-MRSEC Grant No. DMR-0213745.

[1] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004).
[2] M. W. Zwierlein *et al.*, Phys. Rev. Lett. **92**, 120403 (2004).
[3] J. Kinast, S. L. Hemmer, M. E. Gehm, A. Turlapov, and J. E. Thomas, Phys. Rev. Lett. **92**, 150402 (2004).
[4] M. Bartenstein *et al.*, Phys. Rev. Lett. **92**, 203201 (2004).
[5] M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, and W. Ketterle, Nature (London) **435**, 170404 (2005).
[6] A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter* (Springer-Verlag, Berlin, 1980), pp. 13–27.
[7] D. M. Eagles, Phys. Rev. **186**, 456 (1969).
[8] N. Nygaard, G. M. Bruun, C. W. Clark, and D. L. Feder, Phys. Rev. Lett. **90**, 210402 (2003).
[9] M. Rodriguez, G. S. Paraoanu, and P. Törma, Phys. Rev. Lett. **87**, 100402 (2001).
[10] A. Bulgac and Y. Yu, Phys. Rev. Lett. **91**, 190404 (2003).
[11] J. Tempere, M. Wouters, and J. T. Devreese, Phys. Rev. A **71**, 033631 (2005).
[12] P. Pieri and G. C. Strinati, Phys. Rev. Lett. **91**, 030401 (2003).
[13] Q. J. Chen, J. Stajic, S. Tan, and K. Levin, Phys. Rep. **412**, 1 (2005).
[14] P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966).
[15] J. Bardeen, R. Kummel, A. E. Jacobs, and L. Tewordt, Phys. Rev. **187**, 556 (1969).
[16] F. Gygi and M. Schlüter, Phys. Rev. B **43**, 7609 (1991).
[17] Y. Ohashi and A. Griffin, Phys. Rev. A **72**, 063606 (2005).
[18] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Oxford, New York, 2003).
[19] C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2002).
[20] C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).
[21] N. Nygaard, G. M. Bruun, B. I. Schneider, C. W. Clark, and D. L. Feder, Phys. Rev. A **69**, 053622 (2004).
[22] M. Franz and Z. Tesanovic, Phys. Rev. Lett. **80**, 4763 (1998).
[23] Q. J. Chen, J. Stajic, S. N. Tan, and K. Levin, Phys. Rep. **412**, 1 (2005).
[24] M. Machida and T. Koyama, Phys. Rev. Lett. **94**, 140401 (2005).
[25] Y. Yu and A. Bulgac, Phys. Rev. Lett. **90**, 161101 (2003).
[26] R. Sensarma, M. Randeria, T.-L. Ho, e-print cond-mat/0510761.