Magnetic field dependence of the superconducting gap node topology in non-centrosymmetric $CePt_3Si$

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Non-centrosymmetric superconductors, such as $CePt_3Si$ and Li_2PtB_2, are believed to have a line node in the energy gap arising from coexistence of s-wave and p-wave pairing. Using as an example $CePt_3Si$ we show that a weak c-axis magnetic field will remove this line node, since it has no topological stability against time-reversal symmetry breaking perturbations. Conversely a field in the $a - b$ plane is shown to remove the line node on some regions of the Fermi surface, while bifurcating the line node in other directions, resulting in two 'boomerang'-like shapes. These line node topological changes are predicted to be observable experimentally in the low temperature heat capacity.

The existence of nodal points or lines in the energy gap of a superconductor or a Fermi superfliud, such as ^{3}He, is one of the main characteristics of unconventional symmetry pairing states. An important question is whether or not these nodes are accidental or are fully required by the fundamental symmetry of the pairing state. Secondly one can ask whether or not the nodal points or lines are topologically stable, or whether they can in principle be destroyed by small perturbations. This question was discussed in a seminal paper by Volovik[1], in which he showed that point nodes, such as in ^{3}He-A, are diabolical points characterized by a Berry phase and topological charge. Because of this property the nodal structure cannot be removed by small perturbations, such as a magnetic field. Very recently Sato[2] and Volovik[3] have independently, shown that for line nodes of the gap function topological stability is only guaranteed if time reversal symmetry is preserved. The topological structure of the nodal line can be classified as Z_2 (i.e. the group, {0,1}, of integers modulo 2). Perturbations breaking time reversal symmetry remove conservation of the relevant quantum numbers, and hence line nodes are not topologically stable against such perturbations.

It is especially interesting to consider the possible gap nodal structure in the recently discovered non-centrosymmetric superconductors such as $CePt_3Si$[4], Li_2Pt_3B [5], UIr [6], and $CeIrSi_3$ [7]. The absence of inversion symmetry along with parity-violating antisymmetric spin-orbit coupling (ASOC) makes possible in these compounds a simultaneous admixture of singlet and triplet pairing components on the sheets of its, non Kramers degenerate, Fermi surface. Unconventional behavior, including zeroes in the superconducting gap function, is then possible, even if the pair wave function exhibits the full spatial symmetry of the crystal. For example, thermal conductivity experiments suggest in $CePt_3Si$ that the superconducting gap most probably has lines of nodes on the Fermi surface[8], while NMR experiments[9, 10] show evidence for crystal field excitations, as well as the formation of a heavy fermion metallic state. Surprisingly, $1/T_1T$ does not show the usual $T3$ behavior of other Ce based heavy fermion superconductors, but rather a weak Hebel-Slichter like peak below T_c. Most recently it has been argued that the nodal structure of the superconducting gap in Li_2Pt_3B arises due to a relatively large ASOC effects which allow the spin-triplet component to be large in Li_2Pt_3B, producing line nodes in the energy gap as evidenced by the linear temperature dependence of the penetration depth, $\lambda(T)$[5].

In this paper we consider the effect of time reversal symmetry breaking on the nodal topology in the non-centrosymmetric superconductors, using as an example the compound $CePt_3Si$. This material is tetragonal with space group $P4mm$. It is found to have a spin-density wave Neel order at $T_N = 2.2$K, corresponding to an effective moment $0.16\mu_B/Ce$[11] and then superconductivity below about 0.75K[4]. Starting with the model gap nodal structure proposed by Hayashi *et al.*[12], we show that the line node can be completely removed by an arbitrarily weak c-axis magnetic field. In contrast, for $a-b$ plane oriented magnetic fields we show that magnetic fields create additional lines of nodes, splitting the single degenerate node of the time-reversal symmetric ground state into two. Moreover, we show that the double line of nodes does not extend around the whole Fermi sphere but forms a topological "boomerang"-like structure, as shown in Fig. 1. These effects lead to a dramatic increase in the linear T coefficient in C_V/T, which should be visible experimentally in the single crystal samples that are now available. The appearance of these extra line nodes in a magnetic field and their large effect on the physical properties is surprising given the often stated argument that the non Kramers degenerate Fermi surface should suppress the effect of Zeeman interactions on the superconducting state[13]. However, a strong and unusual angle dependence to the paramagnetic susceptibility has already been predicted by Samokhin[14] and Mineev[15] has shown that the paramagnetic limit is expected to be strongly field-angle dependent.

The superconducting state of $CePt_3Si$ has already been subjected to considerable experimental and theoretical effort. As well as the existence of the gap line node[8], a surprisingly high H_{c2} has been observed of about 3.2T for H along (001) and 2.7T for H along (100)[16], exceeding the Pauli limiting field of $H_P \sim 1.2$T. In addition to the weak antiferromagnetism, with $Q = (001/2)$ and an effective moment of about $0.16\mu_B$ per Ce atom, considerably less than the $2.54\mu_B/Ce$ expected for the Ce^{3+} ion $4f_{5/2}$ ground state, well defined crystal field excitations at 1meV and 24meV were also seen[11].

Theoretical models of the superconducting state in $CePt_3Si$ are based upon the existence of a Rashba type spin-orbit coupling

$$\hat{H}_{so} = \alpha \sum_{\mathbf{k},s,s'} \mathbf{g}_{\mathbf{k}}.\sigma_{ss'} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s'} \qquad (1)$$

as studied by Gor'kov and Rashba[17]. Here $\mathbf{g}_{\mathbf{k}} = -\mathbf{g}_{-\mathbf{k}}$ is a real pseudovector, by convention normalized so that $\langle g2_{\mathbf{k}} \rangle_F = 1$ where $\langle \ldots \rangle_F$ denotes an average over the Fermi surface, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices and $c^{\dagger}_{\mathbf{k}s}$ is the usual Fermi field operator. This spin-orbit coupling removes the usual Kramers degeneracy between the two spin states at a given $\mathbf{k}$, and leads to a quasi-particle dispersion $\varepsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} \pm \alpha|\mathbf{g}_{\mathbf{k}}|$ [18], splitting the Fermi surface into two sheets with a $\mathbf{k}$ dependent local spin orientation. The fully-relativistic Fermi surface calculated by Samokhin, Zijlstra and Bose[19] shows three distinct sheets, each of which becomes split into two as a result of the spin-orbit interaction. The spin-orbit coupling in $CePt_3Si$ has the form $\mathbf{g}_{\mathbf{k}} \sim (-k_y, k_x, 0)$ [18], which breaks the parity symmetry $\hat{P}$ and therefore

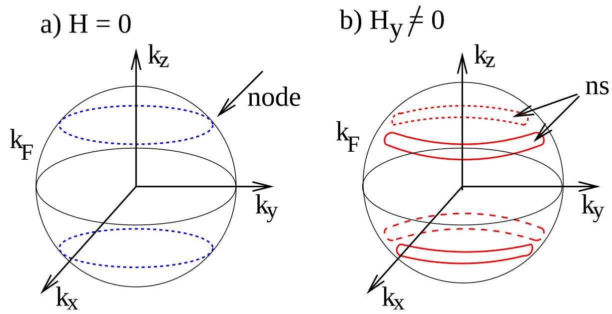

FIG. 1: (color online) Illustration of the influence of the *ab*-plane external magnetic field on the gap line nodes in $CePt_3Si$. (a) zero-field line nodes for $\pm k_z = const$ on one Rashba Fermi surface sheet; (b) $H_y \neq 0$ removes the node along the $\pm k_y$ direction and bifurcates the node elsewhere, yielding "boomerang"-like nodal topology.

mixes singlet and triplet pairing states. A full symmetry analysis [19, 20] shows that conventional s-wave pairing ($\Delta_{\mathbf{k}}$ having full tetragonal symmetry) and a p-wave triplet pairing state with order parameter $\mathbf{d}_{\mathbf{k}}$ parallel to the $\mathbf{g}_{\mathbf{k}}$-vector, $\mathbf{d}_{\mathbf{k}} \sim (-k_y, k_x, 0)$, are able to coexist. If the microscopic pairing interaction strongly favors one type of pairing over the other then that one will be dominant, but in general both gap components are present on a single Fermi surface sheet.

Following Hayashi *et al.*[12] we take the pairing state as the combined s-wave and $\mathbf{d}_{\mathbf{k}}$ state described above. Using the notation of Ref. [21] the mean-field BCS Hamiltonian for this system in the presence of a magnetic Zeeman field can be written

$$H_{MF} = \begin{pmatrix} \epsilon_{\mathbf{k}} + H_z & -i\alpha g_{\mathbf{k}} e^{-i\phi} - iH_y & id_{\mathbf{k}} e^{-i\phi} & \Delta_{\mathbf{k}} \\ i\alpha g_{\mathbf{k}} e^{i\phi} + iH_y & \epsilon_{\mathbf{k}} - H_z & -\Delta_{\mathbf{k}} & id_{\mathbf{k}} e^{i\phi} \\ -id^*_{\mathbf{k}} e^{i\phi} & -\Delta^*_{\mathbf{k}} & -\epsilon_{\mathbf{k}} - H_z & i\alpha g_{\mathbf{k}} e^{i\phi} + iH_y \\ \Delta^*_{\mathbf{k}} & -id^*_{\mathbf{k}} e^{-i\phi} & -i\alpha g_{\mathbf{k}} e^{-i\phi} - iH_y & -\epsilon_{\mathbf{k}} + H_z \end{pmatrix}, \qquad (2)$$

where for brevity we write $\mathbf{g}_{\mathbf{k},x} + i\mathbf{g}_{\mathbf{k},y} = ig_{\mathbf{k}} e^{i\phi}$, with $\phi = \tan^{-1}(k_y/k_x)$. Similarly we write $\mathbf{d}_{\mathbf{k},x} + i\mathbf{d}_{\mathbf{k},y} = id_{\mathbf{k}} e^{i\phi}$ and we have set $H_x = 0$.

In zero external field the diagonalization of this Hamiltonian yields the quasiparticle energy dispersion,

$$E_{1,2}(\mathbf{k}) = \sqrt{(\epsilon_{\mathbf{k}} \mp \alpha g_{\mathbf{k}})^2 + |d_{\mathbf{k}} \mp \Delta_{\mathbf{k}}|^2}. \qquad (3)$$

In the case where both singlet and triplet order parameters, $\Delta_{\mathbf{k}}$ and $d_{\mathbf{k}}$, can be chosen as real, this is the spectrum described by Hayashi *et al.*[12]. Assuming that the p-wave gap component is dominant so that $\Delta_{\mathbf{k}}$ is smaller than the maximum value of $d_{\mathbf{k}}$ on the Fermi surface, then one of the Rashba split sheets of the Fermi surface will have a line node, where $\Delta_{\mathbf{k}} = d_{\mathbf{k}}$ and the other sheet will be nodeless. For a spherical Fermi surface and the simplest gap functions allowed by symmetry, $\Delta_{\mathbf{k}} = \Delta$ and $\mathbf{d}_{\mathbf{k}} = d_0(-k_y, k_x, 0)/k_F$, the nodes are two horizontal circles around the Fermi sphere at $\pm k_z =$ const. as illustrated in Fig. 1(a). As pointed out by Sato[2] the nodes have Z_2 character. They can be removed by simply setting the relative phase between the two complex scalar order parameters $\Delta_{\mathbf{k}}$ and $d_{\mathbf{k}}$ non-zero, as one can readily see from Eq. 3. For the sake of simplicity we ignore in the present study the Doppler shift that arises due to the circulating supercurrent.

Let us now consider what will happen to the lines of nodes when time-reversal symmetry is broken by applying a Zeeman exchange field $\mathbf{H}$. We assume that we are dealing with relatively weak field and therefore the Fulde-Ferrel-Larkin-Ovchinnikov state[22–24] is not present. Let us first consider the case of a c-axis field. In this case $\mathbf{H} \perp \mathbf{g_k}$ and the Hamiltonian (2) can be diagonalized to obtain

$$E_{1,2}(\mathbf{k}, H_z) = \sqrt{\epsilon_{\mathbf{k}}^2 + (\alpha k)^2 + H_z^2 + \Delta_{\mathbf{k}}^2 + k^2|d|^2 \mp \sqrt{4H_z^2\,[\Delta_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}}^2] + [\Delta_{\mathbf{k}} k(d + d^*) + 2\alpha k \epsilon_{\mathbf{k}}]^2}} \quad (4)$$

and $E_{3,4}(\mathbf{k}, H_z) = -E_{1,2}(\mathbf{k}, H_z)$. One can readily see that this spectrum has no node, and so the gap node predicted by Hayashi et al. is not topologically stable against weak z-axis magnetic fields.

To explain the lack of topological stability, consider the normal and superconducting state quasiparticle spectrum near the two Rashba split sheets of the Fermi surface. In Fig.2(a) where we show schematically the energy dispersion $\mathrm{E}_{\mathbf{k}_{||}}$ in a cut through the Fermi surface at $k_z = \pm const.$ We have chosen the value of k_z coinciding with the line node predicted by Hayashi et al., given by the zero of Eq. 3. On the left hand panel of Fig.2(a) we show the normal state electron (e1, e2) and hole (h1,h2) quasiparticle dispersions near the two Rashba Fermi surface sheets. On the right hand side we show the corresponding superconducting state energies from Eq. 3. Clearly one sheet has a finite gap and the other has a node. Now consider the spectrum when a weak c-axis field is applied, as shown in Fig. 2(b). In this case the spectrum becomes fully gapped, and the line node is removed. In effect the original line node is "accidental", arising from a particular cancelation between the s-wave and p-wave gap components $\Delta_{\mathbf{k}}$ and $d_{\mathbf{k}}$ at some particular value of k_z. When the symmetry breaking perturbation H_z is applied the crossing electron and hole-like levels $h2$ and $e2$ in Fig. 2(a), interact and so an avoided level crossing occurs, hence removing the line node.

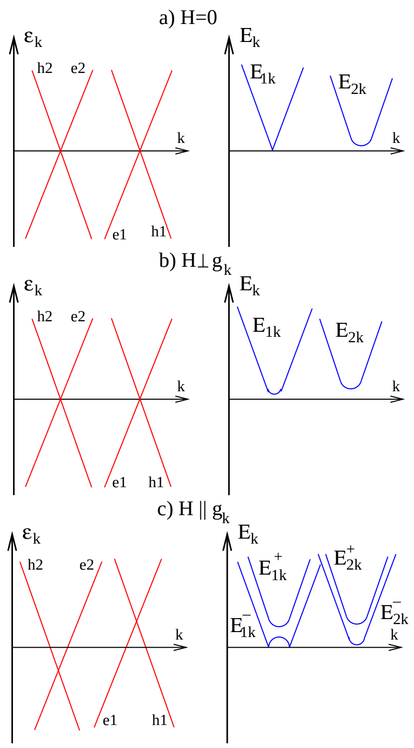

FIG. 2: (color online) Normal state (left) and superconducting state (right) quasiparticle dispersions, ϵ_k and $E_{\mathbf{k}}$, for particles and holes as a function of $k = (k_x 2 + k_y 2)^{1/2}$ for a fixed k_z. From top to bottom, zero field $\mathbf{H} = 0$, $\mathbf{H} \perp \mathbf{g_k}$, and $\mathbf{H} \parallel \mathbf{g_k}$

On the other hand consider the case of a $a - b$ plane magnetic field. The two Fermi surface sheets will be perturbed differently depending upon whether $\mathbf{H} \parallel \mathbf{g_k}$ or $\mathbf{H} \perp \mathbf{g_k}$. The latter case is essentially identical to Fig. 2(b), and so for these parts of the Fermi surface the gap node is removed. On the other hand, for the regions where $\mathbf{H} \parallel \mathbf{g_k}$ the gap node is found to *bifurcate*. The reason for this is illustrated in Fig. 2(c). The field perturbs the two Rashba sheets oppositely, because they have spin components parallel to the applied field $\mathbf{H}$. This can be seen in the normal state spectrum to the left side of Fig. 2(c). The corresponding superconducting state spectrum is shown to the right in Fig. 2(c). The four quasiparticle states no longer obey the symmetry $E_{3,4}(\mathbf{k}, H_y) = -E_{1,2}(\mathbf{k}, H_y)$. A result is that one branch of the quasiparticle spectrum near the original line node now crosses zero twice, while the other remains non-zero. This implies that the gap node bifurcates. Note that the final spectrum can always be defined as positive, consistent with stability of the Fermi sea, after applying a

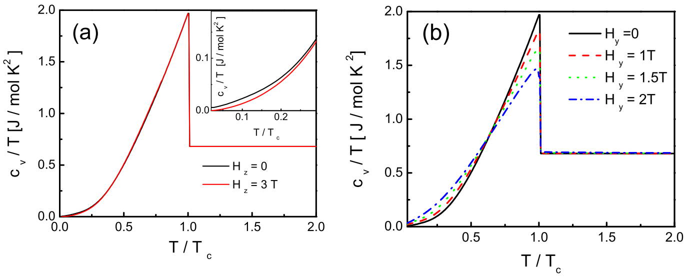

FIG. 3: (color online) Calculated temperature dependence of the specific heat with and without Zeeman field along z-direction(a) and along y-direction(b). The inset shows the low-temperature region for $H_z = 0$ and $H_z = 3$T. Here, we assume the BCS-like temperature dependence of the both p-wave and s-wave components of the superconducting gap with $\mathbf{d_k}(0) = 0.2$meV and $\Delta_{\mathbf{k}}(0) = 0.25\Delta_p(0)$ which gives about the BCS ratio between the magnitude of the superconducting gap and $T_c = 0.75$K. Following experimental findings we adopt $E_f \approx 0.012$eV and estimate $k_F \approx 0.5$ $\AA^{-1}$ which are typical values for the heavy-fermion metals. We further approximate the Rashba splitting of the bands $\alpha \sim 1 \times 10^{-3}$ eV $\AA$.

suitable particle-hole transformation to the quasiparticle states. This sign change results in the bifurcated node, as shown in the right panel in Fig. 2(c).

The final nodal topology for $a - b$ oriented magnetic fields is shown in Fig. 1(b). For $\mathbf{k}$ vectors with $x - y$ components parallel to $\mathbf{H}$ the gap node is removed, while for $\mathbf{k}$ vectors with $x - y$ components perpendicular to $\mathbf{H}$ the gap node bifurcates. Overall this leads to the unusual "boomerang" shaped gap line nodes as shown in Fig. 1(b). This topological structure is consistent with the general Z_2 topological arguments of Sato[2] and Volovik[3]. The Z_2 gap node has two topological invariants, which in the presence of time reversal symmetry are independently conserved, leading to stability of the line node. But the symmetry breaking perturbation $\mathbf{H}$ removes the stability, leading to either node removal or node bifurcation depending on the field orientation.

Experimentally this nodal change should be observable in unusual field dependence of various low temperature properties. In $CePt_3Si$ NMR experiments show both a Hebel-Slichter peak, a signature of the nodeless s-wave superconductor, and power-law behavior of the spin-lattice relaxation at low temperatures consistent with nodal structure of the superconducting gap[9, 10]. The predicted gap topology in Fig. 1 would imply a change in the low temperature power law to exponential for c-axis fields, and a changed pre-factor of the low temperature power law for $a - b$ oriented fields. Similarly the changes in the line node topology upon applied magnetic field results in the change of the thermodynamic characteristics such as heat capacity, C_V/T. In Fig.3 we show our results for the temperature dependence of the specific heat, C_V/T for various Zeeman fields. For c-axis fields the low temperature behavior changes from linear to exponential, but the actual total change is small for physically relevant values of $\mathbf{H}_z$, as shown in Fig.3(a). In contrast for $a - b$ plane fields the formation of the "boomerang"-like structure in the line nodes nodes both reduces the jump in the specific heat at T_c, and leads to a noticeable increase in C_V/T at low temperatures. Furthermore, for larger fields we also find that an even more substantial reduction of the jump occurs. This happens because for large enough exchange fields a new pair of gap nodes develops also on the second Rashba Fermi surface sheet. This is because for larger fields the lower quasi-particle state $E_2^-(\mathbf{k})$, also crosses zero as is evident from Fig.2(c). Most interestingly we find that these effects develop at small enough fields in $CePt_3Si$ to be observed experimentally. For example, measurements of the temperature dependence of the specific heat in an applied magnetic fields for poly-crystalline samples[4] are somewhat consistent with our prediction in Fig. 3(b). However, further studies are necessary on single crystals in order to check our predictions in more detail. Furthermore, it is also interesting to note that similar effects to those we predict for the specific heat could also be observed by other thermodynamic characteristics sensitive to the changes in the low energy density of states in superconductors such as penetration depth, thermal conductivity, spin-lattice relaxation etc.. Calculation of such properties is left to future work.

In conclusion, we have shown that Zeeman field induces an interesting and novel phenomena in the the non-centrosymmetric heavy fermion superconductor $CePt_3Si$. A c-axis field is shown to remove the "accidental" line node, and change the specific heat, C_V/T from linear to exponential at low temperatures. A field in the $a-b$ plane is shown to split the nodes into two 'boomerang'-like structures which will reduce the jump in the C_V/T and enhance the value of C_V/T at zero temperature. These surprising changes result from the changes of the Z_2 topological quantum numbers by the time reversal symmetry breaking perturbation, consistent with the arguments of Sato[2] and Volovik [3].

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[1] G.E. Volovik, Pis'ma Zh. Eksp. Fiz. **46**, 81 (1987) [JETP Lett. **46** 98 (1987)].
[2] M.Sato, Phys. Rev. B **73**, 214502 (2006).
[3] G.E. Volovik, cond-mat/0601372 (unpublished).
[4] E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E.W. Scheidt, A. Gribanov, Yu. Seropegin, H. Noel, M. Sigrist,

and P. Rogl, Phys. Rev. Lett. **92**, 027003 (2004).

[5] H.Q. Yuan, D.F. Agterberg, N. Hayashi, P. Badica, D. Vandervelde, K. Togano, M. Sigrist, and M. B. Salamon, Phys. Rev. Lett. **97**, 017006 (2006).

[6] T Akazawa, H Hidaka, T Fujiwara, T.C. Kobayashi, E. Yamamoto, Y. Haga, R. Settai, and Y. Onuki, J. Phys: Condens. Matter **16**, L29 (2004); T. Akazawa, H. Hidaka, H. Kotegawa, T.C. Kobayashi, T. Fujiwara, E. Yamamoto, Y. Haga, R. Settai, and Y. Onuki, J. Phys. Soc. Jpn. **73**, 3129 (2004).

[7] I. Sugitani, Y. Okuda, H. Shishido, T. Yamada, A. Thamizhavel, E. Yamamoto, T.D. Matsuda, Y. Haga, T. Takeuchi, R. Settai, and Y. Onuki, J. Phys. Soc. Jpn. **75**, 043703 (2006).

[8] K. Izawa, Y. Kasahara, Y. Matsuda, K. Behnia, T. Yasuda, R. Settai, and Y. Onuki, Phys. Rev. Lett. **94**, 197002 (2005).

[9] M. Yogi, Y. Kitaoka, S. Hashimoto, T. Yasuda, R. Settai, T.D. Matsuda, Y. Haga, Y. Onuki, P. Rogl, and E. Bauer, Phys. Rev. Lett. **93**, 027003 (2004).

[10] M. Yogi, H. Mukuda, Y. Kitaoka, S. Hashimoto, T. Yasuda, R. Settai, T.D. Matsuda, Y. Haga, Y. Onuki, P. Rogl, and E. Bauer, J. Phys. Soc. Jpn. **75**, 013709 (2006).

[11] N. Metoki, K. Kaneko, T.D. Matsuda, A. Galatanu, T. Takeuchi, S. Hashimoto, T. Ueda, R. Settai, Y. Onuki, and N. Bernhoeft, J. Phys: Condens. Matter **16**, L207 (2004).

[12] N. Hayashi, K. Wakabayashi, P.A. Frigeri and M. Sigrist, Phys. Rev. B **73** 024504 (2006).

[13] P.A. Frigeri, D.F. Agterberg and M. Sigrist, New Jour. Phys. **6**, 115 (2004).

[14] K.V. Samokhin, Phys. Rev. Lett. **94**, 027004 (2005).

[15] V.P. Mineev, Phys. Rev. B **71**, 012509 (2005).

[16] T. Yasuda, H. Shishido, T. Ueda, S. Hashimoto, R. Settai, T. Takeuchi, T.D. Matsuda, Y. Haga, and Y. Onuki, J. Phys. Soc. Jpn. **73**, 1657 (2004).

[17] L.P. Gor'kov and E.I. Rashba, Phys. Rev. Lett. **87**, 037004 (2001).

[18] P.A. Frigeri, D.F. Agterberg, A. Koga and M. Sigrist, Phys. Rev. Lett. **92**, 097001 (2004).

[19] K.V. Samokhin, E.S. Zijlstra and S.K. Bose, Phys. Rev. B **69**, 094514 (2004).

[20] I.A. Sergienko and S.H. Curnoe, Phys. Rev. B **70**, 214510 (2004).

[21] B.J. Powell, J.F. Annett and B.L. Györffy, J. Phys. A: Math. Gen. **36**, 9289 (2003).

[22] P. Fulde, and R.A. Ferrel, Phys. Rev. **135**, A550 (1964).

[23] A.I. Larkin, and Yu.N. Ovchinnikov, Zh. Eksp. Teor. Fiz **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].

[24] R.P. Kaur, D.F. Agterberg and M. Sigrist, Phys. Rev. Lett. **94**, 137002 (2005).