Ginzburg-Landau theory of noncentrosymmetric superconductors

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The data of temperature dependent superfluid density \( n_s(T) \) in Li\(_2\)Pd\(_3\)B and Li\(_2\)Pt\(_3\)B [Yuan et al., Phys. Rev. Lett. 97, 017006 (2006)] show that a sudden change of the slope of \( n_s(T) \) occur at slightly lower than the critical temperature. Motivated by this observation, we microscopically derive the Ginzburg-Landau (GL) equations for noncentrosymmetric superconductors with Rashba type spin orbit interaction. Cooper pairing is assumed to occur between electrons only in the same spin split band and pair scattering is allowed to occur between two spin split bands. The GL theory of such a system predicts two transition temperatures, the higher of which is the conventional critical temperature \( T_c \) while the lower one \( T^* \) corresponds to the cross-over from a mixed singlet-triplet phase at lower temperatures to only spin-singlet or spin-triplet (depending on the sign of the interband scattering potential) phase at higher temperatures. As a consequence, \( n_s(T) \) shows a kink at this cross-over temperature. We attribute the temperature at which sudden change of slope occurs in the observed \( n_s(T) \) to the temperature \( T^* \). This may also be associated with the observed kink in the penetration depth data of CePt\(_3\)Si. We have also estimated critical field near critical temperature.

I. INTRODUCTION

The spin-orbit (SO) coupling of electrons in noncentrosymmetric crystals lifts the spin degeneracy and hence splits the energy bands. For weak SO coupling, band splitting energy \( E_{SO} \) is smaller than the superconducting energy scales. In this case, pairing potential may still be chosen as a function of spin and momentum of quasiparticles near the Fermi surface unaffected by the SO coupling.\(^1\)\(^-\)\(^3\) In the opposite limit, i.e., when the band splitting energy exceeds the superconducting critical temperature \( T_c \), the electrons with opposite momenta form Cooper pairs only if they are from same nondegenerate band.\(^4\)\(^-\)\(^8\) Interband pairing in this case can be neglected. Due to the lack of inversion symmetry in the underlying crystal, the superconducting order parameter may, in general, be an admixture\(^2\) of spin-singlet and spin-triplet components, i.e., the gap function may be decomposed as \( \Delta_k = [\psi_k \sigma_0 + d_k \cdot \sigma] \psi'_k \), where \( \psi_k \) is the spin-singlet component and \( d_k \) is the spin-triplet component of the order parameter, and \( \sigma \)'s are the Pauli matrices. The spin-triplet component is however possible only in the presence of spin-triplet channel in the pairing interaction potential, even in the presence of SO splitting.

The recent discovery\(^9\) of superconductivity in CePt\(_3\)Si which is noncentrosymmetric, has raised interest in the properties of superconductors without inversion symmetry. A flurry of noncentrosymmetric heavy fermion compounds like Ul\(_r\) (Ref. 10), CeRhSi\(_3\) (Ref. 11), CeIRS\(_3\) (Ref. 12) exhibiting superconductivity have been discovered since then. All of these compounds are strongly correlated: Both antiferro magnetism and superconductivity coexist\(^9\) in CePt\(_3\)Si, in particular. On the other hand recently discovered Li\(_2\)Pd\(_3\)B (Ref. 13) and Li\(_2\)Pt\(_3\)B (Ref. 14) compounds are not of strongly correlated type and thus may be ideally used to explore the properties of noncentrosymmetric superconductivity. The band structure calculation\(^15\) in CePt\(_3\)Si reveals that 500K \( \lesssim E_{SO} \lesssim 2000K \), i.e., \( E_{SO} \) is much larger than \( T_c \) which is reported to be 0.75K. Therefore the pairing between electrons in two different spin split bands can be neglected for CePt\(_3\)Si and so are in the case of Li\(_2\)Pd\(_3\)B and Li\(_2\)Pt\(_3\)B compounds. In this paper, we consider this assumption.

Both the penetration depth data\(^16\) and thermal conductivity data\(^17\) in CePt\(_3\)Si seem to suggest the existence of line nodes in the system. However, a theoretical model\(^18\) consisting of mixed singlet and triplet order parameters with no line node may also explain the penetration depth data\(^19\) at low temperatures. This model reasonably fits also with the data of superfluid density \( n_s(T) \) in Li\(_2\)Pd\(_3\)B and Li\(_2\)Pt\(_3\)B at low temperatures. However this model alone can not explain the sudden change in slope of \( n_s(T) \) at some characteristic temperature that has been clearly observed\(^19\) in these systems, specially in Li\(_2\)Pt\(_3\)B. This motivates us to study Ginzburg-Landau (GL) theory for two component order parameters associated with two spin split bands formed in the presence of SO interaction. In this theory, we have considered attractive intraband pairing potential and attractive or repulsive interband pair scattering potential. As a consequence we show, apart from the conventional superconducting critical temperature, that there is another characteristic temperature \( T^* \) at which superconducting order parameter undergoes a cross-over from a mixed singlet-triplet phase at lower temperatures to only triplet or singlet phase at higher temperatures. The superfluid density shows a kink in its behaviour at the temperature \( T^* \).

The article is organized as follows. In section II, we review some important aspects of the Hamiltonian for a noncentrosymmetric superconductor. It corresponds to two bands with opposite helicity. Following the method of semiclassical gradient expansion\(^20\), we microscopically derive Ginzburg-Landau equations for such a superconductor in section III. Both the intraband pairing potential and interband pair scattering potential have been...
II. NONCENTROSYMMETRIC SUPERCONDUCTORS

We begin this section with a brief introduction to the model Hamiltonian for noncentrosymmetric superconductors. The normal state Hamiltonian\(^1\) for the electrons in a band of lattice without inversion symmetry is

\[
H_0 = \sum_{k,s} \xi_k c_{ks}^\dagger c_{ks} + \sum_{k,s,s'} g_{k} \cdot \sigma_{ss'} c_{ks}^\dagger c_{ks'},
\]

where electrons with momentum \(k\) and spin \(s (= \uparrow\text{ or } \downarrow)\) are created (annihilated) by the operators \(c_{ks}^\dagger (c_{ks})\), \(\xi_k\) is the band energy measured from the Fermi energy \(\epsilon_F\). The second term in the Hamiltonian(1) breaks parity as \(g_{-k} = -g_k\) for a non-centrosymmetric system. For a system like Heavy fermion compound CePt\(_3\)Si which has layered structure, \(H_0\) is considered to be two-dimensional. For such a system of electrons with band mass \(m\), \(\xi_k = \frac{\hbar^2}{2m} - \epsilon_F\) and \(g_k = \alpha n_k\) where \(n_k = \hat{n} \times k\), i.e., the spin-orbit interaction is of Rashba type where \(\alpha\) is called Rashba parameter. Here \(\hat{n}\) represents the axis of non-centrosymmetry which is perpendicular to the plane of the system. Due to the breaking down of the parity, spin degeneracy of the band is lifted; by diagonalizing \(H_0\), one finds two spin-split bands with energies \(\xi_{k\lambda} = \xi_k + \lambda \epsilon_{F} |k|\) where \(\lambda = \pm\) describes helicity of the spin-split bands. Therefore in the diagonalized basis \(H_0\) (1) becomes \(H_0 = \sum_{k,\lambda = \pm} \xi_{k\lambda} c_{k\lambda}^\dagger c_{k\lambda}\) where \(c_{k\lambda} = (c_{k\uparrow} - \lambda \alpha \epsilon_{F} c_{k\downarrow})/\sqrt{2}\) is the electron destruction operator and \(c_{k\lambda}^\dagger = (c_{k\uparrow}^\dagger - \lambda \alpha \epsilon_{F} c_{k\downarrow}^\dagger)/\sqrt{2}\) is the electron creation operator in band \(\lambda\) with momentum \(k\) where \(\hat{\epsilon}_{k\lambda} = -i \exp(-i\phi_k)\) with \(\phi_k\) being the angle of \(k\) with \(\hat{z}\)-axis. The Fermi momenta in these bands are \(k_F = \sqrt{k_F^2 + m^2 \alpha^2} - \lambda \alpha \epsilon_F\) where \(k_F = \sqrt{2m \epsilon_F}\) is the Fermi momentum in the absence of band splitting. The density of electronic states at Fermi energy in these bands may be found as \(\nu_\lambda = \frac{m}{2\pi} \left(1 - \lambda \alpha^2/\sqrt{k_F^2 + m^2 \alpha^2}\right)\).

Band structure calculation\(^15\) on CePt\(_3\)Si reveals that the energy difference between two spin-split bands near \(k_F\) is 50–200 meV which is much larger than the superconducting critical temperature, \(k_B T_c \approx 0.06\) meV. The formation of Cooper pairing between electrons in different spin-split bands may thus be ignored\(^4\)–\(^7\), i.e., \(\langle \hat{c}_{k\lambda} \hat{c}_{-k\lambda} \rangle\) is finite only when \(\lambda' = \lambda\). However the scattering of pairs between two spin-split bands are allowed. The Hamiltonian for the system may then be written as

\[
H = \sum_{k,\lambda = \pm} \xi_{k\lambda} c_{k\lambda}^\dagger c_{k\lambda} + \sum_{k,k',\lambda,\lambda'} V_{\lambda\lambda'}(k,k') c_{k\lambda}^\dagger c_{-k\lambda}^\dagger c_{-k'\lambda'} c_{k'\lambda'}
\]

where \(V_{\lambda\lambda'}(k,k')\) represents intraband pair potential and interband pair scattering potential.

III. GINZBURG-LANDAU EQUATIONS

The total second quantized Hamiltonian in the real space can be written by performing a Fourier transformation of equation (2). It then takes the form

\[
\mathcal{H} = \int dr \varphi_\lambda^\dagger (r) \left( \frac{(p + eA)^2}{2m} + \mu \right) \varphi_\lambda (r) + \int dr dr' \varphi_\lambda^\dagger (r) \varphi_{\lambda'}^\dagger (r') V_{\lambda\lambda'}(r - r') \varphi_{\lambda'} (r') \varphi_\lambda (r)
\]

Here \(\varphi_\lambda (r)\) is the field operator for electrons in band \(\lambda\) at position \(r\) and the repeated indices’s denotes summation. \(V_{\lambda\lambda'}(r - r')\) denotes intraband pairing as well as interband pair scattering potential The vector potential \(A\) which preserves gauge invariance is introduced. From here after we consider unit system: \(\hbar = 1, k_B = 1\) and \(c = 1\). In Gor’kov’s weak coupling theory, the equation of motion of the normal and anomalous Green’s functions in each spin-split band can be written as

\[
\left(i \omega_n - \frac{(p + eA)^2}{2m} + \mu\right) G_\lambda (r, r'; \omega_n) + \int d\omega'' \Delta_\lambda (r, r') F_\lambda (r'', \omega''; \omega_n) = \delta (r - r') \delta (\omega'' - \omega')
\]

\[
-i \omega_n - \frac{(p - eA)^2}{2m} + \mu \right) F_\lambda (r, r'; \omega_n) - \int d\omega'' \Delta_\lambda^* (r, r') G_\lambda (r'', r'; \omega_n) = 0,
\]

where \(G_\lambda (r, r'; \omega_n)\) and \(F_\lambda (r, r'; \omega_n)\) respectively are normal and anomalous quasiparticle Green’s functions in band \(\lambda\), and \(\Delta_\lambda^* (r, r')\) is the gap function which can be written as

\[
\Delta_\lambda (r, r') = -T \sum_{n,\lambda'} V_{\lambda\lambda'} (r, r') F_{\lambda'} (r', r'; \omega_n)
\]

where \(\omega_n = (2n + 1) \pi T\) is the fermionic Matsubara frequency at temperature \(T\). Normal state electronic
Green’s function $\hat{G}_\lambda(r, r'; \omega_n)$ satisfies the equation

$$\left(i\omega_n - \frac{(p + eA)^2}{2m} + \mu\right)G_\lambda(r, r'; \omega_n) = \delta(r - r') \tag{7}$$

In terms of $G_\lambda(r, r'; \omega_n)$, a self consistent solution of Eqs. (4) and (5) becomes

$$G_\lambda(r, r'; \omega_n) = G_\lambda(r, r'; \omega_n) - \int dr_1 dr_2 G_\lambda(r, r_1; \omega_n)\Delta_\lambda(r_1, r_2) \int dr_3 dr_4 G_\lambda(r_2, r_3; -\omega_n)\Delta_\lambda^*(r_3, r_4)G_\lambda(r_4, r'; \omega_n) \tag{8}$$

$$\mathcal{F}^\lambda(r,r'; \omega_n) = \int dr_1 dr_2 G_\lambda(r, r_1; -\omega_n)\Delta_\lambda^*(r_1, r_2) \times \left[G_\lambda(r_2, r'; \omega_n) - \int dr_3 dr_4 G_\lambda(r_2, r_3; \omega_n)\Delta_\lambda(r_3, r_4)\right] \tag{9}$$

In the absence of $A$, the normal state Green’s function is translationally invariant and can be written in momentum space as $\hat{G}_\lambda = 1/(i\omega_n - \xi_{k\lambda})$. In a semiclassical approximation\textsuperscript{20}, the role of $A$ is to generate a phase in the single particle normal state Green’s function:

$$G_\lambda(r, r'; \omega_n) = \hat{G}_\lambda(r, r'; \omega_n) \exp\left(-ie \int_{r'}^r ds \cdot A(s)\right) \tag{10}$$

where the integration is over a straight line path from $r'$ to $r$. Close to the superconducting transition temperature, magnitude of order parameter is small and its smallness allows us to expand $\mathcal{F}^\lambda$ and $\mathcal{G}$ in terms of it for each individual spin split band:

$$G_\lambda(r, r'; \omega_n) = G_\lambda(r, r'; \omega_n) - \int dr_1 dr_2 G_\lambda(r, r_1; \omega_n)\Delta_\lambda(r_1, r_2) \int dr_3 dr_4 G_\lambda(r_2, r_3; -\omega_n)\Delta_\lambda^*(r_3, r_4)G_\lambda(r_4, r'; \omega_n)$$

$$\mathcal{F}^\lambda(r,r'; \omega_n) = \int dr_1 dr_2 G_\lambda(r, r_1; -\omega_n)\Delta_\lambda^*(r_1, r_2) \times \left[G_\lambda(r_2, r'; \omega_n) - \int dr_3 dr_4 G_\lambda(r_2, r_3; \omega_n)\Delta_\lambda(r_3, r_4)\right]$$

Substituting Eq. (12) in Eq.(6) and writing

$$\Delta_\lambda(r, r') = \Delta_{\lambda I}(r, r') + \Delta_{\lambda II}(r, r') \tag{13}$$

we find

$$\Delta_{\lambda I}(r, r') = -T \sum_{n, \lambda'} V_{\lambda\lambda'}(r, r') \int dr_1 dr_2 \Delta_{\lambda'}(r_1, r_2) \Delta_{\lambda'}^*(r_1, r_2) \Delta_{\lambda'}(r_2, r'; \omega_n) \tag{14}$$

$$\Delta_{\lambda II}(r, r') = T \sum_{n, \lambda'} V_{\lambda\lambda'}(r, r') \int dr_1 G_{\lambda'}(r_1, r_2; -\omega_n) \Delta_{\lambda'}^*(r_1, r_2) \Delta_{\lambda'}^*(r_2, r_3; \omega_n) \Delta_{\lambda'}(r_3, r_4)$$

$$\times G_{\lambda'}(r_4, r_5; -\omega_n) \Delta_{\lambda'}^*(r_5, r_6) G_{\lambda'}(r_6, r'; \omega_n) \tag{15}$$

Expressing the order parameter $\Delta_\lambda^*(r_1, r_2)$ in terms of center of mass coordinate $R = (r_1 + r_2)/2$ of the pair and relative coordinate $\rho = r_1 - r_2$ of the pair and making Fourier transform with respect to the relative coordinate, we can express $\Delta_{\lambda I}$ in Eq. (14) as the sum of two terms:

$$\Delta_{\lambda I} = \Delta^*_{\lambda I c} + \Delta^*_{\lambda I g} \tag{16}$$

where

$$\Delta^*_{\lambda I c}(R, k) = -T \sum_{n, \lambda'} \int \frac{d^2k'}{(2\pi)^2} V_{\lambda\lambda'}(k - k') \frac{1}{\omega_n^2 + \xi_{k\lambda'}^2} \Delta^*_{\lambda'}(R, k') \tag{17}$$

$$\Delta^*_{\lambda I g}(R, k) = -T \sum_{n, \lambda'} \int \frac{d^2k'}{2(2\pi)^2} V_{\lambda\lambda'}(k - k') \left\{ \frac{1}{(2m)^2} \left( \omega_n^2 + \xi_{k\lambda'}^2 \right)^2 \left( k_x^2 \Pi_x + k_y^2 \Pi_y \right) + \frac{\xi_{k\lambda'} \Pi_x^2}{2m \left( \omega_n^2 + \xi_{k\lambda'}^2 \right)^2} \right\} \Delta^*_{\lambda'}(R, k') \tag{18}$$
Similarly we find from Eq. (15),
\[
\Delta_{\lambda}^{s}(R, k) = T \sum_{n, \lambda'} \int \frac{d^{2}k'}{(2\pi)^{2}} V_{\lambda\lambda'}(k' - k') \frac{1}{(\omega_{n}^{2} + \xi_{k'}^{2})^{2}} |\Delta_{\lambda'}(R, k')|^{2} \Delta_{\lambda'}^{s}(R, k')
\]  
(19)

We assume the interaction potential to be
\[
V_{\lambda\lambda'}(k' - k') = -V_{\lambda\lambda'}[\Delta_{\lambda}^{s} + \Delta_{\lambda}^{s}] 
\]  
(20)
where interaction strength $V_{\lambda\lambda'} > 0$ for $\lambda = \lambda'$ and it may have either sign when $\lambda \neq \lambda'$. The potential $V_{i} = -V_{\lambda\lambda'} \Lambda_{\lambda} \Lambda_{\lambda'}$ leads to the order parameter $\Delta_{\lambda,1} \Lambda_{\lambda}$ which in turn corresponds to $s$-wave pairing in singlet channel, and $p$-waves for spin up-up and down-down triplet channels. The other part of the potential (20), $V_{2} = -V_{\lambda\lambda'} \Lambda_{\lambda} \Lambda_{\lambda'}$ will help to induce order parameter $\Delta_{\lambda,2} \Lambda_{\lambda}$. This new order parameter corresponds to $d$-wave in singlet channel, and $p$-wave and $f$-wave for spin up-up and down-down triplet channels respectively. Thus we can write the new form of the order parameter as,
\[
\Delta_{\lambda}^{s}(R, k) = \Delta_{\lambda,1}^{s}(R) \Lambda_{\lambda} + \Delta_{\lambda,2}^{s}(R) \Lambda_{\lambda} 
\]  
(21)

Inserting the form of $V_{\lambda\lambda'}(k' - k')$ in Eq. (20) and $\Delta_{\lambda}^{s}(R, k)$ in Eq. (21) into Eqs. (17 – 19), we find
\[
\Delta_{\lambda,1}^{s}(R, k) = \ln \left( \frac{2e^{2}\omega_{D}}{\pi T} \right) \sum_{\lambda'} g_{\lambda\lambda'} \left[ \Delta_{\lambda,1}^{s} + \Delta_{\lambda,2}^{s} \right] 
\]  
(22)
\[
\Delta_{\lambda,2}^{s}(R, k) = -\frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} v_{F\lambda}^{2} \left[ (2\Pi^{2} \Delta_{\lambda,1}^{s} + \Pi_{1}^{2} \Delta_{\lambda,2}^{s} ) \Lambda_{\lambda} + (2\Pi_{1}^{2} \Delta_{\lambda,2}^{s} + \Pi_{2}^{2} \Delta_{\lambda,1}^{s} ) \Lambda_{\lambda} \right] 
\]  
(23)
\[
\Delta_{\lambda,1}^{s}(R, k) = -\frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} \left[ (|\Delta_{\lambda,1}^{s}|^{2} + 2|\Delta_{\lambda,2}^{s}|^{2}) |\Delta_{\lambda,1}^{s} \Lambda_{\lambda} + (2|\Delta_{\lambda,1}^{s}|^{2} + |\Delta_{\lambda,2}^{s}|^{2}) \Delta_{\lambda,2}^{s} \Lambda_{\lambda} \right] 
\]  
(24)

where dimensionless interaction strength $g_{\lambda\lambda'} = \frac{1}{4} V_{\lambda\lambda'} \nu_{\lambda'}$, $\gamma = 0.5772$ is the Euler constant, $\omega_{D}$ is the Debye frequency, $v_{F\lambda}$ is the Fermi velocity for band $\lambda$ and $\alpha = \frac{\gamma(T)}{8(\pi T)^{2}}$. Further $\Pi = -i \nabla R - 2eA(R)$ and $\Pi_{\pm} = \Pi_{x} \pm i \Pi_{y}$.

Summing expressions (22–24) and equating the sum with Eq. (21) and then by comparing coefficients of $\Lambda_{\lambda}^{s}$ and $\Lambda_{\lambda}$ we find the GL equations for each band with primary as well as induced order parameters:
\[
\Delta_{\lambda,1}^{s}(R) = \ln \left( \frac{2e^{2}\omega_{D}}{\pi T} \right) \sum_{\lambda'} g_{\lambda\lambda'} \Delta_{\lambda,1}^{s} \lambda_{1} - \frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} v_{F\lambda}^{2} \left( 2\Pi^{2} \Delta_{\lambda,1}^{s} + \Pi_{1}^{2} \Delta_{\lambda,2}^{s} \right) - \frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} \left( |\Delta_{\lambda,1}^{s}|^{2} + 2|\Delta_{\lambda,2}^{s}|^{2} \right) \Delta_{\lambda,1}^{s} 
\]  
(25)
\[
\Delta_{\lambda,2}^{s}(R) = \ln \left( \frac{2e^{2}\omega_{D}}{\pi T} \right) \sum_{\lambda'} g_{\lambda\lambda'} \Delta_{\lambda,2}^{s} \lambda_{2} - \frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} v_{F\lambda}^{2} \left( 2\Pi_{1}^{2} \Delta_{\lambda,2}^{s} + \Pi_{2}^{2} \Delta_{\lambda,1}^{s} \right) - \frac{\alpha}{8} \sum_{\lambda'} g_{\lambda\lambda'} \left( |\Delta_{\lambda,2}^{s}|^{2} + 2|\Delta_{\lambda,1}^{s}|^{2} \right) \Delta_{\lambda,2}^{s} 
\]  
(26)

Note that gradient of $\Delta_{\lambda,1}^{s}(R)$ leads to the induction of $\Delta_{\lambda,2}^{s}(R)$. A self consistent solution of these order parameters involve simultaneous solution of Eqs. (25) and (26). The transition temperature $T_{c}$ however may be obtained from the linear in $\Delta_{\lambda,1}^{s}(R)$ terms in Eq. (25). Solving the matrix equation, one finds
\[
T_{c} = \left( \frac{2e^{2}\omega_{D}}{\pi} \right) \exp \left[ -\frac{1}{g_{2}} \right] \delta_{1,2} = \frac{1}{2} \left( g_{++} + g_{--} \right) \pm \sqrt{(g_{++} - g_{--})^{2} + 4g_{+-}g_{-+}} 
\]  
(27)

The critical temperature should be determined by the solution $\min(g_{1}, g_{2})$, i.e., $g_{2}$ in contrary to the consideration of Ref. 8. The other solution $g_{1}$ does not have any physical importance. However in a certain physical situation as we discuss in the next section, this redundant solution gets renormalized to a value less than $g_{2}$ and manifests itself to a physical solution. We choose a special situation when $g_{++} = g_{--}$ and $g_{+-} = g_{-+}$, i.e., the intra as well as inter band strengths of interaction are independent of bands although they are different from each other in general. This assumption is reasonable since $g_{\lambda\lambda'}$ is dimensionless and is the product of $V_{\lambda\lambda'}$ and $\nu_{\lambda'}$, i.e., a density of states weighted interaction strength. The matrix $\hat{g}$ is positive definite, i.e., $g_{++} > 0$, $g_{--} > 0$, and $\det(\hat{g}) > 0$. This indicates $g_{+-}$ may have either of the signs. By this choice,
\[
T_{c} = \left( \frac{2e^{2}\omega_{D}}{\pi} \right) \exp \left[ -\frac{1}{g_{++} - |g_{+-}|} \right] 
\]  
(28)
IV. TRANSITION TEMPERATURES

Order parameters $\Delta_{\lambda,1}$ and $\Delta_{\lambda,2}$ consist of both singlet and triplet components: they are $\Delta_{s,l} = (\Delta_{+l} - \Delta_{-l})/2$ and $\Delta_{t,l} = (\Delta_{+l} + \Delta_{-l})/2$ respectively, where $l = 1$ or 2. We thus find the GL equations for $\Delta_{s,1}$ and $\Delta_{t,1}$ derivable from Eq. (25) as

\begin{align}
(1 - \bar{g}_{++} - \bar{g}_{+-}) \Delta_{s,1}^2(R) + \frac{\alpha}{16} (g_{++} + g_{+-}) &\left[ v_{F,1}^2 (2\Pi^2 \Delta_{s,1}(R) + \Pi^2 \Delta_{s,2}(R)) - v_{F,2}^2 (2\Pi^2 \Delta_{s,1}^*(R) + \Pi^2 \Delta_{s,2}^*(R)) \right] \\
+ \alpha (g_{++} + g_{+-}) &\left[ (|\Delta_{t,1}|^2 + 2|\Delta_{s,1}(R)|^2 + 2|\Delta_{t,2}(R)|^2 + 2|\Delta_{s,2}(R)|^2) \Delta_{s,1}^*(R) + \Delta_{s,2}^*(R) \Delta_{t,1}(R) \right] \\
+ 2\Delta_{s,1}(R) \Delta_{s,2}(R) \Delta_{t,2}(R) + 2\Delta_{s,1}(R) \Delta_{s,2}(R) \Delta_{s,2}^*(R) \right] &= 0
\end{align}

(29)

\begin{align}
(1 - \bar{g}_{++} + \bar{g}_{+-}) \Delta_{s,1}^2(R) + \frac{\alpha}{16} (g_{++} - g_{+-}) &\left[ v_{F,1}^2 (2\Pi^2 \Delta_{s,1}^*(R) + \Pi^2 \Delta_{s,2}^*(R)) - v_{F,2}^2 (2\Pi^2 \Delta_{s,1}^*(R) + \Pi^2 \Delta_{s,2}^*(R)) \right] \\
+ \alpha (g_{++} - g_{+-}) &\left[ (|\Delta_{t,1}|^2 + 2|\Delta_{s,1}(R)|^2 + 2|\Delta_{t,2}(R)|^2 + 2|\Delta_{s,2}(R)|^2) \Delta_{s,1}^*(R) + \Delta_{s,2}^*(R) \Delta_{t,1}(R) \right] \\
+ 2\Delta_{s,1}(R) \Delta_{s,2}(R) \Delta_{t,2}(R) + 2\Delta_{s,1}(R) \Delta_{s,2}(R) \Delta_{s,2}^*(R) \right] &= 0
\end{align}

(30)

where $v_{F,1}^2 = v_{F}^2 + v_{F}^2$ and $v_{F,2}^2 = v_{F}^2 - v_{F}^2$. These equations have been written under the assumption that $g_{++} = g_{+-}$ i.e., the dimensionless intraband interaction strength is independent of spin split band and $g_{++} = g_{+-}$ which is rather obvious. We also define $\bar{g}_{\lambda\lambda'} = \ln \left( \frac{2e^\gamma \omega_D}{\pi} \right) g_{\lambda\lambda'}$. Similarly we can use Eq. (29) to obtain the GL equations for other two order parameters $\Delta_{s,2}$ and $\Delta_{t,2}$, which may be obtained by making the replacements $\Delta_{s,1} \leftrightarrow \Delta_{s,2}$, $\Delta_{t,1} \leftrightarrow \Delta_{t,2}$ and $\Pi_{-} \leftrightarrow \Pi_{+}$ in Eqs. (29) and (30).

Equations (29) and (30) clearly show the decoupling of order parameters $\Delta_{s,1}$ and $\Delta_{s,2}$ in their linear order and as their coefficients are unequal, they have two different critical temperatures. The higher one of these two corresponds to the standard critical temperature $T_c$ and the lower one corresponds to the temperature at which the spin-nature of the order parameter changes. The information of this new transition temperature is however hidden in the Eq. (25) as the GL equations for $\Delta_{s,1}$ and $\Delta_{s,2}$ are coupled in their linear order. We also observe from the other two GL equations for $\Delta_{s,2}$ and $\Delta_{t,2}$ that the transition temperature for both the singlet order parameters are same and this is also the case for the two triplet order parameters. Relative magnitude of singlet transition temperature $T_s$ and triplet transition temperature $T_t$ depends on the sign of interband interaction $g_{++}$. Therefore total superfluid density at $T < T_s$, $n_s = |\Delta_{s,1}|^2 + |\Delta_{t,1}|^2 = -\frac{1}{\alpha} \ln \left( \frac{T}{T_s} \right)$

\begin{align}
T_s &= \left( \frac{2e^\gamma \omega_D}{\pi} \right) \exp \left[ -\frac{1}{g_{++} - g_{+-}} \right] (33)
\end{align}

and hence $T_s/T_t = \exp[g_{+-}/(g_{++} - g_{+-})] < 1$. The predicted $T_s$ is then the cross-over temperature $T^*$ below which both singlet and triplet pairing exist and above which only triplet pairing exists.

Assuming $\Delta_{s,2} \ll \Delta_{s,1}$, we find $|\Delta_{s,1}|^2 = -\frac{1}{\alpha} \ln \left( \frac{T}{T_s} \right)$ near $T_s$. Therefore total superfluid density at $T < T_s$,

\begin{align}
T_s &= \left( \frac{2e^\gamma \omega_D}{\pi} \right) \exp \left[ -\frac{1}{g_{++} - g_{+-}} \right] (33)
\end{align}

and hence $T_s/T_t = \exp[g_{+-}/(g_{++} - g_{+-})] < 1$. Above and below $T^*$, superfluid density is then found to be $-(1/\alpha) \ln (T/T_s)$ and $-(1/\alpha) \ln (T/T_s)$ respectively.

Assuming $g_{++} < 0$, one finds

\begin{align}
T_t &= \left( \frac{2e^\gamma \omega_D}{\pi} \right) \exp \left[ -\frac{1}{g_{++} - g_{+-}} \right] (33)
\end{align}

by equating the coefficient of $\Delta_{s,1}$ in Eq. (29) with zero at $T_t$ which is identified as $T_c$ (28). We now look for existence of any other characteristic temperature which could be less than $T_c$. Assuming further that $\Delta_{s,1} = 0$ and $\Delta_{t,2} \ll \Delta_{t,1}$ near $T_t$, we find superfluid density which is entirely due to triplet order parameter, to be

\begin{align}
n_s &= |\Delta_{t,1}|^2 = -\frac{1}{\alpha} \ln \left( \frac{T}{T_t} \right)
\end{align}

(32)

The coefficient of $\Delta_{t,2}^*$ in Eq. (30) is now $1 - \bar{g}_{++} + \bar{g}_{+-} + 3\alpha (g_{++} + g_{+-})|\Delta_{t,1}|^2$. Equating it to zero at $T = T_s$, we find

\begin{align}
T_s &= \left( \frac{2e^\gamma \omega_D}{\pi} \right) \exp \left[ -\frac{1}{g_{++} - g_{+-}} \right] (33)
\end{align}

and hence $T_s/T_t = \exp[g_{+-}/(g_{++} - g_{+-})] < 1$. The predicted $T_s$ is then the cross-over temperature $T^*$ below which both singlet and triplet pairing exist and above which only triplet pairing exists.

Assuming $\Delta_{s,2} \ll \Delta_{s,1}$, we find $|\Delta_{s,1}|^2 = -\frac{1}{\alpha} \ln \left( \frac{T}{T_s} \right)$ near $T_s$. Therefore total superfluid density at $T < T_s$,

\begin{align}
n_s &= |\Delta_{s,1}|^2 + |\Delta_{t,1}|^2 = -\frac{1}{\alpha} \ln \left( \frac{T}{T_s} \right) + \ln \left( \frac{T}{T_t} \right) (34)
\end{align}

Figure 1 shows the variation of $n_s$ with temperature below $T_t$ and around $T_s$. It shows a kink at $T = T_s$.

For attractive interband scattering potential, $g_{++} > 0$ and hence $T_c$ coincides with

\begin{align}
T_t &= \left( \frac{2e^\gamma \omega_D}{\pi} \right) \exp \left[ -\frac{1}{g_{++} + g_{+-}} \right] (35)
\end{align}

becomes cross-over temperature $T^*$ above which the order parameter is fully singlet. In this case, $T_t/T_s = \exp[-g_{+-}/(g_{++}^2 - g_{+-}^2)] < 1$. Above and below $T^*$, superfluid density is then found to be $-(1/\alpha) \ln (T/T_s)$ and $-(1/\alpha) \ln (T/T_s)$ respectively.
We may consider the linearized coupled GL equations for \( s \)-wave and \( t \)-wave, \( s \)-wave being the singlet channel and \( t \)-wave the triplet channel. Equations (37) and (38) suggest that \( \Delta_{s,1} \) and \( \Delta_{s,2} \) leads to the critical field \( H_{c2} \), near critical temperature \( T_c \).

\[ H_{c2} = \frac{2\sqrt{2}}{3(\sqrt{2} - 1)} \frac{1}{\alpha} \ln \left( \frac{T_1}{T} \right) \]

Near critical temperature \( T_c \), the sudden change in \( n_s/T_1 = 0.95 \) becomes

\[ \sum_{n=0}^{\infty} 2(2n+1)a_{n+1}^t \right|_n > + \sqrt{\frac{n}{n-1}} a_n^t \right|_{n-2} > \]

\[ = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) \sum_{n=0}^{\infty} a_{n+1}^t \right|_n > \] (39)

\[ \sum_{n=0}^{\infty} 2(2n+1)a_{n+1}^t \right|_n > + \sqrt{n(n+2)} a_n^t \right|_{n+2} > \]

\[ = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) \sum_{n=0}^{\infty} a_{n+1}^t \right|_n > \] (40)

Equating the coefficients of the lowest Landau level \( |0> \) from Eq. (39) we find

\[ 2a_0^t + \sqrt{2a_0^t} = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) a_0^t \] (41)

which is one of the equations satisfied by \( a_0^t \) and \( a_2^t \). The other equation satisfied by these variables is given by

\[ 5a_2^t + \sqrt{2a_2^t} = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) a_2^t \] (42)

derivable from Eq. (40). The solution of the coupled Eqs. (41) and (42) corresponding to a linear combination of \( a_0^t \) and \( a_2^t \) with the major sharing from the former leads to the critical field

\[ H_{c2} = \frac{2\sqrt{2}}{3(\sqrt{2} - 1)} \frac{1}{\alpha \sqrt{v_{F+}} + v_{F-}} \ln \left( \frac{T_1}{T} \right) \] (43)

V. THE UPPER CRITICAL FIELD

We here estimate the upper critical field near \( T = T_1 > T_s \). If the applied magnetic field is along negative z-axis, then a convenient gauge choice gives \( A = (0, -Hx, 0) \). To simplify the problem by retaining all the essential physics we may consider the linearized coupled GL equations for \( \Delta_{s,1} \) and \( \Delta_{s,2} \). We thus find GL equation for \( \Delta_{s,1} \) from Eq. (29) as

\[ \ln \left( \frac{T}{T_1} \right) \Delta_{s,1}^*(R) = \frac{\nu_{F+} \alpha}{16} (2\Pi_2^2 \Delta_{s,1}^*(R) + \Pi_2^2 \Delta_{s,2}^*(R)) = 0 \]

(37)

and similarly for \( \Delta_{s,2} \), it is given by

\[ \ln \left( \frac{T}{T_1} \right) \Delta_{s,2}^*(R) = \frac{\nu_{F+} \alpha}{16} (2\Pi_2^2 \Delta_{s,2}^*(R) + \Pi_2^2 \Delta_{s,1}^*(R)) = 0 \]

(38)

By defining \( \Pi_\pm = \frac{\Pi_+ \mp \Pi_-}{\sqrt{2} e H} \), it is easy to show that \( \Pi_+ \Pi_- = 1 \). Therefore \( \Pi_\pm \) are regarded as the creation and annihilation operators respectively in occupation number space such that \( \Pi_\pm |n> = \sqrt{n+1}|n+1> \) and \( \Pi_- |n> = \sqrt{n-1}|n-1> \) where \( |n> \) represents \( n \)-th Landau level. Equations (37) and (38) suggest that the characteristic order parameter \( \Delta_0 = 1/\sqrt{\alpha} \) and the coherence length \( \xi_0 = \frac{\sqrt{T_1/T}}{\sqrt{\alpha}} \). The dimensionless order parameters \( \psi_{t,j} = \frac{\Delta_{s,1}}{\Delta_{s,2}} \), \( (j = 1, 2) \) are then may be expressed as a linear combination of Landau levels: \( \psi_{t,j} = \sum_{n=0}^{\infty} a_n^{t,j} |n> \). Therefore Eqs. (37) and (38) become

\[ \sum_{n=0}^{\infty} 2(2n+1)a_{n+1}^t \right|_n > + \sqrt{n(n-1)} a_n^t \right|_{n-2} > \]

\[ = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) \sum_{n=0}^{\infty} a_{n+1}^t \right|_n > \] (39)

\[ \sum_{n=0}^{\infty} 2(2n+1)a_{n+1}^t \right|_n > + \sqrt{n(n+2)} a_n^t \right|_{n+2} > \]

\[ = \frac{1}{K_e H} \ln \left( \frac{T_1}{T} \right) \sum_{n=0}^{\infty} a_{n+1}^t \right|_n > \] (40)

VI. SUMMARY AND DISCUSSION

We have analyzed the critical and cross-over temperatures using equations for order parameters comprising of \( \Delta_{s,1} \) and \( \Delta_{s,1} \) and neglecting the order parameters \( \Delta_{s,2} \) and \( \Delta_{t,2} \). This consideration implies spherically symmetric s-wave in the singlet channel and the triplet channels are of p-waves which have point nodes. On the other hand, the experiments seem to suggest that most of these superconductors, excepting Li2Pd3B, have lines of nodes. For such a case, equations for \( \Delta_{s,2} \) and \( \Delta_{t,2} \) should be considered and we find that the transition and cross-over temperatures remain unaltered.

We observe from the data of temperature dependent super-fluid density \( n_s(T) \) that its slope changes suddenly at \( T \sim 0.9T_c \) for Li2Pd3B. This observation is not however prominent in Li2Pd3B. Since the mixed singlet-triplet phase of Li2Pd3B has very large singlet component compared to the triplet component, the sudden
change in slope of $n_s(T)$ is invisible at the cross-over temperature. On the other hand, Li$_2$Pt$_3$B has comparable amount of singlet and triplet components in the mixed singlet-triplet phase and thus the cross-over temperature is prominent.

The Knight shift measurements$^{21}$ in Li$_2$Pd$_3$B and Li$_2$Pt$_3$B did not show any cross-over temperature whatsoever; the former (latter) shows singlet (triplet) type of data at all temperatures. However, the error bars in these data are huge to conclude this subtle effect. Moreover, we have not considered the effect of impurity which will smoothen this cross-over. The Knight shift measurement in CePt$_3$Si by Yogi et al.$^{22}$ seems to suggest the cross-over temperature is around 0.4$K$, from the point of view of optimistic observation for obvious reason. A more accurate Knight shift measurement in relatively pure systems will directly show the cross-over temperature predicted in this paper. Further observed anomaly$^{23,24}$ in specific heat data of CePt$_3$Si may also be related with this cross-over temperature.

To summarize, we have microscopically derived the Ginzburg-Landau equations for a noncentrosymmetric superconductors like CePt$_3$Si in the presence of interband pair scattering potential. We predict that apart from the conventional transition temperature $T_c$, there is another cross-over temperature $T^*$ at which spin structure of the order parameter changes. The order parameter changes from mixed singlet-triplet phase at lower temperatures to only triplet (singlet) phase for repulsive (attractive) interband scattering potential at higher temperatures. The temperature dependence of superfluid density shows a kink at this cross-over temperature. We also have estimated critical field near the conventional transition temperature.

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