Ginzburg-Landau theory of noncentrosymmetric superconductors

Soumya P. Mukherjee and Sudhansu S. Mandal
Theoretical Physics Department, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India
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The data of temperature-dependent superfluid density $n_s(T)$ in Li_2Pd_3B and Li_2Pt_3B [Yuan *et al.*, Phys. Rev. Lett. **97**, 017006 (2006)] show that a sudden change of the slope of $n_s(T)$ occurs at a temperature 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 which are 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 crossover from a mixed singlet-triplet phase at lower temperatures to only a 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 crossover temperature. We attribute the temperature at which the 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 $CePt_3Si$. We have also estimated the critical field near the critical temperature.

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I. INTRODUCTION

The spin-orbit (SO) coupling of electrons in the noncentrosymmetric crystals lifts the spin degeneracy and hence splits the energy bands. For weak SO coupling, the band splitting energy E_{SO} is smaller than the superconducting energy scales. In that case, the pairing potential may still be chosen as a function of spin and momentum of the 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 the 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 $\Delta_{\mathbf{k}}=[\psi_k\hat{\sigma}_0+\boldsymbol{d}_{\mathbf{k}}\cdot\hat{\boldsymbol{\sigma}}]i\hat{\sigma}_y$, where $\psi_{\mathbf{k}}$ is the spin-singlet component and $\boldsymbol{d}_{\mathbf{k}}$ is the spin-triplet component of the order parameter, and σ's are the Pauli matrices.

The recent discovery[9] of superconductivity in $CePt_3Si$, which is noncentrosymmetric, has raised interest in the properties of superconductors without inversion symmetry. A flurry of noncentrosymmetric heavy-fermion compounds like UIr (Ref. 10), $CeRhSi_3$ (Ref. 11), and $CeIRSi_3$ (Ref. 12) exhibiting superconductivity have been discovered since then. All of these compounds are strongly correlated: Both antiferromagnetism and superconductivity coexist[9] in $CePt_3Si$, in particular. On the other hand, recently discovered Li_2Pd_3B (Ref. 13) and Li_2Pt_3B (Ref. 14) compounds are not of the strongly correlated type and thus may be ideally used to explore the properties of noncentrosymmetric superconductivity. The band structure calculation[15] in $CePt_3Si$ reveals that $500\ \mathrm{K}\lesssim E_{SO}\lesssim 2000\ \mathrm{K}$, i.e., E_{SO} is much larger than T_c which is reported to be 0.75 K. Therefore the pairing between electrons in two different spin-split bands can be neglected for $CePt_3Si$ and so are in the case of Li_2Pd_3B and Li_2Pt_3B compounds. In this paper, we consider this assumption.

Both the penetration depth data[16] and the thermal conductivity data[17] in $CePt_3Si$ 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_2Pd_3B and Li_2Pt_3B at low temperatures. However, this model alone cannot explain the sudden change in slope of $n_s(T)$ at some characteristic temperature that has been clearly observed[19] in these systems, especially in Li_2Pt_3B. This motivates us to study the Ginzburg-Landau (GL) theory for a two-component order parameter associated with two spin-split bands formed in the presence of SO interaction. In this theory, we have considered an attractive intraband pairing potential and attractive or repulsive interband pair scattering potential. As a consequence we have shown that, apart from the conventional superconducting critical temperature, there is another characteristic temperature T^* at which the superconducting order parameter undergoes a crossover from a mixed singlet-triplet phase at lower temperatures to only a triplet or singlet phase at higher temperatures. The superfluid density shows a kink in its behavior at the temperature T^*.

The article is organized as follows. In Sec. II, we review some important aspects of a model Hamiltonian for a noncentrosymmetric superconductor. It corresponds to two bands with opposite helicity. Following the method of semiclassical gradient expansion,[20] we microscopically derive the GL equations for such a superconductor in Sec. III. Both the intraband pairing potential and interband pair scattering potential have been considered. Consequently the GL equations for two bands are coupled. We analyze the GL equations in terms of the singlet- and triplet-order parameters in Sec. IV by combining the GL equations for two separate bands. We find that the new GL equations are decoupled in the linear order of the singlet- and triplet-order parameters. This predicts two different transition temperatures: The higher of these corresponds to the usual superconducting transition temperature, and the lower one describes a transition from a mixed singlet-triplet phase at lower temperatures to only a triplet or singlet phase, depending on the sign of the interband pair scattering potential. We estimate the value of critical magnetic field near T_c in Sec. V. We finally summarize our results and discuss experimental consequences in Sec. VI.

II. NONCENTROSYMMETRIC SUPERCONDUCTORS

We begin this section with a brief introduction of a model Hamiltonian for noncentrosymmetric superconductors. The normal-state Hamiltonian[1–6] for the electrons in a band of a lattice without inversion symmetry is

$$H_0 = \sum_{\mathbf{k},s} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{k},s,s'} \mathbf{g}_{\mathbf{k}} \cdot \boldsymbol{\sigma}_{ss'} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s'}, \tag{1}$$

where the electrons with momentum $\mathbf{k}$ and spin s $(=\uparrow$ or $\downarrow)$ are created (annihilated) by the operators $c^{\dagger}_{\mathbf{k}s}$ $(c_{\mathbf{k}s})$, and $\xi_{\mathbf{k}}$ is the band energy measured from the Fermi energy ϵ_F. The second term in the Hamiltonian (1) breaks parity as $\boldsymbol{g}_{-\mathbf{k}}=-\boldsymbol{g}_{\mathbf{k}}$ for a noncentrosymmetric system. For a system like the heavy-fermion compound $CePt_3Si$ which has layered structure, H_0 is considered to be two dimensional. For such a system of electrons with band mass m, $\xi_{\mathbf{k}}=\frac{\mathbf{k}^2}{2m}-\epsilon_F$ and $\boldsymbol{g}_{\mathbf{k}}=\alpha\boldsymbol{\eta}_{\mathbf{k}}$ where $\eta_k=\hat{n}\times\mathbf{k}$; i.e., the spin-orbit interaction is of Rashba type where α is called the Rashba parameter. Here $\hat{n}$ represents the axis of noncentrosymmetry 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 $\xi_{\mathbf{k}\lambda}=\xi_k+\lambda\alpha|\mathbf{k}|$ where $\lambda=\pm$ describes helicity of the spin-split bands. Therefore, in the diagonalized basis H_0, Eq. (1) becomes $H_0=\Sigma_{\mathbf{k},\lambda=\pm}\xi_{\mathbf{k}\lambda}\tilde{c}^{\dagger}_{\mathbf{k}\lambda}\tilde{c}_{\mathbf{k}\lambda}$, where $\tilde{c}_{\mathbf{k}\lambda}=(c_{\mathbf{k}\uparrow}-\lambda\Lambda^*_{\mathbf{k}}c_{\mathbf{k}\downarrow})/\sqrt{2}$ is the electron destruction operator and $\tilde{c}^{\dagger}_{\mathbf{k}\lambda}=(c^{\dagger}_{\mathbf{k}\uparrow}-\lambda\Lambda_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\downarrow})/\sqrt{2}$ is the electron creation operator in band λ with momentum $\mathbf{k}$ where $\Lambda_{\mathbf{k}}=-i\exp(-i\phi_{\mathbf{k}})$ with $\phi_{\mathbf{k}}$ being the angle of $\mathbf{k}$ with the $\hat{x}$ axis. The Fermi momenta in these bands are $k_F^{\lambda}=\sqrt{k_F^2+m^2\alpha^2}-\lambda m\alpha$ 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 $\nu_{\lambda}=\frac{m}{2\pi}(1-\lambda m\alpha/\sqrt{k_F^2+m^2\alpha^2})$.

A band structure calculation[15] on $CePt_3Si$ 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 $k_BT_c\approx0.06$ meV. The formation of Cooper pairing between electrons in different spin-split bands may thus be ignored;[4–7] i.e., $\langle\tilde{c}_{\mathbf{k}\lambda}\tilde{c}_{-\mathbf{k}\lambda'}\rangle$ is finite only when $\lambda'=\lambda$. However, the scattering of pairs between two spin-split bands is allowed. The Hamiltonian for the system may then be written as

$$H=\sum_{\mathbf{k},\lambda=\pm}\xi_{\mathbf{k}\lambda}\tilde{c}^{\dagger}_{\mathbf{k}\lambda}\tilde{c}_{\mathbf{k}\lambda}+\sum_{\mathbf{k},\mathbf{k}'}\sum_{\lambda,\lambda'}V_{\lambda\lambda'}(\mathbf{k},\mathbf{k}')\tilde{c}^{\dagger}_{\mathbf{k}\lambda}\tilde{c}^{\dagger}_{-\mathbf{k}\lambda}\tilde{c}_{-\mathbf{k}'\lambda'}\tilde{c}_{\mathbf{k}'\lambda'}, \tag{2}$$

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

III. GINZBURG-LANDAU EQUATIONS

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

$$\mathcal{H}=\int d\mathbf{r}\varphi^{\dagger}_{\lambda}(\mathbf{r})[\mathcal{K}_{\lambda}(\boldsymbol{p}+e\boldsymbol{A})-\mu]\varphi_{\lambda}(\mathbf{r}) + \int\int d\mathbf{r}d\mathbf{r}'\varphi^{\dagger}_{\lambda}(\mathbf{r})\varphi^{\dagger}_{\lambda}(\mathbf{r}')V_{\lambda\lambda'}(\mathbf{r}-\mathbf{r}')\varphi_{\lambda'}(\mathbf{r}')\varphi_{\lambda'}(\mathbf{r}). \tag{3}$$

Here $\varphi_{\lambda}(\mathbf{r})$ is the field operator for electrons in band λ at position $\mathbf{r}$, the repeated indices denote summation, and μ is the chemical potential. $V_{\lambda\lambda'}(\mathbf{r}-\mathbf{r}')$ denotes the intraband pairing as well as interband pair scattering potential. The vector potential $\boldsymbol{A}$ which preserves gauge invariance is introduced in the band-dependent kinetic energy operator $\mathcal{K}_{\lambda}(\boldsymbol{p}+e\boldsymbol{A})$, where $\boldsymbol{p}=-i\boldsymbol{\nabla}$. From here after we consider the 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

$$[i\omega_n-\mathcal{K}_{\lambda}(\boldsymbol{p}+e\boldsymbol{A})+\mu]\mathcal{G}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n) + \int d\mathbf{r}''\Delta_{\lambda}(\mathbf{r},\mathbf{r}'')\mathcal{F}^{\dagger}_{\lambda}(\mathbf{r}'',\mathbf{r}';\omega_n)=\delta(\mathbf{r}-\mathbf{r}'), \tag{4}$$

$$[-i\omega_n-\mathcal{K}_{\lambda}(\boldsymbol{p}-e\boldsymbol{A})+\mu]\mathcal{F}^{\dagger}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n) - \int d\mathbf{r}''\Delta^*_{\lambda}(\mathbf{r},\mathbf{r}'')\mathcal{G}_{\lambda}(\mathbf{r}'',\mathbf{r}';\omega_n)=0, \tag{5}$$

where $\mathcal{G}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)$ and $\mathcal{F}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)$, respectively, are the normal and anomalous quasiparticle Green's functions in the band λ, and $\Delta^*_{\lambda}(\mathbf{r},\mathbf{r}')$ is the gap function which can be written as

$$\Delta^*_{\lambda}(\mathbf{r},\mathbf{r}')=-T\sum_{n,\lambda'}V_{\lambda\lambda'}(\mathbf{r},\mathbf{r}')\mathcal{F}^{\dagger}_{\lambda'}(\mathbf{r},\mathbf{r}';\omega_n), \tag{6}$$

where $\omega_n=(2n+1)\pi T$ is the fermionic Matsubara frequency at temperature T. The normal-state electronic Green's function $G_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)$ satisfies the equation

$$[i\omega_n-\mathcal{K}_{\lambda}(\boldsymbol{p}+e\boldsymbol{A})+\mu]G_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)=\delta(\mathbf{r}-\mathbf{r}'). \tag{7}$$

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

$$\mathcal{G}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)=G_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)-\int d\mathbf{r}_1d\mathbf{r}_2G_{\lambda}(\mathbf{r},\mathbf{r}_1;\omega_n) \times\Delta_{\lambda}(\mathbf{r}_1,\mathbf{r}_2)\mathcal{F}^{\dagger}_{\lambda}(\mathbf{r}_2,\mathbf{r}';\omega_n), \tag{8}$$

$$\mathcal{F}^{\dagger}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)=\int d\mathbf{r}_1 d\mathbf{r}_2 G_{\lambda}(\mathbf{r},\mathbf{r}_1;-\omega_n)\times\Delta^*_{\lambda}(\mathbf{r}_1,\mathbf{r}_2)\mathcal{G}_{\lambda}(\mathbf{r}_2,\mathbf{r}';\omega_n). \tag{9}$$

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

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

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

$$\mathcal{G}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)=G_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)-\int d\mathbf{r}_1 d\mathbf{r}_2 G_{\lambda}(\mathbf{r},\mathbf{r}_1;\omega_n)\Delta_{\lambda}(\mathbf{r}_1,\mathbf{r}_2)\times\int d\mathbf{r}_3 d\mathbf{r}_4 G_{\lambda}(\mathbf{r}_2,\mathbf{r}_3;-\omega_n)\times\Delta^*_{\lambda}(\mathbf{r}_3,\mathbf{r}_4)G_{\lambda}(\mathbf{r}_4,\mathbf{r}';\omega_n), \tag{11}$$

$$\mathcal{F}^{\dagger}_{\lambda}(\mathbf{r},\mathbf{r}';\omega_n)=\int d\mathbf{r}_1 d\mathbf{r}_2 G_{\lambda}(\mathbf{r},\mathbf{r}_1;-\omega_n)\Delta^*_{\lambda}(\mathbf{r}_1,\mathbf{r}_2)\times\left[G_{\lambda}(\mathbf{r}_2,\mathbf{r}';\omega_n)-\int d\mathbf{r}_3 d\mathbf{r}_4 d\mathbf{r}_5 d\mathbf{r}_6 G_{\lambda}(\mathbf{r}_2,\mathbf{r}_3;\omega_n)\times\Delta_{\lambda}(\mathbf{r}_3,\mathbf{r}_4)G_{\lambda}(\mathbf{r}_4,\mathbf{r}_5;-\omega_n)\Delta^*_{\lambda}(\mathbf{r}_5,\mathbf{r}_6)G_{\lambda}(\mathbf{r}_6,\mathbf{r}';\omega_n)\right]. \tag{12}$$

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

$$\Delta^*_{\lambda}(\mathbf{r},\mathbf{r}')=\Delta^*_{\lambda_I}(\mathbf{r},\mathbf{r}')+\Delta^*_{\lambda_{II}}(\mathbf{r},\mathbf{r}'), \tag{13}$$

we find

$$\Delta^*_{\lambda_I}(\mathbf{r},\mathbf{r}')=-T\sum_{n,\lambda'}V_{\lambda\lambda'}(\mathbf{r},\mathbf{r}')\int d\mathbf{r}_1 d\mathbf{r}_2 G_{\lambda'}(\mathbf{r},\mathbf{r}_1;-\omega_n)\times\Delta^*_{\lambda'}(\mathbf{r}_1,\mathbf{r}_2)G_{\lambda'}(\mathbf{r}_2,\mathbf{r}';\omega_n), \tag{14}$$

$$\Delta^*_{\lambda_{II}}(\mathbf{r},\mathbf{r}')=T\sum_{n,\lambda'}V_{\lambda\lambda'}(\mathbf{r},\mathbf{r}')\int d\mathbf{r}_{1-6}G_{\lambda'}(\mathbf{r},\mathbf{r}_1;-\omega_n)\times\Delta^*_{\lambda'}(\mathbf{r}_1,\mathbf{r}_2)G_{\lambda'}(\mathbf{r}_2,\mathbf{r}_3;\omega_n)\Delta_{\lambda'}(\mathbf{r}_3,\mathbf{r}_4)\times G_{\lambda}(\mathbf{r}_4,\mathbf{r}_5;-\omega_n)\Delta^*_{\lambda'}(\mathbf{r}_5,\mathbf{r}_6)G_{\lambda'}(\mathbf{r}_6,\mathbf{r}';\omega_n). \tag{15}$$

Expressing the order parameter $\Delta^*_{\lambda}(\mathbf{r}_1,\mathbf{r}_2)$ in terms of the center-of-mass coordinate $\boldsymbol{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$ and the relative coordinate $\boldsymbol{\rho}=\mathbf{r}_1-\mathbf{r}_2$ of the pair and making a Fourier transform with respect to the relative coordinate, we can express $\Delta^*_{\lambda_I}$ in Eq. (14) as the sum of two terms:

$$\Delta^*_{\lambda_I}=\Delta^*_{\lambda_{Ic}}+\Delta^*_{\lambda_{Ig}}, \tag{16}$$

where

$$\Delta^*_{\lambda_{Ic}}(\mathbf{R},\mathbf{k})=-T\sum_{n,\lambda'}\int\frac{d^2\mathbf{k}'}{(2\pi)^2}V_{\lambda\lambda'}(\mathbf{k}-\mathbf{k}')\times\frac{1}{\omega_n^2+\xi^2_{\mathbf{k}'\lambda'}}\Delta^*_{\lambda'}(\mathbf{R},\mathbf{k}'), \tag{17}$$

$$\Delta^*_{\lambda_{Ig}}(\mathbf{R},\mathbf{k})=-T\sum_{n,\lambda'}\int\frac{d^2\mathbf{k}'}{2(2\pi)^2}V_{\lambda\lambda'}(\mathbf{k}-\mathbf{k}')\times\left\{\frac{1}{(2m)^2}\frac{2\xi^2_{\mathbf{k}'\lambda'}-6\omega_n^2}{(\omega_n^2+\xi^2_{\mathbf{k}'\lambda'})^3}(k'_x\Pi_x+k'_y\Pi_y)^2-\frac{1}{2m}\frac{\xi_{\mathbf{k}'}\boldsymbol{\Pi}^2}{(\omega_n^2+\xi^2_{\mathbf{k}'\lambda'})^2}\right\}\Delta^*_{\lambda'}(\mathbf{R},\mathbf{k}'). \tag{18}$$

Similarly we find, from Eq. (15),

$$\Delta^*_{\lambda_{II}}(\mathbf{R},\mathbf{k})=T\sum_{n,\lambda'}\int\frac{d^2\mathbf{k}'}{(2\pi)^2}V_{\lambda\lambda'}(\mathbf{k}-\mathbf{k}')\frac{1}{(\omega_n^2+\xi^2_{\mathbf{k}'\lambda'})^2}\times|\Delta_{\lambda'}(\mathbf{R},\mathbf{k}')|^2\Delta^*_{\lambda'}(\mathbf{R},\mathbf{k}'), \tag{19}$$

where $\boldsymbol{\Pi}=-i\boldsymbol{\nabla}_{\mathbf{R}}-2e\boldsymbol{A}(\mathbf{R})$ with an approximation $\boldsymbol{A}(\mathbf{R}\pm\boldsymbol{\rho}/2)\approx\boldsymbol{A}(\mathbf{R})$.

We assume the interaction potential to be

$$V_{\lambda\lambda'}(\mathbf{k}-\mathbf{k}')=-V_{\lambda\lambda'}\hat{k}\cdot\hat{k}'=-V_{\lambda\lambda'}[\Lambda^*_{\mathbf{k}}\Lambda_{\mathbf{k}'}+\Lambda_{\mathbf{k}}\Lambda^*_{\mathbf{k}'}], \tag{20}$$

where the interaction strength $V_{\lambda\lambda'}>0$ for $\lambda=\lambda'$ and it may have either sign when $\lambda\neq\lambda'$. We thus have considered, contrary to Ref. 5, the crucial interband pair scattering potential which has led to the main conclusion of the present study. The potential $V_1=-V_{\lambda\lambda'}\Lambda^*_{\mathbf{k}}\Lambda_{\mathbf{k}'}$ leads to the order parameter $\Delta_{\lambda,1}\Lambda_{\mathbf{k}}$ 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), $V_2=-V_{\lambda\lambda'}\Lambda_{\mathbf{k}}\Lambda^*_{\mathbf{k}'}$, will help to induce the order parameter $\Delta_{\lambda,2}\Lambda^*_{\mathbf{k}}$. This new order parameter corresponds to d waves in singlet channel and p waves and f waves for spin up-up and down-down triplet channels, respectively. Thus we can write the new form of the order parameter as

$$\Delta^*_{\lambda}(\mathbf{R},\mathbf{k})=\Delta^*_{\lambda,1}(\mathbf{R})\Lambda^*_{\mathbf{k}}+\Delta^*_{\lambda,2}(\mathbf{R})\Lambda_{\mathbf{k}}. \tag{21}$$

Inserting the form of $V_{\lambda\lambda'}(\mathbf{k}-\mathbf{k}')$ as into Eq. (20) and $\Delta^*_{\lambda}(\mathbf{R},\mathbf{k})$ as in Eq. (21) into Eqs. (17)–(19), we find

$$\Delta^*_{\lambda_{Ic}}(\mathbf{R},\mathbf{k}) = \ln\left(\frac{2e^{\gamma}\omega_D}{\pi T}\right)\sum_{\lambda'} g_{\lambda\lambda'}(\Delta^*_{\lambda',1}\Lambda^*_{\mathbf{k}} + \Delta^*_{\lambda',2}\Lambda_{\mathbf{k}}), \tag{22}$$

$$\Delta^*_{\lambda_{Ig}}(\mathbf{R},\mathbf{k}) = -\frac{\alpha}{8}\sum_{\lambda'} g_{\lambda\lambda'}v^2_{F\lambda'}[(2\mathbf{\Pi}^2\Delta^*_{\lambda',1} + \Pi^2_-\Delta^*_{\lambda',2})\Lambda^*_{\mathbf{k}} + (2\mathbf{\Pi}^2\Delta^*_{\lambda',2} + \Pi^2_+\Delta^*_{\lambda',1})\Lambda_{\mathbf{k}}], \tag{23}$$

$$\Delta^*_{\lambda_{II}}(\mathbf{R},\mathbf{k}) = -\alpha\sum_{\lambda'} g_{\lambda\lambda'}[(|\Delta_{\lambda',1}|^2 + 2|\Delta_{\lambda',2}|^2|)\Delta^*_{\lambda',1}\Lambda^*_{\mathbf{k}} + (2|\Delta_{\lambda',1}|^2 + |\Delta_{\lambda',2}|^2)\Delta^*_{\lambda',2}\Lambda_{\mathbf{k}}], \tag{24}$$

where $\Pi_\pm = \Pi_x \pm i\Pi_y$, the dimensionless interaction strength $g_{\lambda\lambda'} = \frac{1}{2}V_{\lambda\lambda'}\nu_{\lambda'}$, $\gamma = 0.5772$ is the Euler constant, ω_D is the Debye frequency, $v_{F\lambda}$ is the Fermi velocity for band λ, and $\alpha = \frac{7\zeta(3)}{8(\pi T)^2}$.

Summing expressions (22)–(24) and equating the sum with Eq. (21) and then by comparing coefficients of $\Lambda^*_{\mathbf{k}}$ and $\Lambda_{\mathbf{k}}$ we find the GL equations for each band with primary as well as induced order parameters:

$$\Delta^*_{\lambda,1}(\mathbf{R}) = \ln\left(\frac{2e^{\gamma}\omega_D}{\pi T}\right)\sum_{\lambda'} g_{\lambda\lambda'}\Delta^*_{\lambda',1} - \frac{\alpha}{8}\sum_{\lambda'} g_{\lambda\lambda'}v^2_{F\lambda'}(2\mathbf{\Pi}^2\Delta^*_{\lambda',1} + \Pi^2_-\Delta^*_{\lambda',2}) - \alpha\sum_{\lambda'} g_{\lambda\lambda'}(|\Delta_{\lambda',1}|^2 + 2|\Delta_{\lambda',2}|^2)\Delta^*_{\lambda',1}, \tag{25}$$

$$\Delta^*_{\lambda,2}(\mathbf{R}) = \ln\left(\frac{2e^{\gamma}\omega_D}{\pi T}\right)\sum_{\lambda'} g_{\lambda\lambda'}\Delta^*_{\lambda',2} - \frac{\alpha}{8}\sum_{\lambda'} g_{\lambda\lambda'}v^2_{F\lambda'}(2\mathbf{\Pi}^2\Delta^*_{\lambda',2} + \Pi^2_+\Delta^*_{\lambda',1}) - \alpha\sum_{\lambda'} g_{\lambda\lambda'}(|\Delta_{\lambda',2}|^2 + 2|\Delta_{\lambda',1}|^2)\Delta^*_{\lambda',2}. \tag{26}$$

Note that the gradient of $\Delta^*_{\lambda,1}(\mathbf{R})$ leads to the induction of $\Delta^*_{\lambda,2}(\mathbf{R})$. A self-consistent solution of these order parameters involves simultaneous solutions of Eqs. (25) and (26). The transition temperature T_c, however, may be obtained from the terms linear in $\Delta^*_{\lambda,1}(\mathbf{R})$ of Eq. (25). Solving the matrix equation, one finds

$$T_c = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{1}{g_2}\right],$$

$$g_{1,2} = \frac{1}{2}[(g_{++} + g_{--}) \pm \sqrt{(g_{++} - g_{--})^2 + 4g_{+-}g_{-+}}]. \tag{27}$$

The critical temperature should be determined by the solution $\min(g_1, g_2)$, i.e., g_2, contrary to the consideration of Ref. 8. The other solution g_1 does not have any physical importance. However, in certain physical situations, as we shall discuss in the next section, this redundant solution gets renormalized to a value less than g_2 and manifests itself as a physical solution. We choose a special situation when $g_{++} = g_{--}$ and $g_{+-} = g_{-+}$; i.e., the intraband as well as interband 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 that g_{+-} may have either of the signs. By this choice,

$$T_c = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{1}{g_{++} - |g_{+-}|}\right]. \tag{28}$$

IV. TRANSITION TEMPERATURES

The 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,[7] where $l = 1$ or 2. We thus find the GL equations for $\Delta_{s,1}$ and $\Delta_{t,1}$ derivable from Eq. (25) as

$$\begin{aligned}(1 - \tilde{g}_{++} - \tilde{g}_{+-})\Delta^*_{t,1}(\mathbf{R}) &+ \frac{\alpha}{16}(g_{++} + g_{+-})\{v^2_{F,1}[2\mathbf{\Pi}^2\Delta^*_{t,1}(\mathbf{R}) + \Pi^2_-\Delta^*_{t,2}(\mathbf{R})] - v^2_{F,2}[2\mathbf{\Pi}^2\Delta^*_{s,1}(\mathbf{R}) + \Pi^2_-\Delta^*_{s,2}(\mathbf{R})]\}\\ &+ \alpha(g_{++} + g_{+-})\{[|\Delta_{t,1}(\mathbf{R})|^2 + 2|\Delta_{s,1}(\mathbf{R})|^2 + 2|\Delta_{t,2}(\mathbf{R})|^2 + 2|\Delta_{s,2}(\mathbf{R})|^2]\Delta^*_{t,1}(\mathbf{R}) + \Delta^{*\,2}_{s,1}(\mathbf{R})\Delta_{t,1}(\mathbf{R})\\ &+ 2\Delta^*_{s,1}(\mathbf{R})\Delta^*_{s,2}(\mathbf{R})\Delta_{t,2}(\mathbf{R}) + 2\Delta^*_{s,1}(\mathbf{R})\Delta_{s,2}(\mathbf{R})\Delta^*_{t,2}(\mathbf{R})\}\\ &= 0,\end{aligned} \tag{29}$$

$$\begin{aligned}(1 - \tilde{g}_{++} + \tilde{g}_{+-})\Delta^*_{s,1}(\mathbf{R}) &+ \frac{\alpha}{16}(g_{++} - g_{+-})\{v^2_{F,1}[2\mathbf{\Pi}^2\Delta^*_{s,1}(\mathbf{R}) + \Pi^2_-\Delta^*_{s,2}(\mathbf{R})] - v^2_{F,2}[2\mathbf{\Pi}^2\Delta^*_{t,1}(\mathbf{R}) + \Pi^2_-\Delta^*_{t,2}(\mathbf{R})]\}\\ &+ \alpha(g_{++} - g_{+-})\{[|\Delta_{s,1}(\mathbf{R})|^2 + 2|\Delta_{t,1}(\mathbf{R})|^2 + 2|\Delta_{s,2}(\mathbf{R})|^2 + 2|\Delta_{t,2}(\mathbf{R})|^2]\Delta^*_{s,1}(\mathbf{R}) + \Delta^{*\,2}_{t,1}(\mathbf{R})\Delta_{s,1}(\mathbf{R})\\ &+ 2\Delta^*_{t,1}(\mathbf{R})\Delta^*_{t,2}(\mathbf{R})\Delta_{s,2}(\mathbf{R}) + 2\Delta^*_{t,1}(\mathbf{R})\Delta_{t,2}(\mathbf{R})\Delta^*_{s,2}(\mathbf{R})\} = 0,\end{aligned} \tag{30}$$

where $v^2_{F,1} = v^2_{F_+} + v^2_{F_-}$ and $v^2_{F,2} = v^2_{F_-} - v^2_{F_+}$. These equations have been written under the assumption that $g_{++} = g_{--}$; i.e., the dimensionless intraband interaction strength is independent of the spin-split band and $g_{+-} = g_{-+}$ which is rather obvious. We also define $\tilde{g}_{\lambda\lambda'} = \ln\left(\frac{2e^{\gamma}\omega_D}{\pi T}\right)g_{\lambda\lambda'}$. Similarly we can use Eq. (26) 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 a decoupling of the order parameters $\Delta_{t,1}$ and $\Delta_{s,1}$ 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 Eq. (25) as the GL equations for $\Delta_{+,1}$ and $\Delta_{-,1}$ 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 temperatures for both singlet-order parameters are the same and this is also the case for the two triplet-order parameters. The relative magnitude of the singlet transition temperature T_s and the triplet transition temperature T_t depends on the sign of the interband interaction g_{+-}.

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

$$T_t = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{1}{g_{++}+g_{+-}}\right] \tag{31}$$

by equating the coefficient of $\Delta_{t,1}$ in Eq. (29) with zero at T_t which is identified as T_c, Eq. (28). We now look for the 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 the superfluid density, which is entirely due to the triplet-order parameter, to be

$$n_s \equiv |\Delta_{t,1}|^2 = -\frac{1}{\alpha}\ln\left(\frac{T}{T_t}\right). \tag{32}$$

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

$$T_s = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{g_{++}-2g_{+-}}{g_{++}^2-g_{+-}^2}\right], \tag{33}$$

and hence $T_s/T_t=\exp[g_{+-}/(g_{++}^2-g_{+-}^2)]<1$. The predicted T_s is then the crossover temperature T^* below which both singlet and triplet pairings 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 the total superfluid density at $T<T_s$,

$$n_s = |\Delta_{s,1}|^2 + |\Delta_{t,1}|^2 = -\frac{1}{\alpha}\left[\ln\left(\frac{T}{T_s}\right)+\ln\left(\frac{T}{T_t}\right)\right]. \tag{34}$$

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

$$T_s = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{1}{g_{++}-g_{+-}}\right] \tag{35}$$

and

$$T_t = \left(\frac{2e^{\gamma}\omega_D}{\pi}\right)\exp\left[-\frac{g_{++}+2g_{+-}}{g_{++}^2-g_{+-}^2}\right] \tag{36}$$

becomes the crossover 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^*, the superfluid density is then found to be $-(1/\alpha)\ln(T/T_s)$ and $-(1/\alpha)[\ln(T/T_s)+\ln(T/T_t)]$, respectively.

V. UPPER CRITICAL FIELD

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

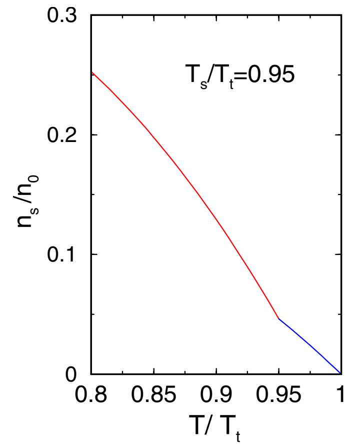

FIG. 1. (Color online) Superfluid density n_s in the units of $n_0=(8\pi^2T_t^2)/[7\zeta(3)]$ as a function of T/T_t for $T_s/T_t=0.95$. T_t is identified as the critical temperature T_c and T_s is identified as the crossover temperature T^* at which the spin symmetry of the order parameter changes.

$$\ln\left(\frac{T}{T_t}\right)\Delta^*_{t,1}(\mathbf{R}) + \frac{v_{F,1}^2\alpha}{16}[2\mathbf{\Pi}^2\Delta^*_{t,1}(\mathbf{R}) + \Pi_-^2\Delta^*_{t,2}(\mathbf{R})] = 0, \tag{37}$$

and similarly for $\Delta_{t,2}$, it is given by

$$\ln\left(\frac{T}{T_t}\right)\Delta^*_{t,2}(\mathbf{R}) + \frac{v_{F,1}^2\alpha}{16}[2\mathbf{\Pi}^2\Delta^*_{t,2}(\mathbf{R}) + \Pi_+^2\Delta^*_{t,1}(\mathbf{R})] = 0. \tag{38}$$

By defining $\tilde{\Pi}_\pm=\frac{\Pi_\pm}{2\sqrt{eH}}$, it is easy to show that $[\tilde{\Pi}_+,\tilde{\Pi}_-]=1$. Therefore $\tilde{\Pi}_\pm$ are regarded as the creation and annihilation operators, respectively, in occupation number space such that $\tilde{\Pi}_+|n\rangle=\sqrt{n+1}|n+1\rangle$ and $\tilde{\Pi}_-|n\rangle=\sqrt{n}|n-1\rangle$ where $|n\rangle$ represents the nth Landau level. Equations (37) and (38) suggest that the characteristic order parameter $\Delta_0=1/\sqrt{\alpha}$ and the coherence length $\xi_0=\sqrt{\frac{v_{F,1}^2\alpha}{8}}$. The dimensionless order parameters $\psi_{t,j}=\frac{\Delta_{t,j}}{\Delta_0},(j=1,2)$ may then be expressed as a linear combination of Landau levels: $\psi_{t,j}{}^*=\sum_{n=0}^{\infty}a_n^{t,j}|n\rangle$. Therefore Eqs. (37) and (38) become

$$\sum_{n=0}^{\infty} 2(2n+1)a_n^{t,1}|n\rangle + \sqrt{n(n-1)}a_n^{t,2}|n-2\rangle = \frac{1}{KeH}\ln\left(\frac{T_t}{T}\right)\sum_{n=0}^{\infty}a_n^{t,1}|n\rangle, \tag{39}$$

$$\sum_{n=0}^{\infty} 2(2n+1)a_n^{t,2}|n\rangle + \sqrt{(n+1)(n+2)}a_n^{t,1}|n+2\rangle = \frac{1}{KeH}\ln\left(\frac{T_t}{T}\right)\sum_{n=0}^{\infty} a_n^{t,2}|n\rangle. \quad (40)$$

Equating the coefficients of the lowest Landau level $|0\rangle$ in Eq. (39) we find

$$2a_0^{t,1} + \sqrt{2}a_2^{t,2} = \frac{1}{KeH}\ln\left(\frac{T_t}{T}\right)a_0^{t,1}, \quad (41)$$

which is one of the equations satisfied by $a_0^{t,1}$ and $a_2^{t,2}$. The other equation satisfied by these variables is given by

$$5a_2^{t,2} + \sqrt{2}a_0^{t,1} = \frac{1}{KeH}\ln\left(\frac{T_t}{T}\right)a_2^{t,2}, \quad (42)$$

derivable from Eq. (40). The solution of the coupled equations (41) and (42) corresponding to a linear combination of $a_0^{t,1}$ and $a_2^{t,2}$ with the major sharing from the former leads to the critical field

$$H_{c2} = \frac{2\sqrt{2}}{3(\sqrt{2}-1)}\frac{1}{e\alpha(v_{F+}^2+v_{F-}^2)}\ln\left(\frac{T_t}{T}\right) \quad (43)$$

near the critical temperature $T_c = T_t$.

VI. SUMMARY AND DISCUSSION

We have analyzed the critical and the crossover temperatures using equations for order parameters comprising of $\Delta_{s,1}$ and $\Delta_{t,1}$ and neglecting the order parameters $\Delta_{s,2}$ and $\Delta_{t,2}$. This consideration implies spherically symmetric *s* waves in the singlet channel and the triplet channels are of *p* waves which have point nodes. On the other hand, the experiments[9,16,17,19] seem to suggest that most of these superconductors, except[19] Li_2Pd_3B, 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 crossover temperatures remain unaltered.

We observe from the data[19] of the temperature-dependent superfluid density $n_s(T)$ that its slope changes suddenly at $T \sim 0.9T_c$ for Li_2Pt_3B. This observation is not, however, prominent in Li_2Pd_3B. Since the mixed singlet-triplet phase of Li_2Pd_3B has a very large singlet component compared to the triplet component,[19] the sudden change in slope of $n_s(T)$ is invisible at the crossover temperature. On the other hand, Li_2Pt_3B has a comparable amount of singlet and triplet components in the mixed singlet-triplet phase and thus the crossover temperature is prominent.

The Knight shift measurements[21] in Li_2Pd_3B and Li_2Pt_3B did not show any crossover 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 the impurity which will smooth this crossover. The Knight shift measurement in $CePt_3Si$ by Yogi *et al.*[22] seems to suggest that the crossover temperature is around 0.4 K, from the point of view of an optimistic observation for obvious reasons. A more accurate Knight shift measurement in relatively pure systems will directly show the crossover temperature predicted in this paper. The further observed anomaly[23,24] in the specific heat data of $CePt_3Si$ may also be related to this crossover temperature.

To summarize, we have microscopically derived the Ginzburg-Landau equations for a noncentrosymmetric superconductors like $CePt_3Si$ in the presence of an interband pair scattering potential. We predict that apart from the conventional transition temperature T_c, there is another crossover temperature T^* at which the spin structure of the order parameter changes. The order parameter changes from a mixed singlet-triplet phase at lower temperatures to only a triplet (singlet) phase for the repulsive (attractive) interband scattering potential at higher temperatures. The temperature dependence of the superfluid density shows a kink at this crossover temperature. We also have estimated the critical field near the conventional transition temperature.

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