Non-Centrosymmetric Superconductors

Guru Kalyan Jayasingh

170260025

ENGINEERING PHYSICS, SENIOR YEAR

Supervised by

Alexander Zyuzin

Researcher, Department of Applied Physics,

Aalto University, Finland

Sumiran Pujari

Assistant Professor, Dept. of Physics, IIT Bombay

Report for PH-587, Bachelor Thesis Project-1 Fall Semester, 2020

Contents

Chapter 1

Introduction

In recent years, an increasing amount of studies have been made on the phenomena of unconventional superconductivity. The original framework of BCS theory described superconductivity as a macroscopic coherent state of Cooper pairs. This was effected by an electron-phonon coupling which leads to an effective attraction between electrons. As worked out by Cooper, the minimal energy configuration enables a contact interaction and hence electrons are required to form Cooper pairs by the most symmetric channel, namely the "s-wave" channel. However, when leaving the realm of electron-phonon coupling, studies have revealed a host of other pairing mechanisms for example spin fluctuation exchange (with promising candidates in nearly magnetic materials), pairing via the p-wave/d-wave/f-wave channels (which can lead to the presence of triplet states), time-reversal breaking in systems, inter-layer BCS type coupling in layered materials etc. Moreover, the role of other orders, for example, Magnetism, has been greatly studied and experiments have been done on materials that have shown superconducting behaviour in the ferromagnetic phase. This opens the possibility of association of superconducting transition with magnetic quantum phase transition. Then there have been examples of materials that have shown multiple superconducting phases and other materials where a superconducting phase develops from a strongly correlated Fermi liquid phase (e.g. Sr2RuO4)[8]. This thesis broadly aims to study one of these alternative mechanisms, namely, the effect of crystal structure symmetry and the specific lack of inversion symmetry on properties of the superconducting phase.

States formed by pairing in a superconductor can be classified according to their parity (for even frequency), namely as even or odd parity. Following the Pauli principle, we can associate even parity with spin-singlet states and odd parity with spin-triplet states. However, this classification, relies on the presence of an inversion centre, so as to make parity a good quantum no. In systems that lack this parity symmetry, a previously forbidden spin-orbit coupling term arises. For example, it has been known that in 2D electron gas, absence of mirror symmetry leads to the occurrence of Rashba spin-orbit coupling, given by

$$\mathcal{H}_{SOC} = \sum_{\vec{k}} \alpha(k_y, -k_x, 0) \cdot \vec{\sigma} \tag{1.1}$$

This when added to the usual quadratic dispersion, leads to energies being $\frac{k^2}{2m} \pm \alpha|k|$, with circular bands[9]. Observe that $\mathcal{H}(\vec{k}) = -\mathcal{H}(-\vec{k})$, thus it is anti-symmetric in its arguments. This is the reason why couplings of these kind come under the broader class of Anti-symmetric spin-orbit coupling (**ASOC**). Now one can ponder over how would the superconducting behaviour change as we go over different values of α, eventually making the spin-orbit coupling strength becomes much greater than Δ, the pairing amplitude? The answer[9] is that we get two following properties of parity broken superconductors:

1. Spin singlet superconductivity remains largely unaffected while we end up destroying two triplet states. This is because for a triplet state to exist, one need $\left|\vec{k}, \uparrow\right\rangle, \left|\vec{k}, \downarrow\right\rangle, \left|-\vec{k}, \uparrow\right\rangle, \left|-\vec{k}, \downarrow\right\rangle$ have to be degenerate. This is guaranteed if we have parity $\hat{\Pi}$ as a symmetry, but lacking the same, this degeneracy breaks.

2. Since parity is no longer a good quantum number, spin singlet and spin triplet states can (and do) mix.

This coupled with the experimental detection[1] of superconductivity in $\mathrm{CeP}t_3\mathrm{Si}$ (inversion asymmetric tetragonal structure) sparked great interest in its pairing mechanism, initially suggesting a mixture of singlet and triplet states. Furthermore, parity breaking can also lead to a two gap superconducting phase which is starkly different from the case of BCS. Finally, recent research has been intensely focusing on Majorana fermions (one particular reason being their use in Quantum computation). Spin triplet superconductors are of great use in this regard[4] and hence a valuable area to direct one's efforts.

1.1 The broad outline of this thesis

The remainder of this report is arranged as follows: In Chapter 2 a brief review of the paper by Samoilenka et al [7] is given, which forms much of the basis for this report. We discuss some non-trivial effects in the magneto-response of materials with spin-orbit coupling, particularly the presence of vortex bound states. Continuing this, in Chapter 3 we take a different route and investigate role of fluctuation in these systems. While their role for conventional BCS is well known[5], we venture to look at two observables: specific heat and diamagnetic susceptibility and try to calculate the role of ASOC in their behaviour near critical point. We finally conclude with some comments on the effect of spin-orbit coupling on these fluctuations.

Chapter 2

Paper Review

The aim of this chapter is to review the paper ”Spiral Magnetic Field and vortex clustering in non-centrosymmetric superconductors”[7] by Samoilenka and Babaev, which presents a microscopic model of the non-centrosymmetric superconductors.
We'll particularly highlight key-approximations and results derived from a microscopic model and set the stage for fluctuational calculations done in the next chapter.

2.1 A microscopic derivation of the Ginzburg Landau model

In systems with lack of inversion symmetry, new terms with, previously not allowed on symmetry considerations, now effect a change in the qualitative properties of a given sample. In case of non-centrosymmetric systems, the so called rashba term leads to one additional term in the GL functional of the superconducting phase.
This paper looks at specific NCS (non-centrosymmetric) superconductors that have space group 'O' or 'T' symmetry (both lack inversion centres, for e.g. O is derived from cubic O_h by excluding it's inversion center).
The paper starts with a model hamiltonian of the BCS kind with a simple Hubbard type attractive potential, of strength given by $V > 0$, and includes spin orbit coupling and a

space dependent magnetic field $\vec{\mathbf{B}}(\vec{\mathbf{x}})$. The hamiltonian is given by

$$H = \sum_{\alpha} E\left(-i\nabla - q\overrightarrow{A}\right)\psi_{\alpha}^{\dagger}\left(\overrightarrow{x},\tau\right)\psi_{\alpha}\left(\overrightarrow{x},\tau\right) - V\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}\psi_{\downarrow}\psi_{\uparrow} + \sum_{\alpha,\beta}\psi_{\alpha}^{\dagger}\left(\overrightarrow{h}\cdot\overrightarrow{\sigma}_{\alpha\beta}\right)\psi_{\beta} \quad (2.1)$$

$$\overrightarrow{h} = \vec{\gamma}\left(-i\nabla - q\overrightarrow{A}\right) - \mu_B\overrightarrow{B} \quad (2.2)$$

$$\overrightarrow{\sigma_{\alpha\beta}} = \left(\overrightarrow{\sigma}\right)_{\alpha\beta} \quad (2.3)$$

where single a particle spectrum is given by $E(-i\boldsymbol{\nabla})$ (which is $\frac{k^2}{2m}$ for free electrons) while $\vec{\gamma}(\vec{k})$ denotes the spin orbit coupling. In case of O/T symmetry, $\vec{\gamma}$ has a simpler form given by $\vec{\gamma}(\vec{k}) \ = \gamma_0\vec{k}$ [2]. Writing a path integral for the same, we replace Ψ from fermionic operators to Grassman fields $a_\alpha(x)$ to obtain

$$S = \int_0^\beta d\tau d\overrightarrow{x} \sum_{\alpha,\beta=\downarrow\uparrow} a_{\alpha}^{\dagger}(\boldsymbol{h}\cdot\boldsymbol{\sigma}_{\alpha\beta})a_{\beta} - Va_{\uparrow}^{\dagger}a_{\downarrow}^{\dagger}a_{\downarrow}a_{\uparrow} \quad (2.4)$$

where

$$\boldsymbol{h} = \left(\partial_T + E - \mu, \overrightarrow{h}\right),\ \boldsymbol{\sigma}_{\alpha\beta} = (\delta_{\alpha\beta}, \overrightarrow{\sigma_{\alpha\beta}})\ \textit{and}\ \overrightarrow{h} = \overrightarrow{\gamma}\left(-i\nabla - e\overrightarrow{A}\left(\overrightarrow{x}\right)\right) - \mu_B\overrightarrow{B}\left(\overrightarrow{x}\right) \quad (2.5)$$

The standard case of $\vec{A}(\vec{x}), \vec{B}(\vec{x})$ varying slowly wrt $\frac{1}{k_F}$ length scale is assumed. Further assumptions which are made are as follows:

$$\mu \gg \omega_D \gg T_c \quad (2.6)$$

$$\gamma_0 k_F \gg \omega_D \gg \mu_B B \quad (2.7)$$

The first of these are valid from standard BCS limits, while the 2nd ones need some explanation: $\mu_B B$ have typical value of $60\mu eV$ for 1 T magnetic fields while ω_D typically have magnitudes in the $25 - 50\ meV$, hence justifies the 2nd inequality. However, the 1st inequality isn't clearly justified since materials have energy split due to spin orbit coupling, given by $\gamma_0 k_F$ (for O symmetry) ranging from 25-200meV in some cases (with many lying in same order as ω_D. See table 1 in [9]). Hence, I think it's a particular limit that the authors wished to take to simplify their calculations for obtaining the GL functional.

We apply a Hubbard-Stratonovich decoupling to the interaction term (similar to BCS case) and write

$$\exp\left[V\int d\overrightarrow{x}d\tau a^{\dagger}_{\uparrow}a^{\dagger}_{\downarrow}a_{\downarrow}a_{\uparrow}\right] = \int D\left[\Delta,\Delta^{\dagger}\right] exp(-\int dtd\overrightarrow{x}\left[\frac{\Delta^{\dagger}\Delta}{V} + \Delta^{\dagger}a_{\downarrow}a_{\uparrow} + \Delta a^{\dagger}_{\uparrow}a^{\dagger}_{x}\right]) \tag{2.8}$$

However, since $h\cdot\sigma_{\alpha\beta}$ isn't diagonal in $a^{\dagger}_{\alpha}, a_{\beta}$ i.e. $\exists$ a $\vec{h}\cdot\vec{\sigma}$ term that mixes spin (this was expected due to inclusion of spin orbit). Hence, we redefine a new grassman field $b \ = (a_{\uparrow}, a_{\downarrow}, a^{\dagger}_{\downarrow}, a^{\dagger}_{\uparrow})$ by expanding our degrees of freedom and write the new H-S transformed partition function as

$$Z \ = \int D[\Delta^{\dagger},\Delta]D[b]e^{-\int d\vec{x}d\tau(b^{T}\frac{H}{2}b+\frac{\Delta^{\dagger}\Delta}{V})} \tag{2.9}$$

where the matrix H is defined as

$$H_0 = \begin{pmatrix} 0 & -h^T \\ h & 0 \end{pmatrix},\ \Lambda = \begin{pmatrix} \delta^{\dagger} & 0 \\ 0 & \delta \end{pmatrix} \tag{2.10}$$

where by T it is meant transpose i.e. taking the matrix operator $h = \boldsymbol{h}\cdot\boldsymbol{\sigma}$ and doing a transpose. Also $\delta \ = \boldsymbol{\sigma}(0,0,i\Delta,0)$ with the usual dot product in $\mathbb{R}^4$. Also, note that for any derivative operator, transpose is defined by $f^T(\frac{\partial}{\partial\tau},\boldsymbol{\nabla}) \ = f(-\frac{\partial}{\partial\tau},-\boldsymbol{\nabla})$.
This form is useful since now integration over fermionic fields can be exactly done due to berezin's formula yielding

$$Z \ = \int D[\Delta^{\dagger},\Delta]e^{\frac{1}{2}ln\ detH-\int d\vec{x}d\tau\frac{\Delta^{\dagger}\Delta}{V}} \tag{2.11}$$

Now a mean field approximation of Δ is made in which one assumes that it doesn't depend on time (i.e. doesn't fluctuate thermally). Then we can write the free energy as

$$F \ = \int\frac{\Delta^2}{V} - \frac{T}{2}Trln\ H \tag{2.12}$$

where by Tr we mean that $H = H(\vec{x},\tau)$ is a matrix for every $\vec{x},\tau$ and we need to take a trace over the same while integration is over $dx, d\tau$. To arrive at the GL functional, we need to expand the 2nd part of trln H in powers of Δ. This is done by the following clever trick:

Define $\hat{f}, \hat{g}$ s.t.

$$\hat{h}\left(-i\nabla\right)\hat{f} = \delta\left(x-x'\right)\delta\left(\tau-\tau'\right) \tag{2.13}$$

$$\hat{g} = e^{\phi\times(x,x')}\hat{f},\ \phi\left(x,x'\right) = i\cdot e\int_{\overrightarrow{x'}}^{x} A\left(\overrightarrow{x_1}\right)d\overrightarrow{x_1} \tag{2.14}$$

$$\hat{h}\left(-i\nabla - e\overrightarrow{A}\right)\hat{g} = \hat{h}\left(-i\nabla - e\overrightarrow{A}\right)\times e^{\phi(x,x')}\hat{f} \tag{2.15}$$

$$= e^{\phi\times(x,x')}\hat{h}\left(-i\nabla\right)\hat{f} = \delta\left(x-x'\right)\delta\left(\tau-\tau'\right) \tag{2.16}$$

Then we have

$$\because \hat{h}\hat{g} = \delta\left(\overrightarrow{x}-\overrightarrow{x'}\right)\delta\left(\tau-\tau'\right) \tag{2.17}$$

$$\Rightarrow H_0^{-1} = \begin{pmatrix} 0 & \hat{g} \\ -\hat{g}^T & 0 \end{pmatrix} \tag{2.18}$$

$$\therefore Tr\log H = Tr\log\left(1+H_0^{-1}\varLambda\right) = \sum_{\gamma=1}^{\infty}\frac{(-1)^{\nu+1}}{v}Tr\left[\left(\hat{g}\hat{\delta}\hat{g}^T\delta^t\right)\right] \tag{2.19}$$

We can further fourier expand $\hat{g}$ to get

$$g\left(\tau-\tau', \overrightarrow{x}-\overrightarrow{x}'\right) = e^{ie\overrightarrow{A}\left(\overrightarrow{x}\right)\times\left(\overrightarrow{x}-\overrightarrow{x},\right)}\times\frac{1}{\beta}\sum_{\omega_n}^{|\omega_n|<\omega_D}\frac{1}{(2\pi)^3}\int d\overrightarrow{k}\,e^{i\overrightarrow{k}\left(\overrightarrow{x}-\overrightarrow{x}'\right)}\times e^{-i\omega_n(\tau-\tau')}f\left(\omega_\eta,\overrightarrow{k}\right) \tag{2.20}$$

This can then be used to expand eqn(2.19) in orders of $\varDelta$. For GL, we clearly need 2nd and 4th order terms as computed in the paper. We'll use the final result (which has been calculated explicitly in the paper) which yields:

$$F = \int d^3\overrightarrow{r}\left[\alpha\left|\psi\right|^2 + \sum_{a=\pm1}K_a\left|\left(v_{aF}D^* - 2a\mu_B\overrightarrow{B}\right)\psi\right|^2 + \beta|\psi|^4\right] + \frac{1}{2}(\vec{B}-\vec{H})^2 \tag{2.21}$$

where all the quantities have been listed in Appendix A. Note that F is clearly bounded from below, hence is a well defined GL functional.

2.2 Rescaled form and Magnetic field configurations

We can redefine variables by

$$\overrightarrow{x} = \frac{1}{\sqrt{-\alpha}}\cdot\left(\frac{\beta}{2\cdot e^2}\right)^{1/4}\overrightarrow{r},\qquad \varDelta = \sqrt{\frac{-\alpha}{2\beta}}\psi$$

$$F = \frac{\sqrt{-\alpha}F'}{2\times(2\times e^2)^{\frac{3}{4}}\beta^{\frac{1}{4}}},\qquad \overrightarrow{A} = \frac{1}{2\times e}\times\frac{r}{x}\overrightarrow{A'}$$

such that the functional looks like

$$F = \int d\overrightarrow{r} \left[\frac{\left(\overrightarrow{B} - \overrightarrow{H}\right)^2}{2} + \sum_{a=\pm 1} \frac{|D_a \Psi|^2}{2k_c} - |\psi|^2 + \frac{|\psi|^4}{2} \right] \tag{2.22}$$

where $D_a = i\boldsymbol{\nabla} - \vec{A} - \chi_a \vec{B}$, $\chi_a = \gamma + a\nu$ (see full definition in Appendix A). We see that new terms in the gauge invariant derivative have come upon: γ is due to SOC, while ν is due to zeeman coupling. Upon extremising eqn(2.22), we get a set of effective GL equations:

$$\sum_a \frac{D_a^2 \psi}{2\kappa_c} - \psi + \psi|\psi|^2 = 0, c.c = 0 \tag{2.23}$$

$$\boldsymbol{\nabla} \times \left[\vec{B} - \vec{H} - \sum_a \chi_a \vec{J}_a \right] = \sum_a \vec{J}_a \tag{2.24}$$

where the new current is defined by $\vec{J}_a = \frac{Re(\psi^* D_a \psi)}{\kappa_c}$. Corresponding boundary conditions are (for $\vec{n}$ being normal to the boundary)

$$\vec{n} \cdot \sum_a D_a \psi = 0 \tag{2.25}$$

$$\vec{n} \times \left[\vec{B} - \vec{H} - \chi_a \vec{J}_a \right] = 0 \tag{2.26}$$

One of the upshot of doing this gymnastic is that we can directly read-off the coherence length by setting $\vec{A} = 0$ in (2.23), which is the only length-scale present in the problem (at 0 field of course) given by

$$\xi = \frac{1}{\sqrt{2\kappa_c}} \tag{2.27}$$

2.3 Magnetic field equations

We now explore the equations accounting for the magnetic response under spin-orbit interaction. We work in the London approximation, which is valid for type-2 superconductors near the lower critical temp (when the 1st vortex starts forming). Under this, we take the density variation to be small as compared to magnetic field decay length-scales (which is valid if $\kappa_{GL} \gg 1$). We'll see later that this can be stated in terms of values of κ_c.

We take $\psi = 0$ at vortex region($r < \xi$), while for $r > \xi$, we recover the bulk phase value $e^{i\phi(\vec{r})}$. Taking the curl of eqn(2.24), we get

$$\left[\frac{\kappa_c}{2} + \gamma^2 + \nu^2\right] \boldsymbol{\nabla} \times \left(\boldsymbol{\nabla} \times \vec{B}\right) + 2\gamma \boldsymbol{\nabla} \times \vec{B} + \vec{B} = -\boldsymbol{\nabla} \times \boldsymbol{\nabla}\phi - \gamma \boldsymbol{\nabla} \times (\boldsymbol{\nabla}\phi) \tag{2.28}$$

This might give the impression that it's impossible to solve for $\vec{B}$ since we don't yet have a form for $\phi(r)$. However, here we're only interested in *greater than* ξ limit, where the RHS is zero (since $\boldsymbol{\nabla} \times \boldsymbol{\nabla}\phi \sim \delta(\vec{r})\hat{z}$). In the paper, to make equations mathematically more transparent, it's re-written in the following form

$$\$\$^{*}\vec{B} = 0, \$ = -\eta + \boldsymbol{\nabla}\times \tag{2.29}$$

$$where\ \eta = \eta_1 + i\eta_2 = \frac{-\gamma + i\tilde{\eta_2}}{\gamma^2 + \tilde{\eta_2}^2}, \tilde{\eta_2} = \sqrt{\frac{\kappa_c}{2} + \nu^2} \tag{2.30}$$

with $\$\$^{*} = \$^{*}\$$ (commuting operators). This leads to the solution of $\vec{B}$ as

$$\overrightarrow{B} = Re\overrightarrow{w}, \quad \$\overrightarrow{w} = 0$$

$$\overrightarrow{w} = \overrightarrow{T} + \frac{1}{\eta} \cdot \left(\nabla \times \overrightarrow{T}\right), \overrightarrow{T} = \nabla \times \left(\overrightarrow{v} f\left(\overrightarrow{r}\right)\right)$$

where we allow $\vec{v}$ to be take values $\vec{v} = const \ / \propto \vec{r}$ for the case of vortices and surface currents. Under this transformation, $\vec{w}$, f are related by

$$\overrightarrow{w} = \eta f \hat{z} - \hat{z} \times \nabla f \tag{2.31}$$

with f satisfying

$$\nabla^2 f + \eta^2 f = 0 \tag{2.32}$$

This leads to a direct form of free energy given by

$$F = \int d\overrightarrow{r} \left\{ \frac{\tilde{n_2}^2}{k_C} \cdot \left(|\nabla f|^2 + |\eta f|^2\right) - \overrightarrow{B} \cdot \overrightarrow{H} \right\} \tag{2.33}$$

There are a few point to note here: Above expressions are valid for both vortices and surface currents (for meissner effect, we set the voritces to 0). It's also general i.e. works both for centrosymmetric and non-centrosymmetric cases. To see a special case of the latter, namely $\gamma, \nu = 0$, we get (2.24) to be the standard GL equation discussed in textbooks. However, the utility of having (2.32) is seen in non-centrosymmetric cases. Using this equation, we'll now investigate meissner state and vortex properties one by one.

2.4 Spiral Meissner State

Consider a superconductor present at half plane $x > 0$. To look at meissner state behaviour, we solve eqn (2.32) to get $f = ce^{i\eta x}$, for c being a complex constant, which is to be derived from the boundary conditions (2.26)

$$\vec{n} \times Re\left[i\frac{\vec{W}}{\eta} - \frac{\kappa_c}{2\tilde{\eta}_2}\vec{H}\right] = 0 \implies c = \frac{-i\kappa_c}{2\eta_2}\tilde{H} \tag{2.34}$$

where $\tilde{H} = H_z + iH_y$ (also we used the fact that $\nabla \times \vec{w} = \eta\vec{w}$ and $\nabla \times \vec{\mathbf{A}} = \vec{\mathbf{B}}$, employing $\vec{\mathbf{B}} = Re\ \vec{\mathbf{w}}$ we get $\vec{\mathbf{A}} = Re\ \frac{\vec{\mathbf{W}}}{\eta}$). Using (2.31), we get the final form of magnetic field as a f(x) as

$$\tilde{B}\ = B_z + iB_y = \ -\frac{i\eta\kappa_c}{2\tilde{\eta}_2}\tilde{H}e^{i\eta x} \propto e^{-\eta_2 x + i\eta_1 x} \tag{2.35}$$

Note: First observe the oscillatory exponential. This means that both B_z, B_y will oscillate with same wavelength and similar to a helix, this'll exhibit a **spiral curve** as it traverses the material. The period of rotation will be $\dfrac{2\pi}{\eta_1}$, while the penetration length will correspond to $\frac{1}{\eta_2}$. Also, since $\eta_1 \propto \gamma$ hence we see a direct macroscopic effect of spin-orbit coupling. If $\gamma = 0$, rotation ceases and we're back to the usual meissner effect. From here, we can assert that γ is a measure of degree of non-centrosymmetricity of the model. The plot of $\vec{B}$ is shown by

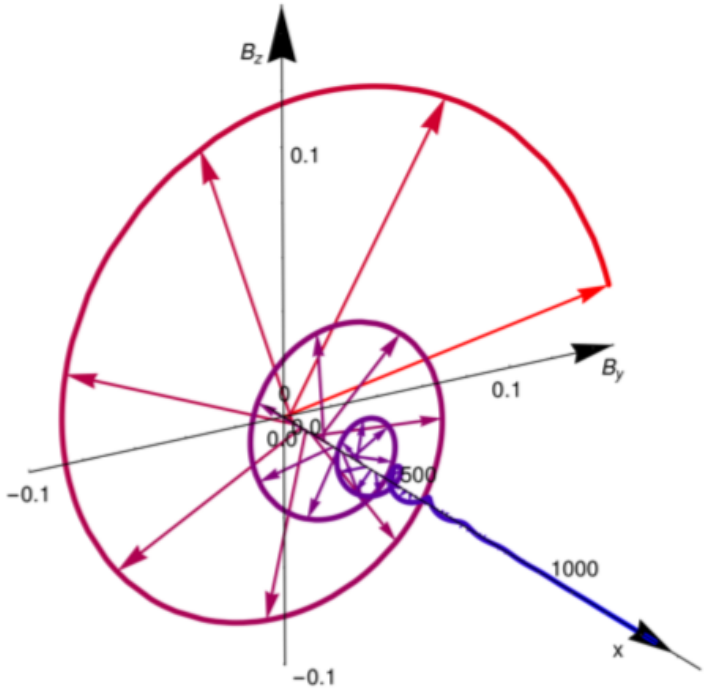

Figure 2.1: Decay of $\vec{B}$ inside the sample. Taken from [7]

2.5 Cross Over to Type 1 at high temperatures

The GL parameter for the theory reads

$$\frac{\lambda}{\xi} = \frac{\sqrt{2\kappa_c}}{\eta_2} = \kappa_c \frac{1 + \frac{2}{\kappa_c}(\gamma^2 + \nu^2)}{\sqrt{1 + \frac{2\nu^2}{\kappa_c}}} \tag{2.36}$$

We see (refer to the list of quantities on Appendix A) that $\frac{\gamma}{\nu}$ is temp independent, while both of them have strong temp dependence (with factors of $T^{3/4}$ in it). We also have $\gamma, \nu \propto \sqrt{|\alpha|}$ with $\frac{\gamma}{\nu} =$ *const*. This has two consequences:

- Near T_c, $\alpha \to 0$, hence $\kappa_{GL} = \kappa_c$
- As T is lowered, κ_{GL} increases. This means that if we started with a type 1 sample near T_c, at lower temperatures, the material can support vortices and turn type 2, provided non-centrosymmetricity (i.e. γ) is strong enough to achieve $\lambda > \xi$. This behaviour was reported in non-centrosymmetric superconductor AuBe[6].

2.6 Magnetic field inside a vortex

We first setup the equations for a single vortex. In order to do so, we need to solve (2.32) in the case of a single cortex placed at $x, y = (0, 0)$ (and assuming that it's translationally invariant along z-direction). In polar coordinates this leads to

$$\rho^2 f_{\rho\rho} + \rho f_\rho + \eta^2\rho^2 f + f_{\theta\theta} = 0 \tag{2.37}$$

This is solved by expanding in Hankel functions as

$$f = \sum_{j=-\infty}^{\infty} c_j e^{i\,j\theta}\mathcal{H}_j^{(1)}(\eta\rho) \tag{2.38}$$

We select hankel functions of 1st kind since they conform to $f(\rho \to \infty) \to 0$. To figure out the coefficients c_j, we match the RHS of (2.28) to get an equivalent condition

$$\boldsymbol{\nabla}^2 f + \eta^2 f = -2\pi\eta n\delta(x, y) \tag{2.39}$$

for a vortex with a phase winding n. This leads to

$$\boldsymbol{\nabla} \times \boldsymbol{\nabla}\phi = 2\pi n\hat{z}\delta(x, y) \;= n\hat{z}\boldsymbol{\nabla}^2 ln\rho \tag{2.40}$$

where the 2nd equality can be easily arrived by appealing to the same in 3D, where it well known from electrodynamics texts (for e.g. Griffiths). Since only $\mathcal{H}_0^{(1)} \to \frac{2i}{\pi} ln\,\rho,\; for \rho \to$

0, we discard c_j for $j \neq 0$. This leads to $\vec{B}$ given by

$$\vec{B} = Re\Big[\frac{i\pi}{2} n\eta \, (\eta\hat{z} - \hat{z} \times \boldsymbol{\nabla} f)\mathcal{H}_0^{(1)}(\eta\rho)\Big] \tag{2.41}$$

In polar coordinates, it leads to

$$\vec{B} = \; Re\Big[\frac{i\pi}{2} n\eta^2 \Big(0, \mathcal{H}_1^{(1)}, \mathcal{H}_0^{(1)}\Big)\Big] \tag{2.42}$$

If we take the limit $\rho \to \infty$, we find that $\mathcal{H}_1^{(1)} \to -i\mathcal{H}_0^{(1)} \propto \frac{e^{i\eta\rho}}{\sqrt{\rho}}$. This yields

$$\tilde{B} = \; B_z + iB_\theta \; \propto \frac{e^{i\eta\rho}}{\sqrt{\rho}} \tag{2.43}$$

hence a spiral like behaviour for magnetic field inside vortices too. Note that the period of the spiral will still be determined by $\eta_1 \propto \gamma$, hence SOC has the general feature of effecting spiral decay of magnetic field - both for vortices and for meissner state.
The plot for the same looks like

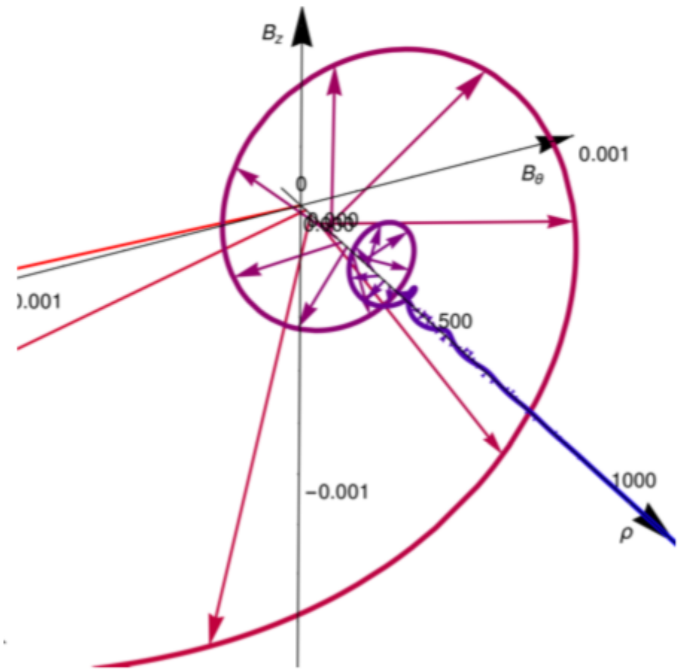

Figure 2.2: Spiral decay of the magnetic field inside a vortex. Taken from [7]

Using eqn(2.33), we can obtain the energy of a vortex $\mathcal{F}$ (note that this is gibbs free energy) as

$$\mathcal{F}_{vortex} = 2\pi n(nH_{c1} + H) \tag{2.44}$$

where H_{c1} is given by

$$H_{c1} = \frac{\tilde{\eta}_2}{\kappa_c}\Big[\eta_1\, arctan\frac{\eta_1}{\eta_2} + \eta_2\, ln\frac{2e^{-\gamma_{euler}}}{|\eta|\xi}\Big] \quad (2.45)$$

2.7 Intervortex interactions and bound states

One of the key results of the paper is the oscillatory nature of the interaction between vortices. Consider a set of vortices with cores at $\vec{r}_i$ with windings n_i respectively. Then (2.32) becomes

$$\boldsymbol{\nabla}^2 f + \eta^2 f = -2\pi\eta\sum_i n_i\delta(x - x_i, y - y_i) \equiv \eta\vec{\boldsymbol{\delta}} \quad (2.46)$$

which yields a simple solution from linearity as

$$f = \sum_i \frac{i\pi}{2}\eta n_i \mathcal{H}_0^{(1)}(\eta|\vec{r} - \vec{r}_i|) \quad (2.47)$$

Now we can extract the net energy of vortices by doing doing this integral, which is exactly calculable since it involves only δ functions. And now we subtract the initial energies of single vortices to get the net result, which is

$$U(R) \propto n_1 n_2 e^{-\eta_2 R} cos(\eta_1 R + \phi_0) \quad (2.48)$$

This shows that interactions are **non-monotonic** and hence the system will form vortex-vortex pairs, preferably at distances corresponding to local minima of U, appearing at periods of $\frac{2\pi}{\eta_1}$. The graph for the same is plotted below. Exact temperature dependence of U is due to other parameters like κ_C that appear in the expression (which brevity has been suppressed).
One way to get an intuitive idea of why such oscillatory behaviour can be expected is to recall that vortices feature a circularly polarized magnetic field (one that decays spirally). Hence when we superimpose two or more of these vortices, we get an interference pattern, formed at regular intervals of $\frac{2\pi}{\eta_1}$. The authors suggest[7] that this can lead to formation of vortex lattice with intervortex distance being at one of the minima.

2.8 Conclusions

This paper explores a model of NCS superconductors, starting from a microscopic hamiltonian. The Ginzburg-landau functional (positively defined in this case) is extracted from mean field approximation. Using that, we see the stark difference of behaviours from usual BCS superconductors in terms of magnetic field response. First of all, meissner effect is non-trivial due to presence of spin orbit coupling and shows a spiral decay. The same is

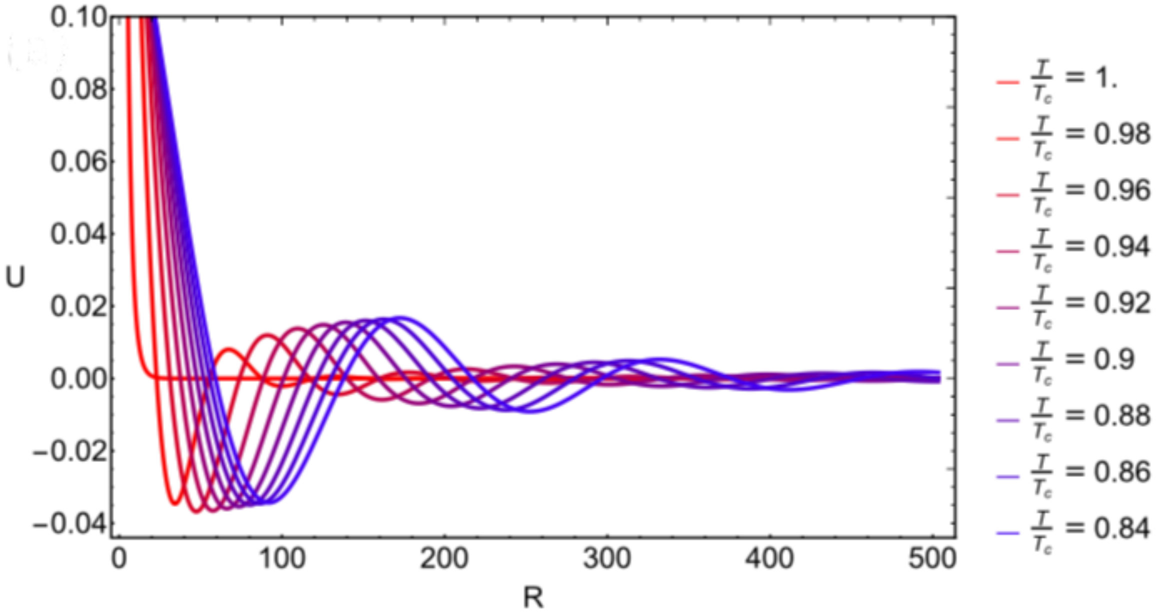

Figure 2.3: Intervortex interaction as a function of temperature. Taken from [7]

also observed for magnetic field of vortices. Finally, we see a non-monotonic behaviour of vortices, which can lead to bound states (vortex lattice) and also a cross-over to type 1 superconductors. We conclude this chapter by stating that this model also offers other behaviors like vortex-boundary interactions which we haven't considered here. We rest this discussion here and now focus on the fluctuational characteristics of NCS materials in the next chapter.

Chapter 3

Fluctuation studies

3.1 Introduction

In general theories of superconductivity, the notion of quasi-particles find a natural place: namely that the BCS problem is essentially an uncoupled problem of bogoliubons, vacuum of which is represented by the BCS ground state. BCS also utilised the idea of mean field theory, which is tantamount to the hubbard stratonovich transformation done in the previous chapter. However, it's almost natural to ask if one needs to consider fluctuations over MFT or quasiparticle description. The grand success of BCS theory lies in the fact that fluctuation corrections are negligible wrt MFT answers, thus rendering the approximation impeccable.

However, in materials like high temperature and organic superconductors or even lower dimensional superconducting systems, the observed phenomena are starkly different from those predicted by mean field ansatz(either by GL or BCS). The transition from normal to superconducting phase appears to be much more smeared out and precursor effects of the superconducting phase appear in the normal phase, even far from T_c. This is characterised by increase of specific heat, diamagnetic susceptibility, conductivity etc. in the vicinity of transition. Moreover, fluctuations have been shown to have dynamical consequences as well, with smearing of resistive transition in thin films detected experimentally(see the paragraph after eqn (10.1) in [5]). Inspired from these observations, this chapter tries to investigate the effect of fluctuation in NCS superconductors in the GL framework. Importantly, we're motivated to understand the role of spin orbit coupling in fluctuations. The basic paper that is followed is given by Larkin and Varlamov[5].

3.2 Fluctuation in superconductors

Fluctuation deals with cooper pairs that are out of the condensate. They differ from well-defined quasi-particles in a few ways

1. They have finite lifetime, inverse of which is of the order of their binding energy. The lifetime is given by

$$\tau_{GL} = \frac{\pi\hbar}{8k_B(T - T_c)} \tag{3.1}$$

τ diverges as T reaches T_c. This is has been derived from a microscopic theory for fluctuations(see relevant sections of the paper by Larkin and Varlamov). In contrast, for well-defined quasi-particles, the energy has to be much larger than it's inverse lifetime.

2. They have large size $\xi_{fluc}(T)$.
ξ_{fluc} is defined as the distance that the pairs travel/move during their lifetime τ_{GL}. The movement is estimated to be a free electron type (i.e. diffusive for dirty superconductors and ballistic in clean ones). For clean superconductors, ξ_{fluc} comes in the same order as ξ_{BCS}.

3. Treatment in **Rayleigh-Jeans sense**: Fluctuation pairs, instead of being Boltzmann particles, are rightly described by **classical fields**. Their distribution is mostly in the sense of BEC with lower moments

$$n(p) \;=\; \frac{1}{e^{E(p)\beta} - 1} \sim \frac{1}{\beta E(p)} \tag{3.2}$$

And GL gives us $E(p)$ near the critical point(quadratic). It can be shown that[5]

$$n_{s_{fluc}} \sim \xi_{fluc}^{-1} \tag{3.3}$$

This is different from BCS, where $n_s \sim \xi_{bcs}^{-2}$.

4. **Microscopic** vs **macroscopic** treatment of fluctuating copper pairs:
Contributions of the fluctuations have both microscopic (quantum) and macroscopic (like classical fields) effects. Quantum effects include quantum interference in the pairing process, renormalization of the density of one-electron states in the normal phase etc.
However, quantities like specific heat, diamagnetic susceptibility can be treated by direct cooper pair contributions and hence be treated in GL framework.

3.3 Fluctuation calculations for model hamiltonian

To perform these calculations, we take the form of GL outlined in eqn(2.21). This is has the form

$$F = \int d^3\overrightarrow{r} \left[\alpha\left|\psi\right|^2 + \sum_{a=\pm 1} K_a \left|\left(v_{aF} D^* - 2a\mu_B \overrightarrow{B}\right)\psi\right|^2 + \beta|\psi|^4\right] + \frac{1}{2}(\vec{B} - \vec{H})^2 \tag{3.4}$$

with the constants defined as (see appendix A for a complete list)

$$\alpha = N\ln\frac{T}{T_c}, K_a = 7\frac{\zeta\left(3\right)}{6\cdot\left(4\pi T\right)^2}\cdot N_a \tag{3.5}$$

$$\beta = \frac{7\zeta\left(3\right)}{\left(4\times\pi T\right)^2}N, N = \frac{N_+ + N_-}{2}, v_{aF} = E'(k_{aF}) + a\gamma_0 \tag{3.6}$$

3.4 Non-critical Fluctuations: Specific Heat

Now we calculate one of the simplest of observables, specific heat, using fluctuation theory. This will later be extended to the more experimentally relevant susceptibility calculation in the coming section.

3.4.1 Mean Field Jump

First calculating the mean field-jump discontinuity in C_v in case of $\vec{\mathbf{B}} = 0$.

$$F = \int dV\left[a\left|\varphi\right|^2 + \frac{b}{2}\cdot\left|\varphi\right|^4 + \gamma\left|\nabla\varphi\right|^2\right] \tag{3.7}$$

where a is same as α in the earlier equation. Let $\boldsymbol{2b = \beta, a_1 = N}$

$$\left|\varphi\right|^2 = -\frac{a}{b}, F = -\frac{a^2}{2b}V = -\frac{V}{2b}a_1^2\log^2\left(1+\epsilon\right) \tag{3.8}$$

This gives

$$C_V = \frac{-1}{VT_c}\cdot\frac{\partial^2 F}{\partial\varepsilon^2} = \frac{a_1^2}{2bT_c}\cdot\frac{\partial^2}{\partial\varepsilon^2}\cdot\log^2(1+\varepsilon) \tag{3.9}$$

$$= \left(\frac{a_1^2}{2bT_c}\right)\cdot\frac{\partial}{\partial\varepsilon}\cdot\left[2\cdot\log\left(1+\varepsilon\right)\cdot\frac{1}{1+\varepsilon}\right]\Big|_{\varepsilon=0} \tag{3.10}$$

$$\Rightarrow \mathit{\Delta} C_{mF} = \frac{a_1^2}{bT_c} \tag{3.11}$$

Note that till this is mean field solution, where we haven't included fluctuations (as can be seen from the standard GL expression in eqn(3.8)).

3.4.2 Fluctuation Contribution: $T > T_C$

Here mean field vanishes and only fluctuations contribute. We assume small fluctuations and neglect the quartic term for now. Also, we currently work in 3D. Now we have

$$F = \int dV \left[a \left|\overline{\psi}\right|^2 + \gamma \left(\nabla \overline{\psi}\right)^2 \right] \tag{3.12}$$

$$\overline{\psi} = \varphi_{mF} (0 = 0) + \varphi \tag{3.13}$$

$$F[\varphi] = \int dV \left[a \left|\varphi\right|^2 + \gamma \cdot \left|\nabla \varphi\right|^2 \right] \tag{3.14}$$

$$\Rightarrow F = -T_c \sum_{\vec{k}} \log \frac{\pi T_c}{a_1 \log(1+\varepsilon) + \gamma k^2} \tag{3.15}$$

where $\epsilon = \frac{T - T_c}{T_c}$ (reduced temperature, assumed small here for near T_c analysis).
Note: In doing the above functional integral, we didn't employ saddle point estimation to find free energy. This is simply because the saddle point contribution is already accounted for in the mean field ($\phi_{mF} = 0$), while we consider only fluctuations over this mean field (average of which is the mean field value). Hence, in fluctuation theory, one takes into account **all** possible fluctuations, without extremising $\mathcal{F}$.
Computing C_V we have

$$\delta C_+ = \frac{-1}{VT_c} \cdot \frac{\partial^2 F}{\partial \varepsilon^2} = \frac{-1}{VT_c} \cdot \frac{\partial^2}{\partial \varepsilon^2} \times \left[-T_c \sum_{\vec{k}} log \frac{\pi T_c}{a_1 \log(1+\varepsilon) + \gamma k^2} \right] \tag{3.16}$$

$$\Rightarrow \delta C_+ = \sum_{\vec{k}} \frac{a_1}{V} times \frac{1}{(1+\varepsilon)^2} \left[\frac{1}{a_1 \log(1+\varepsilon) + \gamma k^2} + \frac{a_1}{(a_1 \log(1+\varepsilon) + \gamma k^2)^2} \right] \tag{3.17}$$

Here the 1st term diverges, while the second term is convergent.

For the 1st term we evaluate the integral to be

$$\sum_{\vec{k}} \frac{a_1}{(1+\varepsilon)^2} \times \frac{1}{V} \times \frac{1}{a_1 \cdot \log(1+\varepsilon) + \gamma k^2} \tag{3.18}$$

$$= \frac{a_1}{(1+\varepsilon)^2} \times \frac{1}{2 \cdot \pi^2} \times \left[\frac{k}{\gamma} - \frac{\sqrt{a_1 \log(1+\varepsilon)} \cdot \tan^{-1}\left(\sqrt{\frac{\gamma}{a}} k\right)}{\gamma^{1.5}} \right] \tag{3.19}$$

$$= tends\ to\ \rightarrow \infty, for\ k \in [(0, \infty)] \tag{3.20}$$

The first linear term in k is divergent for $k \to \infty$. To avoid that, we put $k_{max} = \frac{1}{\xi} \to 0$

as $\epsilon \to 0$. The validity of this ultraviolet cutoff is natural since GL works only for length-scales larger than ξ.

Therefore the 1st integral isn't singular for $|T - T_c| \ll 1$ (infact it just vanishes). Computing the second integral we have

$$\delta C_{+} \sim \int_0^\infty dk \frac{k^2 dk}{\left(\alpha \log\left(1+\varepsilon\right) + \gamma k^2\right)^2} \tag{3.21}$$

$$\Rightarrow \delta C = \frac{a_1^2}{2\pi^2} \cdot \left(\frac{\pi}{4}\right) \times \frac{1}{\sqrt{\alpha \cdot 1\eta\left(1+\varepsilon\right) \cdot \gamma^3}} \sim \frac{1}{\sqrt{\varepsilon}}, \varepsilon \to 0^+ \tag{3.22}$$

Comparing with [5], we see a similar fluctuation scaling for BCS materials as well. This is simply because $\gamma, \nu \propto \sqrt{-\alpha} \to 0$ near T_c, hence it behaves as usual superconductor. We confirm this by calculating the same below T_c.

3.4.3 Fluctuation Contribution for $T < T_C$

Similar to $T > T_C$ calculation, we perform the same manipulations here, keeping in mind to impose UV-cutoff as and when necessary.

$$F = a\psi^2 + \frac{b\psi^4}{2} + \frac{T}{2} \sum_{\vec{k}} \left(\log \frac{\pi T_c}{a + b\psi^2 + \gamma k^2} + \log \frac{\pi T_c}{3b\psi^2 + a + \gamma k^2} \right) \tag{3.23}$$

$$T < T_c, a\psi^2 + b = 0 \tag{3.24}$$

$$\Rightarrow F = a\psi^2 + \frac{b\psi^4}{2} + \frac{T}{2} \sum_{\vec{k}} \left[\log \frac{\pi T_c}{\gamma k^2} + \log \frac{\pi T_c}{2b\psi^2 + \gamma k^2} \right] \tag{3.25}$$

$$C = \frac{1}{VT_c} \cdot \frac{\partial^2 F}{\partial \varepsilon^2} = -\frac{1}{2V} \cdot \frac{\partial^2}{\partial \varepsilon^2} \sum_{\vec{k}} \log \frac{\pi T_c}{2b\psi^2 + \gamma k^2} \tag{3.26}$$

$$= \frac{1}{2V} \times \frac{\partial^2}{\partial \varepsilon^2} \sum_{\vec{k}} \log \frac{\pi T_c}{-2a\psi^2 + \gamma k^2} \tag{3.27}$$

$$= \frac{a_1}{V} \sum_{\vec{n}} \left(\frac{-1}{\left(1+\varepsilon\right)^2} \cdot \frac{1}{\left(\gamma k^2 - 2a\right)} + \frac{1}{1+\varepsilon} \cdot \frac{-1}{\left(\gamma k^2 - 2a\right)^2} \cdot \left(\frac{-2a_1}{1+\varepsilon}\right) \right) \tag{3.28}$$

Now the 1st integral is divergent while the 2nd one is convergent.
Similar to $T > T_C$ case, the 1st one will give non-singular contribution. So we calculate the 2nd term for singular behaviour

$$\delta C = \frac{a_1^2}{\pi^2} \int_0^\infty \frac{k^2 dk}{\left(\gamma k^2 - 2a\right)^2} = \frac{a_1^2}{2 \cdot \pi^2} \cdot \frac{\pi}{4} \cdot \frac{2}{\sqrt{-2a_1 ln\left(1+\varepsilon\right) \cdot \gamma^3}} \tag{3.29}$$

$$\Rightarrow \delta C_{-} = \frac{1}{\sqrt{|\varepsilon|}}, \varepsilon \to 0^- \tag{3.30}$$

Again similar power law scaling as BCS. This confirms the observation that near T_c, this model behaves like a BCS superconductor.

3.4.4 Ginzburg-Levanyuk No.

Specify the Ginzburg-Levanyuk no.(Gi) as the value of reduced temperature at which mean field jump to specific heat equals the contribution due to fluctuations.
This means

$$\Delta C_{Mean\ field} = \Delta C_{fluctuations} \tag{3.31}$$

$$\implies \frac{a_1^2}{bT_c} = \frac{a_1^2}{2\pi^2} \cdot \left(\frac{\pi}{4}\right) \times \frac{1}{\sqrt{\alpha \cdot 1\eta\,(1+Gi)\cdot\gamma^3}} \tag{3.32}$$

$$\implies \xi_{\varepsilon\,=\,Gi} = \sqrt{\frac{\gamma}{\alpha(Gi)}} = \frac{8\pi\gamma^2}{bT_C} \tag{3.33}$$

This puts a practical restriction on the application of fluctuation theory beyond the reduced temperatures set by Gi. This is because we've calculated the above quantities under the assumption that fluctuations are **small**, which isn't true near the critical point. Near the critical point, interactions between fluctuations (characterized by ϕ^4 term) become important and can be treated using methods of critical phenomena (using methods of renormalization group). We'll not delve into that, but shall present an easier alternative approximation scheme which was found to be in excellent agreement with experiments on Bi-Sb thin films (Grossman et al [3]).

3.5 Critical Fluctuations: HF Approximation

Following [3] to look at critical fluctuations, we use a self consistent Hartree Fock Approximation amounting to the replacement

$$|\Psi|^4 = 2 \cdot |\Psi|^2 < |\Psi|^2 > - < |\Psi|^2 >^2 \tag{3.34}$$

and then use this to determine $< |\Psi|^2 >$ self consistently. *Grossman* etal do this to observe specific heat that varies monotonically and reaches the jump value predicted from mean field theory. Proceeding the same way we see

$$F=\int d\overrightarrow{x}\left[\alpha\left|\psi\right|^{2}+\sum_{a=\pm1}\left(K_{a}v_{aF}^{2}\right)\cdot\left|\nabla\varphi\right|^{2}+\beta\left|\psi\right|^{4}\right] \tag{3.35}$$

$$\left|\psi\left(\overrightarrow{r}\right)\right|^{4}=2\cdot\left|\psi\left(\overrightarrow{r}\right)\right|^{2}\langle\left|\psi\right|^{2}\rangle-\langle(\psi)^{2}\rangle^{2} \tag{3.36}$$

$$\langle\left|\psi\right|^{2}\rangle=\eta \tag{3.37}$$

$$F=\int d\overrightarrow{x}\left[\left(a+2\beta\eta\right)\cdot\left|\psi\left(\overrightarrow{r}\right)\right|^{2}+\sum_{a=\pm1}K_{a}v_{aF}^{2}\left|\nabla\psi\left(\overrightarrow{r}\right)\right|\right]^{2} \tag{3.38}$$

$$\sum_{a=\pm1}K_{a}v_{aF}^{2}=\mathit{\Gamma}\ (define) \tag{3.39}$$

Thus HF approximation amounts to replacing $a\rightarrow a+2\eta\beta$. Now the self consistency becomes

$$\eta=\langle\left|\psi\right|^{2}\rangle=\frac{1}{V}\sum_{\overrightarrow{k}}\frac{k_{B}T}{a+2\beta\eta+\mathit{\Gamma}k^{2}} \tag{3.40}$$

$$\tag{3.41}$$

At $T=T_{c}\Rightarrow a_{c}+2\beta_{c}\eta_{c}=0$, therefore

$$\eta_{c}=\frac{1}{V}\sum_{\overrightarrow{k}}\frac{k_{B}T_{c}}{\mathit{\Gamma}k^{2}}=\int\frac{d^{3}k}{\left(2\cdot\pi\right)^{3}}\cdot\frac{k_{B}T_{c}}{\mathit{\Gamma}k^{2}}=\frac{1}{2\cdot\pi^{2}}\times\int_{0}^{k_{max}}dk\frac{k_{B}T_{c}}{\mathit{\Gamma}} \tag{3.42}$$

$$\tag{3.43}$$

Now we set $k_{max}=\frac{1}{\xi}$, selecting the minimum ξ to get a good approximation to the integral.
In[3], they set this to ξ_{0} (pippard's coherence length), however, since we're looking at a region where $|\epsilon|<Gi$, we put the minimum ξ as $\xi_{\varepsilon\,=\,Gi}$ (note that this is the fluctuation coherence length and not the BCS coherence length). This leads to

$$\Rightarrow\eta_{c}=\frac{1}{2\cdot\pi^{2}}\cdot\frac{k_{B}T_{c}}{\mathit{\Gamma}}\cdot\frac{1}{\xi_{Gi}} \tag{3.44}$$

3.5.1 Shift of Critical Temperature

We have the new T_C where $a_c + 2\beta_c\eta_c = 0$, which gives

$$a_c = -2\beta_c\eta_c = -2\beta_c \cdot \frac{1}{2\cdot\pi^2}\cdot\frac{k_BT_c}{\mathit{\Gamma}}\cdot\frac{1}{\xi_{Gi}} \tag{3.45}$$

$$\Rightarrow N\log\left(\frac{T_c}{T_c^0}\right) = -\frac{\beta_c}{\pi^2}\cdot\frac{k_BT_c}{\mathit{\Gamma}}\cdot\frac{1}{\xi_{Gi}} \tag{3.46}$$

$$\Longrightarrow T_c = T_c^0\cdot exp(\frac{-\beta_c}{\pi^2}\cdot\frac{k_BT_c}{\mathit{\Gamma}}\cdot\frac{1}{N\xi_{Gi}}) \tag{3.47}$$

3.5.2 C_v in $|\varepsilon| \ll Gi$ region

With F defined eqn.(3.38), we compute the free energy similarly to non-critical cases as

$$F = -T_c\sum_{\vec{k}}\log\frac{\pi T_c}{(\alpha+2\beta\eta)+\gamma k^2} \tag{3.48}$$

Now proceeding similarly, we can calculate $C_V \sim \dfrac{\partial^2 F}{\partial\varepsilon^2}$ for which we'd require knowledge of $\frac{\partial\eta}{\partial\varepsilon}$ - This has to be calculated using eqn(3.40). A series expansion can be done in ϵ for the same. However since we know that in 3D, Gi is quite small for BCS and this model essentially behaves like BCS near T_c, the correction due to fluctuation is small. Therefore, we leave the computation of the same for the time being and focus on the more interesting observable: Diamagnetic susceptibility.

3.6 Fluctuation Diamagnetism

Since fluctuation induced diamagnetism eventually leads to meissner effect as we reduce the temperature, we can expect it to be small wrt diamagnetic susceptibility of a superconductor. However, it can be comparable or even exceed the value of diamagnetic/paramagnetic susceptibility of a normal metal (see equation 10.58 in [5]). It can be shown, using langevin formula for diamagnetic susceptibility, that the fluctuation correction can be of the order of pauli paramagnetism (but opposite in sign). Hence, we expect that investigating this observable in presence of spin orbit coupling might show an interesting response.

For calculations on BCS superconductors, the reader if referred to [5] section 10.2.4.

3.6.1 Calculation for the model hamiltonian

This section follows the idea outlined in [5] - section 10.2.4, "GL Treatment of Fluctuation Magnetization".

GL free energy as derived in (2.21)

$$F=\int d^3\overrightarrow{r}\left[\alpha\left|\psi\right|^2+\sum_{a=\pm1}K_a\left|\left(v_{aF}D^*-2a\mu_B\overrightarrow{B}\right)\psi\right|^2\right]+\frac{1}{2}(\vec{B}-\vec{H})^2 \tag{3.49}$$

For weak magnetic field and non-critical fluctuations, we neglect the last term (assuming fluctuations are small enough to allow $\vec{B}\sim\vec{H}$).
Expanding the term in the bracket we have a new form

$$\sum_{a=\pm1}K_a\left(v_{aF}^2\left|D\psi\right|^2-2\mu_B\left[a\cdot v_{aF}\right]\overrightarrow{B}\left[\psi^*D^*\psi+\psi D\psi^*\right]+4\mu_B^2B^2\left|\psi\right|^2\right)$$

With

$$D=-i\nabla-2\cdot e\overrightarrow{A}$$

Rewriting the free energy we have

$$F=\int d^3\overrightarrow{r}\left[\left(\alpha+4\mu_B^2B^2\sum_{a=\pm1}K_a\right)\cdot\left|\psi\right|^2+\left(\sum_{a=\pm1}K_av_{aF}^2\right)\cdot\left|D\psi\right|^2-2\mu_B\left(\sum_{a=\pm1}K_aav_{aF}\right)\overrightarrow{B}\cdot\overrightarrow{j}\right]$$
$$\overrightarrow{j}=\psi^*D^*\psi+\psi D\psi^*$$

We, for the time being, ignore the contribution of B^2 to α in the 1st term for weak field B. Also, we take the magnetic field to be along $\hat{z}$ i.e. $\vec{B}=B_0\hat{z}$. Thus free energy is kept explicitly linear in B at the GL level.

$$\overrightarrow{j}\cdot\overrightarrow{B}=j_zB_z=B_0j_z=B_0\left[\psi^*\cdot\left(i\partial_z\right)\psi+\psi\left(-i\partial_z\right)\psi^*\right]$$

Redefining quantities, we have

$$a=\left(\alpha+4\mu_B^2B^2\sum k_a\right)\sim\alpha$$
$$\gamma=2\mu_B\sum_{a=\pm1}K_aav_{aF}$$
$$\delta=\sum K_av_{aF}^2$$

$$F=\int d^3\overrightarrow{r}\left[a\left|\psi\right|^2-\gamma\cdot\overrightarrow{j}\cdot\overrightarrow{B}+\delta\cdot\left|D\psi\right|^2\right] \tag{3.50}$$

This gives us the GL length-scale

$$\xi^2 = \frac{\delta}{|\alpha|} \tag{3.51}$$

Comment: $\xi \rightarrow 0$ at T$\rightarrow 0\ K$.

We expand ψ in terms of the landau levels and choose a gauge s.t. $A_z = 0$.

$$\psi = \sum_{\eta,k} \phi_\eta \left(\overrightarrow{r}\right) \cdot e^{ikz} \cdot c_{\eta,k}$$
$$\phi_\eta \left(\overrightarrow{r}\right) = \phi_m \left(x - x_0\right) \exp\left[ik_y y\right]$$
$$\eta = \left(m, k_y\right)$$

This makes the free energy $F[\psi]$ as

$$\Rightarrow F\left[\psi\right] = \sum_{\eta,k} \left[a + 2kB_0\gamma + \delta.2M \cdot E\left(\eta,k\right)\right] \cdot \left|c_{\eta,k}\right|^2 \tag{3.52}$$

where

$$E\left(\eta,k\right) = \hbar\omega_c \left[m + \frac{1}{2}\right] + \frac{k^2}{2M} \tag{3.53}$$
$$\overrightarrow{j} \cdot \overrightarrow{B} \rightarrow -2kB_0 \tag{3.54}$$

where $\omega_c = = \frac{2eB}{M}$. We evaluate this sum to be

$$Z = \int D\left(\psi\right) \cdot e^{-\beta F[\psi]} \tag{3.55}$$
$$\Rightarrow F = -T \sum_{\eta,k} \log \frac{\pi T}{a + 2kB_0\gamma + \delta.2M \cdot E\left(\eta,k\right)} \tag{3.56}$$
$$\Rightarrow F = -T \sum_{m,k_y,k} log \frac{\pi T}{a + 2kB_0\gamma + \delta \cdot 2M \cdot \left[\hbar\omega_c \left(m + \frac{1}{2}\right) + \frac{k^2}{2M}\right]} \tag{3.57}$$
$$\Rightarrow F = -T \times \frac{SB}{\Phi_0} \sum_{m,k} \log \frac{\pi T}{a + 2kB\gamma + \delta.2M \cdot \left[\omega_c \left(m + \frac{1}{2}\right) + \frac{k^2}{2M}\right]} \tag{3.58}$$

This sum is divergent.
Cause of divergence is the physical inapplicability of GL theory at shortwavelength fluctuations. To bypass this, we put k_{max} and n_{max} cutoffs defined by

$$
\begin{aligned}
&k_{\max}^2 \sim \xi^{-2} \sim \frac{a}{\delta} \sim \frac{N \cdot \left(\ln \frac{T}{T_c}\right)}{\delta} \sim \frac{N \cdot \ln(1+\varepsilon)}{\delta} \\
&\varepsilon = \frac{T - T_c}{T_c}
\end{aligned}
$$

In this model, $\alpha = \ N\ ln\ (\frac{T}{T_c})$. For the m-cutoff, we have

$$
\begin{aligned}
m\omega_c &\sim \frac{k^2}{2M} \sim \frac{\xi^{-2}}{2M} \\
\implies m_{\max} &\sim \frac{\xi^{-2}}{2M\omega_c}, \omega_c = \frac{2eB}{M} = \frac{2B}{M\phi_0} \\
&\sim \frac{a}{\delta} \times \frac{1}{2 \times \frac{2B}{\Phi_0}} \\
&\sim \frac{a\Phi_0}{4B\delta}
\end{aligned}
$$

The sum highlighted in (3.58) should then be used to calculate the 0 field susceptibility $\chi\,(\vec{B} = 0)$.

Note: In what follows, a factor of 2 has been absorbed making 2e $\equiv$ e. However, this doesn't change the qualitative results, since from what follows, we can rescale $e \to 2e$ in the final expression to get the exact answer.

A similar expression for the conventional bcs superconductor (i.e. with $\gamma, \nu = 0$) was worked out in [8]. We reformulate the same approach for this by using eq (8) highlighted in their calculation.

This amounts to redefination as follows:

$$A\,(B, k) = a + 2kB\gamma + \delta k^2 \tag{3.59}$$

$$= a - \frac{B^2\gamma^2}{\delta} + (K')^2 = A'(B, k) \tag{3.60}$$

$$K' = k\sqrt{\delta} + \frac{B\gamma}{\sqrt{\delta}} \tag{3.61}$$

Note that this changes just the k-summation by a factor $\sqrt{\delta}$, leaving the rest of the calculation same. With this, the approximation used in [8] eqn(9) gets modified for our case to become

$$\frac{\left(a - \frac{B^2\gamma^2}{\delta}\right) \cdot \pi}{B\delta e} \gg 1 \implies \frac{B^2\gamma^2}{\delta} + \frac{\delta Be}{\pi} \ll a \tag{3.62}$$

Now, proceeding similar to the same paper (i.e. [8]), the approximation produces

$$\mathcal{F}=\sum_k\left(-\frac{TS}{\Phi_0}\right)\int_0^\infty \log\frac{\pi k_BT}{A\left(B,k\right)+2Bet\delta}dt\cdot B+2\sum_{n=1}^{\infty}(-1)^n\cdot\left(\frac{-TS}{2\delta}\right)\sum_k\frac{\left(e\delta B\right)^2}{\left(n\pi\right)^2}\cdot\frac{1}{A\left(B,k\right)} \tag{3.63}$$

Now, we simplify the second term.

$$2\sum_{n=1}^{\infty}(-1)^n\cdot\left(\frac{-TS}{2\delta}\right)\sum_k\frac{\left(e\delta B\right)^2}{\left(n\pi\right)^2}\cdot\frac{1}{A\left(B,k\right)} \tag{3.64}$$

$$=\sum_k 2*\left(\frac{-TS}{2\delta}\right)*\frac{-\pi^2}{12}*\frac{1}{A\left(B,k\right)} \tag{3.65}$$

$$=\int\frac{dk}{2\pi}\frac{T\delta Se^2}{12}B^2\int\limits_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{1}{A(B,k)} \tag{3.66}$$

$$=\frac{T\delta Se^2}{12}B^2*\frac{\pi}{\sqrt{\delta}}\left[\frac{1}{\sqrt{a}}+\frac{1}{2}\frac{B^2\gamma^2}{\delta a^{1.5}}+....\right] \tag{3.67}$$

where we use the integral

$$\int\limits_{-\infty}^{\infty}\frac{dk}{2\pi}\;\frac{1}{a+\delta k^2+2Bk\gamma}\;=\frac{1}{\sqrt{\delta}}\frac{\pi}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}} \tag{3.68}$$

$$=\frac{\pi}{\sqrt{\delta}}\left[\frac{1}{\sqrt{a}}+\frac{1}{2}\frac{B^2\gamma^2}{\delta a^{1.5}}+....\right] \tag{3.69}$$

where we could expand it in a power series in lieu of (3.62) i.e. in powers of $\frac{B^2\gamma^2}{a\delta}$(since $\delta>0$, we can proceed with it's use).
For the 1st term, we have In doing sum over m, the first term in eqn(**??**) is given by

$$\sum_k\left(-\frac{TS}{\Phi_0}\right)\int_0^\infty\log\frac{\pi k_BT}{A\left(B,k\right)+2Bet\delta}dt\cdot B$$
$$=\sum_k-\frac{TS}{2\delta}\int_0^\infty\log\frac{\pi k_BT}{A\left(B,k\right)+\dfrac{2B\delta t}{\Phi_0}}\cdot\frac{2B}{\Phi_0}dt\delta$$
$$=-\frac{TS}{2\delta}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_0^\infty\log\frac{\pi k_BT}{A\left(B,k\right)+z}dz$$

where

$$A(B,k)=\;a+2kB\gamma+\delta k^2$$

This is a divergent integral, hence we leave it as such, although later we'll use to compute χ. A point to note is that setting $\gamma=0$ here will make the whole integral independent of B, hence for χ calculation, it can be skipped without loss of generality (this is precisely what happens in BCS). However, for this case, we need to retain it.

Collecting all terms together, we have

$$F = \frac{T\delta Se^2}{12}B^2 * \frac{\pi}{\sqrt{\delta}}\left[\frac{1}{\sqrt{a}} + \frac{1}{2}\frac{B^2\gamma^2}{\delta a^{1.5}} + ...\right] - \frac{TS}{2\delta}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_0^{\infty}\log\frac{\pi k_B T}{A\,(B,k)+z}dz \quad (3.70)$$

There are some comments we can make here:

1. The same formula for BCS superconductors has the form

$$F = F^{(0))} + \frac{1}{2}\frac{V}{6\pi}(\frac{e}{\bar{h}c})^2 T\xi_{GL}B^2 \quad (3.71)$$

   which, when compared to the 1st term, shows that we get the same form as BCS plus a contribution due to ASOC in form of B^4 term in $\mathcal{F}$ (without considering the 2nd term).

2. The eqn(3.70) looks faulty, since it features $\frac{1}{a^t}$ for increasing t, which near T_c, should blow more and more strongly as $a \to 0$. However, the result is only valid if $\frac{B^2\gamma^2}{a\delta} \ll 1$, which is a subset of the general condition mentioned in (3.62), hence both $\frac{B^2\gamma^2}{a}$ is always $\lll 1$.

To calculate susceptibility, we need to evaluate the 2nd term first. Proceeding, we have

$$-\chi = \frac{\partial^2 F_{2nd\,term}}{\partial B^2} = \frac{-TS}{2\delta}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_0^{\infty}dz\frac{4k^2\gamma^2}{(a+2Bk\gamma+\delta k^2+z)^2} \quad (3.72)$$

$$= \frac{-TS\gamma^2}{\pi\delta}\frac{1}{\delta^{1.5}}\int_{-\infty}^{\infty}\left(K' - \frac{B\gamma}{\sqrt{\delta}}\right)^2\frac{dK'}{K'^2 + (a - \frac{B^2\gamma^2}{\delta})} \quad (3.73)$$

where $\mathbf{K'} := \sqrt{\delta}k + \frac{B\gamma}{\sqrt{\delta}}$, $\mathbf{K'}\ \varepsilon\ [\frac{-\sqrt{\delta}}{\xi} + \frac{B\gamma}{\sqrt{\delta}}, \frac{\sqrt{\delta}}{\xi} + \frac{B\gamma}{\sqrt{\delta}}]$. Proceeding we have

$$= \frac{-TS\gamma^2}{\pi}\frac{1}{\delta^{2.5}}\left\{\frac{B^2\gamma^2}{\delta}\pi\frac{1}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}} + 2\xi^{-1} - 2\sqrt{a-\frac{B^2\gamma^2}{\delta}}\,tan^{-1}\Big(\frac{\xi^{-1}}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}}\Big)\right\} \quad (3.74)$$

$$\implies \chi = \frac{TS\gamma^2}{\pi}\frac{1}{\delta^{2.5}}\Bigg\{\frac{B^2\gamma^2}{\delta}\pi\frac{1}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}} + 2\frac{\sqrt{\delta}}{\xi} + \sqrt{a-\frac{B^2\gamma^2}{\delta}}\,tan^{-1}\Big(\frac{\frac{-\sqrt{\delta}}{\xi}+\frac{B\gamma}{\sqrt{\delta}}}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}}\Big) \quad (3.75)$$

$$-\sqrt{a-\frac{B^2\gamma^2}{\delta}}\,tan^{-1}\Big(\frac{\frac{\sqrt{\delta}}{\xi}+\frac{B\gamma}{\sqrt{\delta}}}{\sqrt{a-\frac{B^2\gamma^2}{\delta}}}\Big)\Bigg\} \quad (3.76)$$

where we employed the cutoffs for $\mathbf{K'}$ in the last integral.

Since tan^{-1} is a bounded function, we don't get any divergence for small 'a' from the last two terms. To leading order of B, γ (we're trying to look at susceptibility for small field i.e. essentially 0 field susceptibility), the susceptibility behaves as

$$\chi \sim c1 * \gamma^2 + c2 * \frac{B^2\gamma^4}{\sqrt{a}} + ... \tag{3.77}$$

where c1,c2 are constants. This is what we get from (3.76).

Now we can subsequently calculate χ from (3.70) to get a complete expression. We notice that SOC leads to a B^2 dependence of χ_{net} with coefficient proportional to γ^2 at the lowest order. There's also a $\chi \sim \frac{\gamma^2}{\xi}$ dependence, which might be relevant.
Calculation of the same yields

$$\chi = \frac{-T\delta S e^2}{12} * \frac{\pi}{\sqrt{\delta}}\left[2\frac{1}{\sqrt{a}} + \frac{6B^2\gamma^2}{\delta a^{1.5}} + ...\right] + c1 * \gamma^2 + c2 * \frac{B^2\gamma^4}{\sqrt{a}} + ... \tag{3.78}$$

where $c_2 = \frac{TSB^2}{\delta^{3.5}}\frac{1}{\sqrt{a - \frac{B^2\gamma^2}{\delta}}}$, and c_1 can similarly be read off by from (3.76). Barring the exact nature of constants, we see that the functional dependence of χ becomes non-linear once spin orbit coupling is allowed. However, addition of such doesn't alter the temperature dependence of χ and hence it gives the same dependence as BCS in the $\gamma \to 0$ asymptotic limit. Moreover, it should be clarified that χ can depend on B^2 even in absence of γ as remarked in [8]. This however, isn't obtained under GL framework and requires use of diagrammatic techniques.

Chapter 4

Conclusion

In this report we've managed to get a brief idea of the relation between superconductivity and crystal symmetry. As we saw in chapter 2, a inversion asymmetric crystal shows unconventional magneto-response with spiral decay in meissner state and shows vortex bound states. Moreover, solutions worked out in the paper were non-perturbative (employing only London approximation) and hence present this behaviour at a dominant level. Spin orbit coupling is manifestly observed in the handedness of the spiral and NCS superconductors feature a strong temperature dependence in their magnetic response. Crossover to type 1 superconductivity is also expected at high temperatures, which is definitely a beyond standard Ginzburg-Landau phenomenon.
Next we study the effect of thermal fluctuations in these systems. We find that while the fluctuational specific heat features the same temperature dependence as standard BCS, diamagnetic susceptibility has a non-linear contribution on B coming from the spin orbit coupling strength. Along with this, we also calculate other quantities like Ginzburg-levanyuk no. and shift of critical temperature. At this point, we rest our current line of investigation, which was primarily to look for interesting consequences of spin-orbit coupling at the level of Ginzburg landau framework. Our future direction involves trying to look at topological superconductors and see if insights gained from this study might be useful to study properties related to vortices, magneto-response etc in that domain.

This project was envisaged by my advisor Dr. Alexander Zyuzin, who helped me throughout the course of several months with constant and sincere support. I am indebted to him for his guidance and for allowing me to pursue my own chain of investigation, whenever I felt the urge to do so. Also, I would also like to thank my co-guide Prof. Sumiran Pujari for his help during this project. Discussions with him greatly motivated me to simplify several aspects of superconductivity and revise my standings on several other topics.

Appendices

Appendix A

List of quantities

1. $D = -i\nabla - 2 \cdot e\overrightarrow{A}$: The gauge invariant derivative
2. $v^2 = -\alpha K_+ K_- \left(\sum_{a=\pm1} v_{aF}\right)^2 4\mu_B^2 \kappa_c^2 \cdot \left(\frac{2 \cdot e}{\beta}\right)^{\frac{3}{2}} = -\alpha . v_1^2$: Arises due to zeeman coupling to the magnetic field
3. $\alpha = N \ln \frac{T}{T_c}$: The coefficient in front of the GL functional for NCS superconductors. Its sign determines the stable minima of F, hence the configuration of the order parameter.
4. $K_a = 7\frac{\zeta(3)}{6 \cdot (4\pi T)^2} \cdot N_a$: N_a is the density of states at fermi level in one of the ASOC split band with dispersion relation as $\frac{k^2}{2m} + a \cdot \gamma k,\ a = \pm 1$.
5. $N = \frac{N_+ + N_-}{2}$: Avg of dos at E_{aF} of each ASOC split band
6. $\beta = \frac{7\zeta(3)}{(4\pi T)^2} N$
7. $T_c = 2e^{\gamma_{euler}} \omega_D \frac{e^{\left(\frac{-1}{NV}\right)}}{\pi}$: Transition temperature of the superconducting phase in the model
8. $\beta = 7\frac{\zeta(3)}{(4\pi T)^2} N$
9. $\kappa_c = \sqrt{\frac{\beta}{2e^2}} \frac{1}{\sum\limits_{a=\pm1} K_a v_{aF}^2}$: Not to be confused with GL parameter. However, near T_c, the superconductor behaves like a material with GL parameter κ_C.
10. v_{aF} = fermi velocity at each spin orbit split band (i.e. $a = \pm 1$ represents each of the bands).

Bibliography

[1] E. Bauer et al. "Heavy Fermion Superconductivity and Magnetic Order in Noncentrosymmetric $CePt_3Si$". In: *Phys. Rev. Lett.* 92 (2 Jan. 2004), p. 027003. DOI: 10.1103/PhysRevLett.92.027003. URL: https://link.aps.org/doi/10.1103/PhysRevLett.92.027003.

[2] Ernst Bauer and Manfred Sigrist. *Non-centrosymmetric superconductors: introduction and overview*. Vol. 847. Springer Science & Business Media, 2012.

[3] S Grossmann, PH Richter, and C Wissel. "Self consistent theory of fluctuations near D-dimensional superconducting phase transitions". In: *Solid State Communications* 11.3 (1972), pp. 433–436.

[4] A Yu Kitaev. "Unpaired Majorana fermions in quantum wires". In: *Physics-Uspekhi* 44.10S (Oct. 2001), pp. 131–136. ISSN: 1468-4780. DOI: 10.1070/1063-7869/44/10s/s29. URL: http://dx.doi.org/10.1070/1063-7869/44/10S/S29.

[5] AI Larkin and AA Varlamov. "Fluctuation phenomena in superconductors". In: *Superconductivity*. Springer, 2008, pp. 369–458.

[6] Drew J. Rebar et al. "Fermi surface, possible unconventional fermions, and unusually robust resistive critical fields in the chiral-structured superconductor AuBe". In:

Phys. Rev. B 99 (9 Mar. 2019), p. 094517. DOI: 10.1103/PhysRevB.99.094517. URL: https://link.aps.org/doi/10.1103/PhysRevB.99.094517.

[7] Albert Samoilenka and Egor Babaev. “Spiral magnetic field and bound states of vortices in noncentrosymmetric superconductors”. In: *Physical Review B* 102.18 (2020), p. 184517.

[8] Albert Schmid. “Diamagnetic Susceptibility at the Transition to the Superconducting State”. In: *Phys. Rev.* 180 (2 Apr. 1969), pp. 527–529. DOI: 10.1103/PhysRev.180.527. URL: https://link.aps.org/doi/10.1103/PhysRev.180.527.

[9] M Smidman et al. “Superconductivity and spin–orbit coupling in non-centrosymmetric materials: a review”. In: *Reports on Progress in Physics* 80.3 (Jan. 2017), p. 036501. ISSN: 1361-6633. DOI: 10.1088/1361-6633/80/3/036501. URL: http://dx.doi.org/10.1088/1361-6633/80/3/036501.

URKUND

Document Information

Analyzed document	170260025.pdf (D90001279)
Submitted	12/18/2020 8:07:00 AM
Submitted by	Guru Kalyan Jayasingh
Submitter email	guru.k@iitb.ac.in
Similarity	2%
Analysis address	journals.iitb@analysis.urkund.com

Sources included in the report

SA	**Licentiate-2.pdf** Document Licentiate-2.pdf (D32165114)	2
W	URL: https://www.vibgyorpublishers.org/content/ijope/ijope-2-006.xml Fetched: 12/18/2020 8:08:00 AM	1
SA	**DanielFinalReport.pdf** Document DanielFinalReport.pdf (D53948358)	3