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Topologically non-trivial superconductivity in spin–orbit-coupled systems: bulk phases and quantum phase transitions

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Abstract. Topologically non-trivial superconductivity has been predicted to occur in superconductors with a sizable spin–orbit (SO) coupling in the presence of an external Zeeman splitting. Two such systems have been proposed: (a) s-wave superconductor pair potential is proximity induced on a semiconductor and (b) pair potential naturally arises from an intrinsic s-wave pairing interaction. As it is now well known, such systems in the form of a two-dimensional (2D) film or 1D nano-wires in a wire network can be used in topological quantum computation. When the external Zeeman splitting Γ crosses a critical value Γ_c, the system passes from a regular superconducting phase to a non-Abelian topological superconducting phase. In both cases (a) and (b) that we consider in this paper, the pair potential Δ is strictly s-wave in both the ordinary and the topological superconducting phases, which are separated by a topological quantum critical point at $\Gamma_c = \sqrt{\Delta^2 + \mu^2}$, where μ ($\gg \Delta$) is the chemical potential. On the other hand, since $\Gamma_c \gg \Delta$, the Zeeman splitting required for the topological phase ($\Gamma > \Gamma_c$) far exceeds the value ($\Gamma \sim \Delta$) above which an s-wave pair potential is expected to vanish (and the system to become non-superconducting) in the absence of SO coupling. We are thus led to the situation that the topological superconducting phase appears to set in a parameter

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regime at which the system is actually non-superconducting in the absence of SO coupling. In this paper, we address the question of how a pure s-wave pair potential can survive a strong Zeeman field to give rise to a topological superconducting phase. We show that the SO coupling is the crucial parameter for the quantum transition into and the robustness of the topologically non-trivial superconducting phase realized for $\Gamma \gg \Delta$.

Contents

1. Introduction

Recently, topologically non-trivial superconductivity has been theoretically predicted to occur in two classes of systems with spin–orbit (SO) coupling. These are: (a) SO coupled semiconductors in which s-wave superconducting pair potential is induced by the proximity effect [1–3] and (b) SO coupled systems with superconductivity due to intrinsic s-wave pairing interaction [4, 5]. A third system—the surface of a three-dimensional (3D) strong topological insulator (TI)—can also support topological superconductivity when the latter is proximity induced [6]. In this paper, we will ignore the latter and concentrate only on (a) and (b). In both classes (a) and (b), the SO coupling is a consequence of the breakdown of the structural space inversion (SI) symmetry. We will take the resultant SO coupling to be of the Rashba type. A system in class (a) can be artificially grown as a heterostructure consisting of an SO coupled semiconductor in proximity contact with an s-wave superconductor [3]. An example of class (b) is a non-centrosymmetric superconductor [7] or an s-wave Feshbach resonant system with an accompanying SO coupling and Zeeman splitting both of which can be created in a cold fermion atomic system [8, 9]. There is also another class (class (c)) of topological superconductors with non-Abelian statistics, which have been studied extensively in recent literature. Here, the topological nature arises entirely from intrinsic chiral p-wave superconductivity without having any underlying s-wave superconductivity in the system. Some examples of class (c) are the even-denominator 5/2 fractional quantum Hall effect [10], superconducting strontium ruthenate [11], A-phase of superfluid He-3 [12] and superfluid ultracold fermionic gases based directly on the p-wave Feshbach resonance [13]. These class (c) non-Abelain superconductors are effectively

equivalent to being spinless, i.e. completely spin polarized, and are therefore immune to any Zeeman splitting to the leading order. We do not discuss the class (c) systems in this paper, since the main conceptual issue being addressed in this paper does not apply to these systems.

The topologically non-trivial superconducting systems mentioned above are characterized by order parameter defects, such as a vortex and a sample edge, which carry a unique bound state at zero excitation energy [14]. These bound zero energy modes, called Majorana fermion modes after E Majorana [15], can actually be thought of as particles that are their own anti-particles [16]. In other words, they are represented by second quantized operators γ which satisfy the hermiticity condition $\gamma^\dagger = \gamma$. This is strikingly different from the regular fermionic modes for which the second quantized operators $c^\dagger \neq c$. Because of the existence of the zero-energy Majorana modes, a 2D non-Abelian topological superconductor with $2N$ vortices each carrying a single Majorana mode constitutes a system with a 2^N-fold ground state degeneracy protected by an excitation gap [17]. When a Majorana fermion mode in a given order parameter defect is adiabatically moved (braided) around another Majorana mode, the initial state transforms into another one that is a different linear combination in the same ground state manifold. These unitary transformations within the ground state manifold are manifestations of the non-Abelian statistics of the Majorana fermions. The non-Abelian statistics of the Majorana fermions has recently come under intense focus because of its potential application in fault-tolerant topological quantum computation (TQC) [18, 19]. Both the 2D SO coupled superconducting film and its 1D version as quantum nanowires in a wire network have been proposed as potential platforms for TQC [1, 20–26]. In this paper, we will not discuss the Majorana fermion modes or their potential application to TQC. Instead we will focus on the bulk superconducting phases and the quantum phase transitions (QPTs) by exploring the interplay among the SO coupling, Zeeman splitting and the s-wave pairing interactions.

Both systems in classes (a) and (b) are in an ordinary (non-topological) superconducting phase in the absence of an externally imposed Zeeman splitting. The Zeeman splitting, which can be applied either by a parallel magnetic field [27] or by the proximity effect of a nearby magnetic insulator [1–3], creates a gap between the two SO bands as shown in figure 1. From mean-field calculations [1, 3], it is clear that when such a Zeeman splitting Γ crosses a critical value, $\Gamma_c = \sqrt{\Delta^2 + \mu^2}$, where Δ is the s-wave superconducting pair potential and μ is the chemical potential, the system makes a transition to a topological non-Abelian superconducting phase. The critical Zeeman splitting corresponds to the value at which the underlying Fermi surface in the absence of superconductivity shifts from being at both SO bands to occupying only the lower SO band (figure 1). Thus, at this value of the Zeeman splitting, the underlying system changes from having two Fermi surfaces (one in each band) to having just one.

Since μ usually far exceeds Δ, the critical value of the Zeeman splitting Γ_c also far exceeds Δ. Therefore, in the absence of SO coupling, Γ_c far exceeds the Zeeman splitting ($\Gamma \sim \Delta$) above which an s-wave pair potential should decay to zero. The loss of an s-wave pair potential due to a strong Zeeman splitting is due to the fact that for $\Gamma \gtrsim \Delta$ the formation of a spin–singlet pair potential with zero net momentum is impossible (for the discussion of topological phase transition induced by Zeeman splitting we will ignore the states with non-zero values of the Cooper pair momentum). Now let us emphasize the fact that in both the cases we consider in this paper (the superconducting pair potential that is proximity induced and the superconducting pair potential due to an intrinsic on-site pairing interaction), the pair potential is strictly s-wave in both the ordinary and the topologically non-trivial superconducting phases. The fact that the pair potential is s-wave when it is proximity induced from an s-wave superconductor is

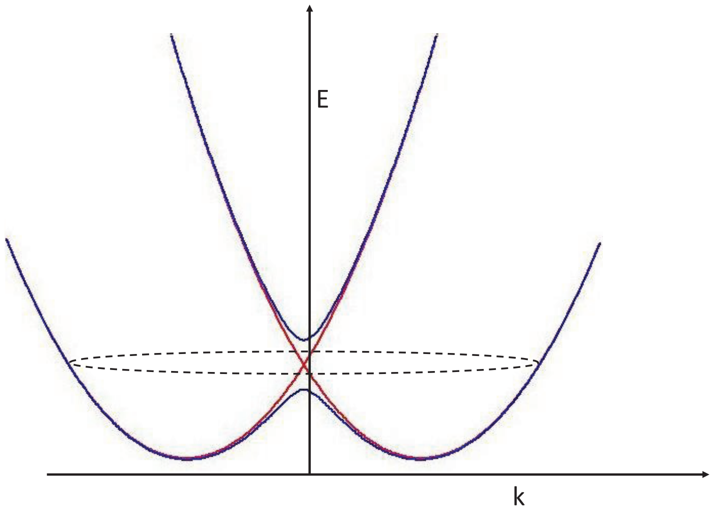

Figure 1. The two SO bands with (blue curves) and without (red curves) Zeeman splitting are shown schematically. With Zeeman splitting the bands have a band gap at the origin. When the Zeeman splitting is large enough so that the chemical potential (dotted circle) lies in the gap, the system has only one Fermi surface and the ordinary superconducting phase gives way to a topologically non-trivial superconducting phase.

self-evident. That it remains s-wave (and is not a mixture of s- and p-waves due to the SO coupling) even when the pair potential is due to an intrinsic on-site pairing interaction is not so obvious. In this case, the pure s-wave symmetry of the pair potential follows from the fact that the intrinsic pairing interaction we consider is spatially local, and thus the formation of a p-wave component of the pair potential is forbidden by the fermion anticommutation relation (for a more detailed discussion, see section 5). Since the pair potential is purely s-wave in both classes (a) and (b) and in both phases (ordinary and topological) in each, how an s-wave pair potential survives a strong Zeeman splitting $\Gamma \gg \Delta$ to realize the topologically non-trivial phase is the central conceptual question we address in this paper.

The basic conceptual issue being discussed here is the topic often alluded to as the Chandrasekhar–Clogston (CC) limit [28, 29] in ordinary s-wave superconductivity, which states, in effect, that an s-wave superconductor, where the Cooper pairing is between spin-up and spin-down electrons near the Fermi surface, cannot withstand a Zeeman splitting larger than the superconducting gap. This is because then spin splitting exceeds the superconducting gap energy, making it impossible for a superconducting ground state to develop. On first sight, it appears that the condition on the Zeeman splitting needed for superconductivity in [1–3] far exceeds this limit, thus destroying all superconductivity! This has caused some confusion about the very existence of the topological superconducting phase either using a heterostructure [1–3] where s-wave superconductivity is induced by proximity effect or using SO-coupled systems with intrinsic s-wave pairing interactions [4].

The mean-field calculations of [1–3] are not enough to resolve this question. This is because a mean-field theory is not just a postulate to assume the existence of a mean-field pair potential in the Hamiltonian H as is done in these works; one is also required to establish the finiteness of the pair potential by satisfying the self-consistent gap equation. In other words,

we need to satisfy the Bardeen–Cooper–Schrieffer (BCS) self-consistent gap equation with a strong Zeeman potential ($\Gamma > \sqrt{\mu^2+\Delta^2}$) to check whether a non-zero s-wave pair potential Δ gives a consistent solution. This will ensure that the mean field H in [1–3] is not flawed to begin with, and our Bogoliubov–de Gennes (BdG) solution of the Majorana fermion is not a spurious mathematical result with no physical connection. In this paper, we conduct this study by self-consistently solving the appropriate BCS gap equations in the presence of attractive s-wave pairing interaction, SO coupling and an externally applied Zeeman splitting. *Note that satisfying such a gap equation is a requirement for superconducting pair potential when it is derived from the microscopic pairing interactions. However, when the pair potential is proximity induced on a SO-coupled system by a nearby s-wave superconductor, the gap equation need not be satisfied. In this case, the SO-coupled system simply 'inherits' the pair potential of the nearby superconductor.*

For the case of intrinsic pairing interactions, we show that the s-wave pair potential indeed remains non-zero even beyond the Zeeman splitting above which it would be lost in the absence of SO coupling. In fact, in the non-Abelian phase the non-zero value of the pair potential crucially depends on and *increases* with the SO coupling constant, which is consistent with the fact that it is zero in the absence of the SO coupling. A simple intuitive way to understand this starts by recalling how s-wave superconductivity is destroyed by a Zeeman splitting. In the absence of SO coupling, the two spin bands are shifted by an energy gap proportional to the Zeeman splitting Γ. With increasing Γ it becomes increasingly difficult for the system to create s-wave spin–singlet pairs with zero net momentum. Finally, when Γ crosses a value $\sim\Delta$ the s-wave pair potential vanishes. The critical Zeeman splitting, $\Gamma_c = \sqrt{\Delta^2+\mu^2}$, needed for the topological phase transition is thus squarely beyond the acceptable Zeeman splitting the pair potential can sustain. It is now important to realize that, in the presence of the SO coupling, the two SO bands cannot simply be viewed as 'spin-up' and 'spin-down' bands. Instead, they both have a non-zero minority spin amplitude coexisting with the majority spin component. Therefore, even when the Zeeman splitting is large enough to make the Fermi surface lie only in the lower band, spin–singlet s-wave pairs cannot be completely lost. If the superconductivity is due to an intrinsic pairing interaction the gap equation shows that the pair potential, although always non-zero, decays with increasing Zeeman couplings. However, the magnitude of the pair potential in the non-Abelian phase can be increased by increasing the magnitude of the SO coupling, which therefore enables a stable non-Abelian phase in the phase diagram. Alternatively if the superconductivity is due to the proximity effect, there is no need of satisfying the self-consistent gap equation. In this case, which applies to the heterostructure geometry, the superconducting pair potential is simply 'inherited' from the adjacent s-wave superconductor (section 8).

2. Hamiltonian

We assume that the quasi-2D electron system is described by the Hamiltonian model

$$H = H_0 + H_{\rm SO} + H_\Gamma + H_{\rm int}, \tag{1}$$

where H_0 describes the bulk conduction electrons, $H_{\rm SO}$ is the SO interaction term, H_Γ represents the Zeeman coupling and $H_{\rm int}$ represents the electron–electron interaction. Explicitly, we have

$$H_0 = \sum_{\boldsymbol{p},\sigma} \xi_{\boldsymbol{p}} c^\dagger_{\boldsymbol{p}\sigma} c_{\boldsymbol{p}\sigma}, \tag{2}$$

$$H_{SO} = \alpha \sum_{\boldsymbol{p},\sigma,\sigma'} c^{\dagger}_{\boldsymbol{p}\sigma} (p_y \tau_x - p_x \tau_y)_{\sigma,\sigma'} c_{\boldsymbol{p}\sigma'}, \tag{3}$$

$$H_{\Gamma} = \Gamma \sum_{\boldsymbol{p}} \left(c^{\dagger}_{\boldsymbol{p}\uparrow} c_{\boldsymbol{p}\uparrow} - c^{\dagger}_{\boldsymbol{p}\downarrow} c_{\boldsymbol{p}\downarrow} \right), \tag{4}$$

$$H_{\text{int}} = \frac{1}{2} \sum_{\boldsymbol{p},\boldsymbol{p}',\boldsymbol{q}} \sum_{\sigma,\sigma'} V(q) c^{\dagger}_{\boldsymbol{p}+\boldsymbol{q}\sigma} c^{\dagger}_{\boldsymbol{p}'-\boldsymbol{q}\sigma'} c_{\boldsymbol{p}'\sigma'} c_{\boldsymbol{p},\sigma}, \tag{5}$$

where $\xi_{\boldsymbol{p}} = p^2/2m - \mu$ is the bulk spectrum (measured relative to the chemical potential μ), α is the strength of the Rashba SO coupling, Γ represents the Zeeman field, $V(q)$ is the short-ranged interaction potential (we will later restrict ourselves to an on-site pairing interaction, $V(q)$ independent of q, natural for s-wave order), $\tau_{x(y)}$ are Pauli matrices and $c^{\dagger}_{\boldsymbol{p}\sigma}$ ($c_{\boldsymbol{p}\sigma}$) is the creation (annihilation) operator corresponding to the single-particle state with momentum $\boldsymbol{p}$ and spin σ. It is convenient to work in the spinor basis provided by the eigenfunctions $\phi_{\lambda}(\boldsymbol{p})$ of the single-particle Hamiltonian $H_0 + H_{SO}$,

$$\phi_{\lambda}(\boldsymbol{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i}\lambda \mathrm{e}^{\mathrm{i}\theta_{\boldsymbol{p}}} \end{pmatrix}, \tag{6}$$

where $\lambda = \pm$ and $\mathrm{e}^{\mathrm{i}\theta_{\boldsymbol{p}}} = (p_x + \mathrm{i} p_y)/p$. The corresponding eigenvalues are

$$\epsilon_{\lambda}(\boldsymbol{p}) = \xi_{\boldsymbol{p}} + \lambda \alpha p. \tag{7}$$

The electron c-operators can be expressed in terms of the annihilation operators $a_{\boldsymbol{p}\lambda}$ associated with the spinor eigenstates as

$$c_{\boldsymbol{p}\sigma} = \sum_{\lambda} \phi_{\lambda}(\boldsymbol{p},\sigma) a_{\boldsymbol{p}\lambda}. \tag{8}$$

Using the spinor representation, the Hamiltonian becomes

$$H_0 + H_{SO} = \sum_{\boldsymbol{p},\lambda} \epsilon_{\lambda}(\boldsymbol{p}) a^{\dagger}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}\lambda}, \tag{9}$$

$$H_{\Gamma} = \Gamma \sum_{\boldsymbol{p},\lambda} a^{\dagger}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}-\lambda}, \tag{10}$$

$$H_{\text{int}} = \frac{1}{2} \sum_{\boldsymbol{p},\boldsymbol{p}',\boldsymbol{q}} \sum_{\lambda,\lambda',\mu,\mu'} V(q) \chi_{\lambda\lambda'}(\boldsymbol{p}+\boldsymbol{q},\boldsymbol{p}) \chi_{\mu\mu'}(\boldsymbol{p}'-\boldsymbol{q},\boldsymbol{p}') a^{\dagger}_{\boldsymbol{p}+\boldsymbol{q}\lambda} a^{\dagger}_{\boldsymbol{p}'-\boldsymbol{q}\mu} a_{\boldsymbol{p}'\mu'} a_{\boldsymbol{p}\lambda}, \tag{11}$$

where

$$\chi_{\lambda\lambda'}(\boldsymbol{p}_1,\boldsymbol{p}_2) = \tfrac{1}{2} \left(1 + \lambda\lambda' \, \mathrm{e}^{-\mathrm{i}(\theta_{\boldsymbol{p}_1} - \theta_{\boldsymbol{p}_2})} \right) \tag{12}$$

is the scalar product of two spinors, $\phi_{\lambda}(\boldsymbol{p}_1)$ and $\phi_{\lambda'}(\boldsymbol{p}_2)$.

3. Superconducting gap equations

To derive the gap equations, we first introduce the regular and anomalous Green functions as

$$\mathcal{G}_{\lambda\lambda'}(\boldsymbol{p},\tau-\tau') = -\langle T_{\tau} a_{\boldsymbol{p}\lambda}(\tau) a^{\dagger}_{\boldsymbol{p}\lambda'}(\tau') \rangle, \tag{13}$$

$$\mathcal{F}_{\lambda\lambda'}(\boldsymbol{p},\tau-\tau') = \lambda\langle T_\tau a_{\boldsymbol{p}\lambda}(\tau)a_{-\boldsymbol{p}\lambda'}(\tau')\rangle, \tag{14}$$

$$\mathcal{F}^{+}_{\lambda\lambda'}(\boldsymbol{p},\tau-\tau') = \lambda\langle T_\tau a^{\dagger}_{\boldsymbol{p}\lambda}(\tau)a^{\dagger}_{-\boldsymbol{p}\lambda'}(\tau')\rangle, \tag{15}$$

where T_τ is the time ordering operator and the operators $a_{\boldsymbol{p}\lambda}(\tau)$ are in the Heisenberg representation. The correlation functions $\mathcal{F}_{\lambda\lambda'}(\boldsymbol{p}) = \mathcal{F}_{\lambda\lambda'}(\boldsymbol{p},0+)$ have the properties

$$\mathcal{F}_{\lambda\lambda}(-\boldsymbol{p}) = -\mathcal{F}_{\lambda\lambda}(\boldsymbol{p}), \quad \mathcal{F}^{+}_{\lambda\lambda}(-\boldsymbol{p}) = \mathcal{F}^{*}_{\lambda\lambda}(\boldsymbol{p}), \tag{16}$$

$$\mathcal{F}_{+-}(-\boldsymbol{p}) = \mathcal{F}_{-+}(\boldsymbol{p}), \quad \mathcal{F}^{+}_{+-}(-\boldsymbol{p}) = \mathcal{F}^{*}_{-+}(\boldsymbol{p}). \tag{17}$$

The definitions (14) and (15) of the anomalous correlation functions follow the convention used by Gor'kov and Rashba [30].

Following the standard procedure, we write the equations of motion for the Green functions using the time evolution of the a-operators, $\partial_\tau a_{\boldsymbol{p}\lambda}(\tau) = [H, a_{\boldsymbol{p}\lambda}]$. We have

$$\begin{aligned}
&[-\partial_\tau - \epsilon_\lambda(\boldsymbol{p})]\mathcal{G}_{\lambda\lambda'}(\boldsymbol{p},\tau-\tau') - \Gamma\mathcal{G}_{-\lambda\lambda'}(\boldsymbol{p},\tau-\tau') + \sum_{\boldsymbol{q},\mu,\mu_1,\lambda_1} V(\boldsymbol{p}-\boldsymbol{q})\chi_{\lambda\mu}(\boldsymbol{p},\boldsymbol{q})\chi_{\lambda_1\mu_1}\\
&\qquad\times(-\boldsymbol{p},-\boldsymbol{q})\lambda_1\mu_1\mathcal{F}_{\mu_1\mu}(-\boldsymbol{q},0+)\mathcal{F}_{\lambda_1\lambda'}(-\boldsymbol{p},\tau-\tau') = \delta_{\lambda\lambda'}\delta(\tau-\tau'),\\
&[-\partial_\tau + \epsilon_\lambda(\boldsymbol{p})]\mathcal{F}^{+}_{\lambda\lambda'}(-\boldsymbol{p},\tau-\tau') - \Gamma\mathcal{F}^{+}_{-\lambda\lambda'}(-\boldsymbol{p},\tau-\tau') - \lambda\sum_{\boldsymbol{q},\mu,\mu_1,\lambda_1} V(\boldsymbol{p}-\boldsymbol{q})\chi_{\mu\lambda}\\
&\qquad\times(-\boldsymbol{q},-\boldsymbol{p})\chi_{\mu_1\lambda_1}(\boldsymbol{q},\boldsymbol{p})\mu\mathcal{F}_{\mu\mu_1}(-\boldsymbol{q},0+)^{+}\mathcal{G}_{\lambda_1\lambda}(-\boldsymbol{p},\tau-\tau') = 0.
\end{aligned} \tag{18}$$

The gap function can be defined as

$$\Delta_{\lambda\lambda_1}(\boldsymbol{p}) = \lambda_1 \sum_{\boldsymbol{q},\mu,\mu_1} V(\boldsymbol{p}-\boldsymbol{q})\chi_{\lambda\mu}(\boldsymbol{p},\boldsymbol{q})\chi_{\lambda_1\mu_1}(-\boldsymbol{p},-\boldsymbol{q})\mu_1\mathcal{F}_{\mu_1\mu}(-\boldsymbol{q},0+). \tag{19}$$

Introducing the definition of the gap function in equation (18), we have

$$\begin{aligned}
&[-\partial_\tau - \epsilon_\lambda(\boldsymbol{p})]\mathcal{G}_{\lambda\lambda'}(\boldsymbol{p},\tau-\tau') - \Gamma\mathcal{G}_{-\lambda\lambda'}(\boldsymbol{p},\tau-\tau') + \sum_{\lambda_1}\Delta_{\lambda\lambda_1}(\boldsymbol{p})\mathcal{F}^{+}_{\lambda_1\lambda'}(-\boldsymbol{p},\tau-\tau')\\
&\qquad= \delta_{\lambda\lambda'}\delta(\tau-\tau'),\\
&[-\partial_\tau + \epsilon_\lambda(\boldsymbol{p})]\mathcal{F}^{+}_{\lambda\lambda'}(-\boldsymbol{p},\tau-\tau') - \Gamma\mathcal{F}^{+}_{-\lambda\lambda'}(-\boldsymbol{p},\tau-\tau') + \sum_{\lambda_1}\Delta^{*}_{\lambda_1\lambda}\mathcal{G}_{\lambda_1\lambda}(\boldsymbol{p},\tau-\tau') = 0.
\end{aligned} \tag{20}$$

Defining the Fourier transforms of the correlation functions in the usual way, $\mathcal{G}_{\lambda\lambda'}(\boldsymbol{p},\tau) = k_{\mathrm{B}}T\sum_n \mathrm{e}^{-\mathrm{i}\omega_n\tau}\mathcal{G}_{\lambda\lambda'}(\boldsymbol{p},\mathrm{i}\omega_n)$, the set of equations of motion can be expressed in a matrix form as

$$\begin{pmatrix} \mathrm{i}\omega_n - \epsilon_+ & -\Gamma & \Delta_{++} & \Delta_{+-}\\ -\Gamma & \mathrm{i}\omega_n - \epsilon_- & \Delta_{-+} & \Delta_{--}\\ \Delta^{*}_{++} & \Delta^{*}_{-+} & \mathrm{i}\omega_n + \epsilon_+ & -\Gamma\\ \Delta^{*}_{+-} & \Delta^{*}_{--} & -\Gamma & \mathrm{i}\omega_n + \epsilon_- \end{pmatrix} \begin{pmatrix} \mathcal{G}_{++}\\ \mathcal{G}_{-+}\\ \mathcal{F}^{+}_{++}\\ \mathcal{F}^{+}_{-+} \end{pmatrix} = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \tag{21}$$

where the arguments of the Green functions have been omitted for simplicity. A similar set of equations, which can be obtained from (21) by switching the + and − labels, couples $\mathcal{G}_{--}$, $\mathcal{G}_{+-}$, $\mathcal{F}_{--}$ and $\mathcal{F}_{+-}$. The superconducting spectrum can be obtained from the condition that the determinant of the 4×4 matrix in equation (21) vanish taking $\mathrm{i}\omega_n \to E$. Also, by solving the system of equations of motion for $\mathcal{F}_{\lambda\lambda'}$ and introducing the solutions in equation (19) we obtain

the self-consistent gap equations. In general, we have $\Delta_{\lambda\lambda}(\boldsymbol{p}) = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta_p}[\Delta_{0s}(\boldsymbol{p}) + \lambda\Delta_{0a}(\boldsymbol{p})]$, where the symmetric and antisymmetric components of the diagonal gap functions are

$$\Delta_{0s}(\boldsymbol{p}) = -\sum_{\boldsymbol{q}} \frac{V(\boldsymbol{p}-\boldsymbol{q}) + V(\boldsymbol{p}+\boldsymbol{q})}{2} \frac{\mathrm{i}}{2}[\mathcal{F}_{++}(-\boldsymbol{q},0) + \mathcal{F}_{--}(-\boldsymbol{q},0)]\mathrm{e}^{\mathrm{i}\theta_q}, \tag{22}$$

$$\Delta_{0a}(\boldsymbol{p}) = -\mathrm{i}\sum_{\boldsymbol{q}} \frac{V(\boldsymbol{p}-\boldsymbol{q}) - V(\boldsymbol{p}+\boldsymbol{q})}{2} \Big[(\mathcal{F}_{++} - \mathcal{F}_{--})\cos(\theta_{\boldsymbol{p}} - \theta_{\boldsymbol{q}})\mathrm{e}^{\mathrm{i}\theta_q} + \mathrm{i}(\mathcal{F}_{+-} - \mathcal{F}_{-+})\sin(\theta_{\boldsymbol{p}} - \theta_{\boldsymbol{q}})\mathrm{e}^{\mathrm{i}\theta_q}\Big]. \tag{23}$$

Similarly, the off-diagonal gap functions can be expressed as $\Delta_{\lambda-\lambda}(\boldsymbol{p}) = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta_p}[\Delta_{1s}(\boldsymbol{p}) + \lambda\Delta_{1a}(\boldsymbol{p})]$, with

$$\Delta_{1s}(\boldsymbol{p}) = -\sum_{\boldsymbol{q}} \frac{V(\boldsymbol{p}-\boldsymbol{q}) - V(\boldsymbol{p}+\boldsymbol{q})}{2} \frac{\mathrm{i}}{2}[\mathcal{F}_{+-}(-\boldsymbol{q},0) + \mathcal{F}_{-+}(-\boldsymbol{q},0)]\mathrm{e}^{\mathrm{i}\theta_q}, \tag{24}$$

$$\Delta_{1a}(\boldsymbol{p}) = -\mathrm{i}\sum_{\boldsymbol{q}} \frac{V(\boldsymbol{p}-\boldsymbol{q}) - V(\boldsymbol{p}+\boldsymbol{q})}{2} \Big[\mathrm{i}(\mathcal{F}_{++} - \mathcal{F}_{--})\sin(\theta_{\boldsymbol{p}} - \theta_{\boldsymbol{q}})\mathrm{e}^{\mathrm{i}\theta_q} + (\mathcal{F}_{+-} - \mathcal{F}_{-+})\cos(\theta_{\boldsymbol{p}} - \theta_{\boldsymbol{q}})\mathrm{e}^{\mathrm{i}\theta_q}\Big]. \tag{25}$$

Note that $\Delta_{js}(-\boldsymbol{p}) = \Delta_{js}(\boldsymbol{p})$ and $\Delta_{ja}(-\boldsymbol{p}) = -\Delta_{ja}(\boldsymbol{p})$, i.e. Δ_{js} and Δ_{ja} represent the singlet and triplet components of the gap functions, respectively.

4. Assumption of local interaction

Instead of solving the complicated coupled set of gap equations above, we simplify matters by considering the case of strictly local interactions. In other words, we neglect the momentum dependence of the interaction potential, $V(\boldsymbol{p}) = V_0 < 0$. Then the only non-vanishing component of the superconducting gap is the singlet component, $\Delta_{0s} = \Delta$, and it becomes momentum independent. Since by a Zeeman splitting the singlet component of the gap function will be the most affected, we can make this approximation to examine the fate of the superconducting condensate with increasing Zeeman potential.

For a strictly local attractive interaction, the superconducting spectrum is given by

$$E^2_{1(2)}(\boldsymbol{k}) = \xi_{\boldsymbol{k}}^2 + \alpha_k^2 + \Gamma^2 + |\Delta|^2 \mp 2\sqrt{\xi_{\boldsymbol{k}}^2\alpha_k^2 + \Gamma^2(\xi_{\boldsymbol{k}}^2 + |\Delta|^2)}, \tag{26}$$

where $\alpha_k = \alpha k$. Solving the kinetic equations for $\mathcal{F}_{++}$ and $\mathcal{F}_{--}$ and using equation (22) we obtain the gap equation for the strictly local attractive interaction,

$$k_{\mathrm{B}}T\sum_n \frac{-V_0}{2}\sum_{\boldsymbol{q}}\left[\frac{1}{\omega_n^2 + E_1^2} + \frac{1}{\omega_n^2 + E_2^2} - \frac{\Gamma^2}{\sqrt{\xi_{\boldsymbol{q}}^2\alpha_q^2 + \Gamma^2(\xi_{\boldsymbol{q}}^2 + |\Delta|^2)}}\left(\frac{1}{\omega_n^2 + E_1^2} - \frac{1}{\omega_n^2 + E_2^2}\right)\right] = 1. \tag{27}$$

Taking the zero-temperature limit and performing the summation over the frequencies we obtain

$$1 = \frac{-V_0}{2}\sum_{\boldsymbol{q}}\left[\frac{1}{2E_1(\boldsymbol{q})} + \frac{1}{2E_2(\boldsymbol{q})} - \frac{\Gamma^2}{\sqrt{\xi_{\boldsymbol{q}}^2\alpha_q^2 + \Gamma^2(\xi_{\boldsymbol{q}}^2 + |\Delta|^2)}}\left(\frac{1}{2E_1(\boldsymbol{q})} - \frac{1}{2E_2(\boldsymbol{q})}\right)\right]. \tag{28}$$

5. Anomalous correlation functions and gap functions in the *c*-operator representation

To obtain a deeper understanding of the singlet–triplet mixing in superconductors with SO coupling [30], it is useful to determine the expressions for the anomalous correlation functions and of the gap functions in terms of the original electron operators. We first express the c-operators in terms of a-operators, $c_{\boldsymbol{p}\uparrow} = (a_{\boldsymbol{p}+} + a_{\boldsymbol{p}-})/\sqrt{2}$ and $c_{\boldsymbol{p}\downarrow} = -\mathrm{i}\mathrm{e}^{\mathrm{i}\theta_p}(a_{\boldsymbol{p}+} - a_{\boldsymbol{p}-})/\sqrt{2}$, and we obtain for the singlet and triplet anomalous correlation functions the expressions

$$\begin{aligned}\langle T_\tau c_{-\boldsymbol{p}\downarrow}(\tau)c_{\boldsymbol{p}\uparrow}(\tau')\rangle &= \frac{\mathrm{i}}{2}\mathrm{e}^{\mathrm{i}\theta_p}\big[\mathcal{F}_{++}(-\boldsymbol{p},\tau-\tau') + \mathcal{F}_{--}(-\boldsymbol{p},\tau-\tau') + \mathcal{F}_{+-}(-\boldsymbol{p},\tau-\tau') \\ &\quad + \mathcal{F}_{-+}(-\boldsymbol{p},\tau-\tau')\big], \\ \langle T_\tau c_{-\boldsymbol{p}\sigma}(\tau)c_{\boldsymbol{p}\sigma}(\tau')\rangle &= \tfrac{1}{2}\mathrm{e}^{(1-\sigma)\mathrm{i}\theta_p}\big[\mathcal{F}_{++}(-\boldsymbol{p},\tau-\tau') - \mathcal{F}_{--}(-\boldsymbol{p},\tau-\tau') \\ &\quad + \sigma\mathcal{F}_{+-}(-\boldsymbol{p},\tau-\tau') - \sigma\mathcal{F}_{-+}(-\boldsymbol{p},\tau-\tau')\big],\end{aligned} \tag{29}$$

where the $\mathcal{F}$ anomalous functions are given by equations (14) and (15). In the limit of local interactions we can determine the explicit dependence of the $\mathcal{F}$ functions on the parameters of the model using equation (21), and we have $(\mathcal{F}_{\lambda\lambda'} + \mathcal{F}_{-\lambda-\lambda'}) \propto \Delta_{0s}(\mathbf{p})$ and $(\mathcal{F}_{\lambda\lambda'} - \mathcal{F}_{-\lambda-\lambda'}) \propto \mathrm{i}\alpha p\,\mathrm{e}^{-\mathrm{i}\theta_p}\Delta_{0s}(\mathbf{p})$. Consequently, in the c-operator representation both the singlet and the triplet components of the anomalous correlation function are proportional to the s-wave gap, $\langle T_\tau c_{-\boldsymbol{p}\downarrow}(\tau)c_{\boldsymbol{p}\uparrow}(\tau')\rangle \propto \Delta_{0s}(\mathbf{p})$ and $\langle T_\tau c_{-\boldsymbol{p}\sigma}(\tau)c_{\boldsymbol{p}\sigma}(\tau')\rangle \propto \mathrm{i}\alpha\Delta_{0s}(\mathbf{p})(p_x - \mathrm{i}\sigma p_y)$, respectively.

We emphasize that, in the limit of local pairing interaction, the anomalous correlation function in the c-operator representation has both singlet and triplet components, but the corresponding gap function is purely s-wave. To show this property explicitly, we can re-derive the gap equations in the c-operator representation and, instead of equation (20), we obtain

$$\begin{aligned}(-\partial_\tau - \xi_{\boldsymbol{p}} - \sigma\Gamma)G_{\sigma\sigma'}(\boldsymbol{p},\tau-\tau') - \sigma\alpha p G_{-\sigma\sigma'}(\boldsymbol{p},\tau-\tau') + \sum_{\sigma_1}\Delta_{\sigma_1\sigma}(\boldsymbol{p})\langle T_\tau c^\dagger_{\boldsymbol{p}\sigma'}c^\dagger_{-\boldsymbol{p}\sigma_1}\rangle \\ = \delta_{\sigma\sigma'}\delta(\tau-\tau'),\end{aligned} \tag{30}$$

where $G_{\sigma\sigma'}(\boldsymbol{p},\tau-\tau') = -\langle T_\tau c_{\boldsymbol{p}\sigma}(\tau)c^\dagger_{\boldsymbol{p}\sigma'}(\tau')\rangle$ is the normal Green function and the gap functions are defined as

$$\Delta_{\sigma\sigma'}(\boldsymbol{p}) = -\sum_{\boldsymbol{q}} V(\boldsymbol{p}-\boldsymbol{q})\langle c_{-\boldsymbol{p}\sigma}(\tau)c_{\boldsymbol{p}\sigma'}(\tau)\rangle. \tag{31}$$

The equal time anomalous correlation $\langle c_{-\boldsymbol{p}\sigma}(\tau)c_{\boldsymbol{p}\sigma'}(\tau)\rangle$ can be expressed in terms of $\mathcal{F}_{\lambda\lambda'}(0)$. Explicitly, we have

$$\begin{aligned}\Delta_{\downarrow\uparrow}(\boldsymbol{p}) &= -\sum_{\boldsymbol{q}}\frac{V(\boldsymbol{p}-\boldsymbol{q})+V(\boldsymbol{p}+\boldsymbol{q})}{2}\frac{\mathrm{i}}{2}\mathrm{e}^{\mathrm{i}\theta_q}\big[\mathcal{F}_{++}+\mathcal{F}_{--}\big] - \sum_{\boldsymbol{q}}\frac{V(\boldsymbol{p}-\boldsymbol{q})-V(\boldsymbol{p}+\boldsymbol{q})}{2} \\ &\quad\times\frac{\mathrm{i}}{2}\mathrm{e}^{\mathrm{i}\theta_q}\big[\mathcal{F}_{+-}+\mathcal{F}_{-+}\big], \\ \Delta_{\uparrow\uparrow}(\boldsymbol{p}) &= -\sum_{\boldsymbol{q}}\frac{V(\boldsymbol{p}-\boldsymbol{q})-V(\boldsymbol{p}+\boldsymbol{q})}{2}\frac{1}{2}\big[\mathcal{F}_{++}-\mathcal{F}_{--}\big] - \sum_{\boldsymbol{q}}\frac{V(\boldsymbol{p}-\boldsymbol{q})+V(\boldsymbol{p}+\boldsymbol{q})}{2} \\ &\quad\times\frac{1}{2}\big[\mathcal{F}_{+-}-\mathcal{F}_{-+}\big].\end{aligned}$$

In the limit of strictly local interactions $V(\boldsymbol{p}-\boldsymbol{q}) = V(\boldsymbol{p}+\boldsymbol{q}) = V_0$ and $(\mathcal{F}_{+-} - \mathcal{F}_{-+}) \propto q_x - \mathrm{i}q_y$ and, consequently, the triplet component vanishes, $\Delta_{\uparrow\uparrow} = \Delta_{\downarrow\downarrow} = 0$. Alternatively, the expression for the singlet component of the gap becomes identical with the right-hand side (rhs) of equation (22); hence we have $\Delta_{\downarrow\uparrow}(\boldsymbol{p}) = \Delta_{0s}(\boldsymbol{p}) = \Delta$. We conclude that in a superconductor with SO coupling and on-site pairing interactions, the anomalous correlation function is characterized by a mixture of singlet and triplet components, yet the gap function has purely s-wave symmetry. A p-wave component of the gap can develop only in the presence of non-local pairing interactions. As a consequence, in a system with strictly local pairing interaction, if the singlet anomalous correlation vanishes, the superconducting gap as well as all the other components of the anomalous correlation function will vanish.

6. Analysis of the gap equation

We first analyze the gap equation, equation (28), in some special cases for which the solutions are well known. This will serve as a test for the validity of our analytical calculations. By putting $\Gamma = 0$ and $\alpha = 0$, which corresponds to the standard BCS case of a local attractive interaction with no SO coupling and Zeeman splitting, we find $E_1 = E_2 = \sqrt{\xi_q^2 + |\Delta|^2}$. In this case, from equation (28) we recover the standard BCS gap equation,

$$1 = \frac{-V_0}{2} \sum_{\boldsymbol{q}} \frac{1}{\sqrt{\xi_q^2 + |\Delta|^2}}, \tag{32}$$

where the summation over $\boldsymbol{q}$ should be performed over states satisfying $|\xi_{\boldsymbol{q}}| < \omega_{\mathrm{D}}$, with ω_{D} being some cut-off Debye energy scale. As is well known [31], since the integral on the rhs diverges in the limit $|\Delta| \to 0$, in this case a non-zero solution for Δ exists for any $V_0 < 0$.

Next we take the system with $\Gamma = 0$, $\alpha \neq 0$. In this case, $E_{1(2)} = \sqrt{(\xi_{\boldsymbol{q}} \mp \alpha_q)^2 + |\Delta|^2}$. The gap equation now becomes

$$1 = \frac{-V_0}{4} \sum_{\boldsymbol{q}} \left[\frac{1}{\sqrt{(\xi_{\boldsymbol{q}} - \alpha_q)^2 + |\Delta|^2}} + \frac{1}{\sqrt{(\xi_{\boldsymbol{q}} + \alpha_q)^2 + |\Delta|^2}} \right]. \tag{33}$$

As in the previous case, the integrals on the rhs of equation (33) diverge when $|\Delta| \to 0$; hence a non-vanishing solution for Δ exists for any $V_0 < 0$.

To establish the familiar result that s-wave superconductivity is destroyed by Zeeman splitting (in the absence of SO coupling), we consider the special case, $\Gamma \neq 0$ and $\alpha = 0$. In this case $E_{1(2)} = |\sqrt{\xi_{\boldsymbol{q}}^2 + |\Delta|^2} \mp \Gamma|$, and the gap equation becomes

$$1 = \frac{-V_0}{2} \sum_{\boldsymbol{q}} \frac{1}{\sqrt{\xi_q^2 + |\Delta|^2}}, \tag{34}$$

where the summation over $\boldsymbol{q}$ is done over states satisfying $|\xi_{\boldsymbol{q}}| < \omega_{\mathrm{D}}$ and $\sqrt{\xi_{\boldsymbol{q}}^2 + |\Delta|^2} > \Gamma$. The second constraint results from the cancellation of two terms from equation (28) that diverge in the limit $|\Delta| \to 0$. Since the integral on the rhs of the gap equation no longer diverges, a non-zero solution for Δ exists only for $|V_0|$ larger than a critical value. This implies that for a given strength of the attractive potential $|V_0|$, no non-zero solution for Δ can be found above a critical value of the Zeeman potential Γ.

Finally, we consider the most general case of a non-zero Zeeman potential as well as a non-zero SO coupling, $\Gamma \neq 0$, $\alpha \neq 0$. The gap equation is then given by equation (28). The exact cancelation of the divergent terms that characterizes the $\alpha = 0$ case does no longer hold and the rhs of equation (28) becomes arbitrarily large in the limit $|\Delta| \to 0$. Consequently, a non-vanishing solution for Δ exists for *any* negative value of V_0. This implies that Δ does not vanish for any value of Γ, or, in other words, the pair potential cannot be completely destroyed by a Zeeman splitting in the presence of a non-zero SO coupling. This is in agreement with a similar result derived earlier in a different context [7]. Nonetheless, at large values of Γ the superconducting pair potential decreases exponentially with the strength of the Zeeman splitting as we show in the next section.

7. Numerical solution and quantum phase transitions (QPTs)

Next, we determine the general solution of the gap equation by solving equation (28) numerically. We address two distinct cases: (i) the high carrier concentration regime, when the chemical potential μ (i.e. the Fermi energy in our zero-temperature limit) represents the largest energy scale in the problem, $\mu \gg \omega_D, \Gamma, \alpha k_F, \Delta(0)$, and (ii) low carrier concentration, when $\omega_D > \mu, \Gamma, \alpha k_F, \Delta(0)$. Here, ω_D is the analogue of the Debye frequency (i.e. the characteristic energy cut-off for the intrinsic pairing interaction), αk_F is the strength of the SO interaction at the Fermi wave vector and $\Delta(0)$ is the value of the superconducting gap at zero Zeeman splitting. The zero-field gap is a measure of the pairing interaction strength, and in fact one can use V_0 instead of $\Delta(0)$ as an independent parameter. The Debye frequency acts as a cut-off in equation (28), i.e. the summation over $\boldsymbol{q}$ of a function $f(\boldsymbol{q}, E_i(\boldsymbol{q}))$ is restricted to the values of the wave vector satisfying $E_i(\boldsymbol{q}) < \omega_D$.

To obtain the self-consistent numerical solution for the gap, we define the function

$$\theta(\Delta) = \frac{-V_0}{2} \sum_{\boldsymbol{q}} \left[\frac{1}{2E_1(\boldsymbol{q})} + \frac{1}{2E_2(\boldsymbol{q})} - \frac{\Gamma^2}{\sqrt{\xi_{\boldsymbol{q}}^2 \alpha_{\boldsymbol{q}}^2 + \Gamma^2(\xi_{\boldsymbol{q}}^2 + |\Delta|^2)}} \left(\frac{1}{2E_1(\boldsymbol{q})} - \frac{1}{2E_2(\boldsymbol{q})} \right) \right] - 1. \tag{35}$$

With this notation, equation (28) becomes $\theta(\Delta) = 0$. This equation is characterized by two qualitatively different regimes that are controlled by the relative strength of the SO interaction and the zero-field gap. If $2\alpha k_F \gtrsim \Delta(0)$, $\theta(\Delta)$ is a monotonically decreasing function that starts from large positive values at $\Delta \to 0$ and equation (35) has always one non-vanishing solution. By contrast, when $2\alpha k_F < \Delta(0)$, the function $\theta(\Delta)$ becomes non-monotonic for certain values of the Zeeman field Γ, which means that equation (35) can have multiple non-vanishing solutions for a given set of parameters. To illustrate this situation, we show in figure 2 the function $\theta(\Delta)$ for a system with large carrier concentration ($\mu = 0.5$ eV) and extremely low SO interaction ($\alpha = 0.5$ meV Å in panel (a) and $\alpha = 1$ meV Å in panel (b), i.e. $2\alpha k_F = 0.2$ meV and $2\alpha k_F = 0.4$ meV, respectively). The Debye frequency is $\omega_D = 25$ meV and the zero-field gap is $\Delta(0) = 0.5$ meV. At low Zeeman splitting, $\theta(\Delta)$ vanishes at a single point $\Delta \approx 0.5$ meV, but increasing Γ leads to a local minimum in $\theta(\Delta)$ that goes to zero for $\Gamma \approx 0.318$ meV. Further increasing the Zeeman splitting leads to three non-vanishing solutions $\Delta_1(\Gamma) > \Delta_2(\Gamma) > \Delta_3(\Gamma)$ (see figure 2), where $\Delta_1(\Gamma)$ and $\Delta_3(\Gamma)$ are the 'low field' and 'high field' solutions, respectively, and $\Delta_2(\Gamma)$ is an unstable solution. The 'low field' and 'high field' solutions coexist in some range of Zeeman field strengths, suggesting that the system undergoes a precipitous drop in

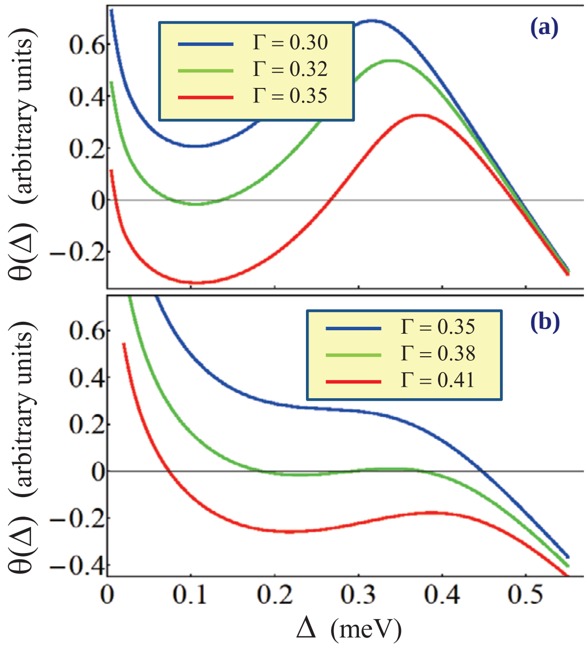

Figure 2. The behavior of the function $\theta(\Delta)$ (equation (35)) with Δ. The values of Δ at which $\theta(\Delta)=0$ are the solutions of the self-consistent gap equation. (a) $\theta(\Delta)$ with Δ for various values of the Zeeman splitting Γ for a small value of the SO coupling constant α ($2\alpha k_{\mathrm{F}}=0.2\,\mathrm{meV}$) and large $\mu=0.5\,\mathrm{eV}$. Initially, for smaller values of the Zeeman splitting there is just one solution for Δ. With increasing the values of Γ, there are three solutions for Δ, one of which (the one in the middle) is unstable. The lower (higher) solution for Δ is the high (low) field solution that co-exists in a region of co-existence. With Γ going up, the high field solution becomes smaller but is never zero. Consequently, there is no true first-order transition in the presence of a small α, even though there is a first-order-like precipitous drop in Δ at some values of Γ, which is a remnant of the first-order transition for $\alpha=0$. (b) $\theta(\Delta)$ with Δ for increasing values of Γ with a fixed large $\mu=0.5\,\mathrm{eV}$ and *a larger SO coupling* $2\alpha k_{\mathrm{F}}=0.4\,\mathrm{meV}$. $\theta(\Delta)$ is now monotonically decreasing and the resultant unique solution for Δ decreases with increasing the values of Γ. The rate of decrease of this solution with Γ is much lower and continuous. As in the case of smaller α, there is no QPT.

Δ akin to a field-tuned first-order phase transition. The coexistence region shrinks as the strength of the SO coupling increases (see figure 2(b)) and vanishes at a value $\alpha_{\mathrm{c}}\approx 1.1\,\mathrm{meV}\,\mathrm{\AA}$. We note that in real systems such as non-centrosymmetric superconductors, the strength of the SO coupling is usually larger than this critical value and, consequently, the first-order-like precipitous drop in Δ may not be observable. In cold fermion systems, the SO coupling constant can be used as a tuning parameter to interpolate between these two behaviors.

The dependence of the solution to the gap equations on Γ is shown in figure 3. The coexistence region can be easily seen for $\alpha=0.5\,\mathrm{meV}\,\mathrm{\AA}$ (green line in figure 3), corresponding to the (stable) solutions of the equation $\theta(\Delta)=0$ for the θ function shown in figure 2(a).

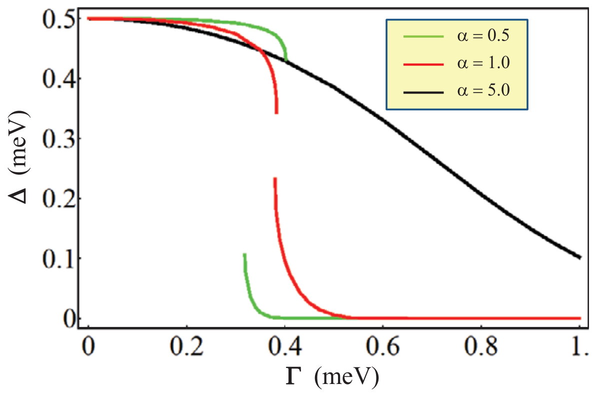

Figure 3. The solution of the gap equation (see figure 2) plotted against the Zeeman splitting Γ for various values of the SO coupling constant α (in meV Å). For small values of α, the superconducting gap falls discontinuously with Γ, but it is never strictly zero in the presence of SO coupling. Consequently, there is only a first-order-like crossover, which is a remnant of the true first-order phase transition with Γ for $\alpha = 0$. For larger values of α (black curve), the decay of the superconducting pair potential with Zeeman splitting is much slower and continuous. It falls exponentially (but is never strictly zero) only for higher fields $\Gamma > 2\alpha k_F$.

Note the exponential decay of the 'high field' solution Δ_3 with increasing Γ. Practically the superconducting gap is negligible ($\Delta < 1\,\mu$eV) for $\Gamma > 0.41$ meV. The coexistence region shrinks as we approach the critical SO coupling (red line in figures 3 and 2(b) and then, for $\alpha > \alpha_c$, the gap equation has a continuous solution $\Delta(\Gamma)$ that decreases monotonically with the Zeeman field (black line in figure 3). Note that at high fields, $\Gamma > 2\alpha k_F$, the gap decreases exponentially. However, the energy scale for the SO coupling, $2\alpha k_F$, can be significant in realistic systems (tens of meV) and the high field regime may not be attainable, i.e. the gap will not vanish for any realistic value of the Zeeman field.

The existence of a first-order-like drop in Δ that ends at a critical value of the SO coupling α_c is generic, i.e. this feature is present at any value of the carrier density. However, to realize a topologically non-trivial non-Abelian regime, it is necessary to satisfy the condition $\Gamma^2 > \mu^2 + \Delta^2$. Consequently, we study the solutions of the gap equation in the low-density regime, where the chemical potential, the Zeeman field, the SO interaction and the superconducting order parameter are comparable. *In particular, we address the following question: is it possible to realize the condition for the existence of a topologically non-trivial non-Abelian phase while maintaining a reasonable superconducting gap?* Before presenting the results, we note that in the low-density regime the zero-field gap has a strong dependence on the chemical potential. More precisely, for a given set of parameters V_0, ω_D and α, the zero-field gap $\Delta(0)$ decreases with μ. In our calculations, we fix V_0 at a value that corresponds to $\Delta(0) = 0.4$ meV at $\mu = 2$ meV and, at lower carrier densities (i.e. lower values of μ), we calculate the zero-field gap using the gap equation. Also, we note that, as we vary the Zeeman splitting Γ, the chemical potential of a system with fixed carrier density n remains constant as long as the high-energy band E_2 has non-zero occupation. For higher values of Γ, i.e. when the bands split, we determine

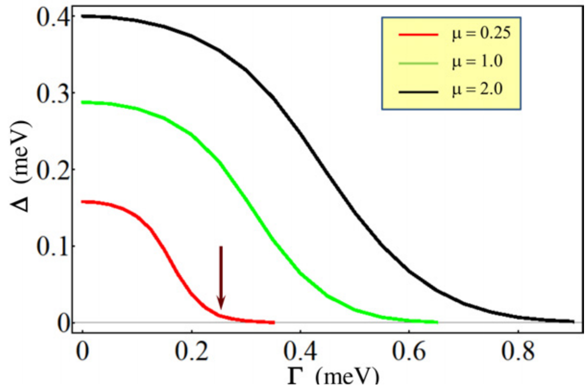

Figure 4. The solution of the gap equation plotted against the Zeeman splitting Γ for three different values of μ for a fixed value of the SO coupling constant $\alpha = 0.1$ eV Å. The value of α is large enough so that Δ remains continuous with Γ. For larger values of μ (black and green curves), Δ becomes inappreciably small for $\Gamma \geqslant \mu$. For the red curve, however, Δ is appreciable (0.02 meV) for $\Gamma \geqslant \mu = 0.25$ meV. Since to the right of this Γ it is possible to satisfy $\Gamma^2 > \mu^2 + \Delta^2$, the system is in a topologically non-trivial phase in this region. Therefore, somewhere above $\Gamma = 0.25$ meV (shown with an arrow), there is a topological QPT from a regular superconducting phase (to the left of the arrow) to a topologically non-trivial non-Abelian phase (to the right of the arrow).

the chemical potential $\mu = \mu(n, \Gamma)$ corresponding to the fixed carrier density. The values of μ provided below represent zero-field values.

Figure 4 shows the dependence of the solution of the gap equation on the Zeeman splitting for three different values of the chemical potential (i.e. three carrier densities), $\mu = 2.0$, 1 and 0.25 meV. The Debye frequency is taken as $\omega_D = 25$ meV and the Rashba coupling is $\alpha = 0.1$ eV Å, i.e. the system is characterized by a strong SO coupling. For these parameters the system is above the critical value of α for the discontinuous fall of Δ and hence Δ is now a continuous function of Γ. Before analyzing the plots in figure 4, remember that in order to satisfy the conditions for the non-Abelian s-wave phase ($\Gamma^2 > \mu^2 + \Delta^2$), an appreciable Δ when Γ has crossed $\sim \mu$ is needed. Coming back to figure 4 note that, similar to figure 3 (black curve), Δ falls with increasing the values of Γ. For the black and green curves (higher μ), Δ becomes inappreciably small (although it is never zero) by the time Γ becomes $\sim \mu$. However, for the red curve ($\mu = 0.25$ meV) there is a residual superconducting pair potential $\Delta \approx 0.02$ meV for $\Gamma \geqslant \mu$, i.e. the system is in a topologically non-trivial non-Abelian phase. Moreover, as shown in figure 5, the magnitude of this residual s-wave pair potential increases with α and thus can be increased by increasing the value of the SO coupling. Therefore, for these parameter values, there is topological quantum phase transition (TQPT) when Γ crosses the critical value $\Gamma_c = \sqrt{\mu^2 + \Delta^2}$ (shown with an arrow in figure 4). The TQPT separates a regular (non-topological) superconducting phase ($\Gamma < \Gamma_c$) from a topological non-Abelian superconducting phase ($\Gamma > \Gamma_c$). From our self-consistent mean-field theory, we find this TQPT to be continuous; that is, there is no change in Δ at the critical value of the Zeeman splitting.

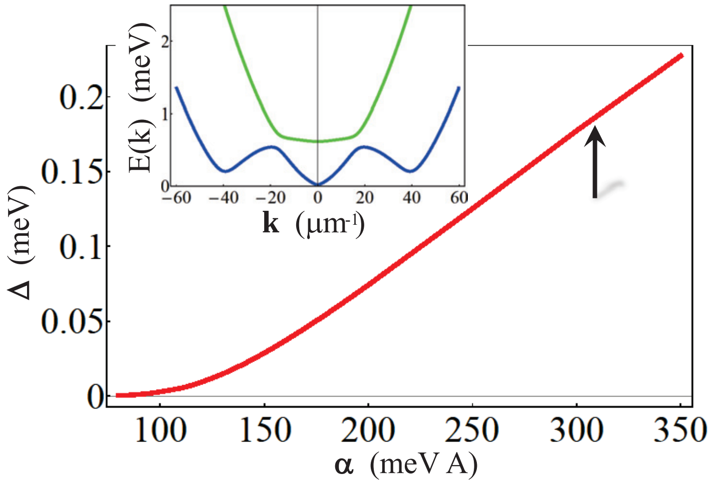

Figure 5. Dependence of the superconducting pair potential Δ in the topological phase on the strength of Rashba SO coupling α. The system is characterized by a chemical potential at zero magnetic field $\mu_0 = 0.25$ meV (see the red curve in figure 4 for the dependence of Δ on Γ). The Zeeman splitting is fixed at $\Gamma = 0.3$ meV. With these parameters the system is in a non-Abelian phase for $\alpha = 0.1$ eV Å. The superconducting pair potential increases monotonically with α. For $\alpha \geqslant 303$ meV Å (black arrow) the condition $\Gamma^2 > \mu^2 + \Delta^2$ is no longer satisfied and the system undergoes another topological QPT to an ordinary superconducting phase (at large α). The inset shows the two excitation energies, equation (26), of which the smaller one (blue curve) vanishes at $k = 0$ at this α-tuned TQPT.

8. Topological quantum phase transition (TQPT) in the proximity induced case

An alternative and perhaps more robust way to create a topologically non-trivial non-Abelian superconductor is to induce a superconducting pair potential in an SO coupled semiconductor by the proximity effect [1–3]. Ideally, for the proximity-effect-induced superconductivity, the pairing interaction resides in a parent s-wave superconductor such as Al or Nb, while the quasi-particles of interest are confined to a 2D or 1D semiconductor layer on the surface of the superconductor. The proximity effect has been shown to create a topological superconductor similar to the ones discussed above on the surface state of a TI [6, 32, 33] and also in a 2D semiconductor layer [3].

Physically, the proximity effect arises from multiple Andreev reflections of electrons in a semiconductor that is connected to a superconductor by tunneling. For most realistic cases, there is no pairing interaction in the semiconductor. Thus, strictly speaking the superconducting pair potential vanishes in the semiconductor and at first glance it appears that there is no superconductivity induced in the semiconductor. However, the superconducting order parameter defined by $\langle \psi_\sigma^\dagger(\boldsymbol{r})\psi_{\sigma'}^\dagger(\boldsymbol{r}')\rangle$ is found to remain non-zero in the semiconductor layer. Furthermore, the multiple Andreev reflections open a gap in the spectrum of quasi-particles that are localized in the semiconductor layer. The spectra of such quasi-particles can be shown to be identical to quasi-particles with an *effective* pairing potential in the semiconductor layer [32]. Therefore, from the point of the quasi-particle spectrum, which is the only property that is relevant to

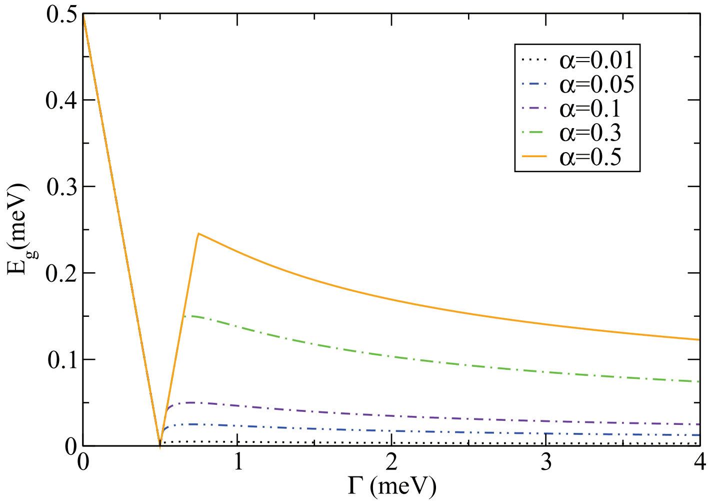

Figure 6. Quasi-particle gap E_g versus Zeeman coupling Γ for various values of SO interaction α. The strength of the SO coupling in the inset is such that $\alpha = 0.3$ corresponds to 0.1 eV Å. The proximity-induced pair potential and chemical potential are taken to be $\Delta_{\rm eff} = 0.5$ meV and $\mu = 0.0$. The quasi-particle gap vanishes at the critical value $\Gamma_c = \sqrt{\Delta_{\rm eff}^2 + \mu^2}$. Above the critical point, SO coupling opens a quasi-particle gap that is proportional to α in the small α limit.

the definition of a topological superconductor, the proximity to a superconductor induces a superconducting quasi-particle gap in the semiconductor.

The proximity effect can be induced by even weak tunneling between the semiconductor and the superconductor. Therefore, the quasi-particle spectrum in the semiconductor does not affect the pairing potential in the superconductor significantly. *Specifically, for the proximity-induced superconductivity case, the self-consistency effects that were important in the discussions in the previous sections become insignificant.* Furthermore, if the Zeeman potential is also induced by proximity effect from a magnetic insulator on the other surface of the semiconductor, there is no direct tunneling between the superconductor and the magnetic insulator and therefore no suppression of the order parameter in the superconductor [3]. Thus, in contrast to the discussions in the previous sections, where the Zeeman-potential-induced topological phase transition was accompanied by significant changes in the pair potential Δ, the pair potential Δ in the proximity induced case remains unaffected by the Zeeman splitting.

The TQPT in both cases (the proximity induced case and the case when the pair potential is due to an intrinsic pairing interaction) can be characterized by the closing of the superconducting quasi-particle gap (shown in figure 6) as the Zeeman potential is raised from $\Gamma = 0$ past the critical value $\Gamma_c = \sqrt{\Delta^2 + \mu^2}$. In the proximity-induced case, Δ is the proximity-induced effective pair potential and μ is the Fermi energy in the semiconductor. The quasi-particle gap $E_g(\boldsymbol{k})$ (minimum of $E_{1(2)}(\boldsymbol{k})$ in equation (26)) closes at $k = 0$ exactly when Γ passes through Γ_c (figure 6), indicating the existence of a QPT even though the superconducting pair potential Δ remains perfectly continuous. The quasi-particle gap for $\Gamma > \Gamma_c$ shows a linear dependence on the SO coupling strength α at small α [3]. Here it is appropriate to mention a caveat for the case where the Zeeman potential is not proximity induced but is instead induced by a magnetic

field [20, 21, 27]. In this case, the Zeeman potential also suppresses the superconducting pair potential in the parent s-wave superconductor. However, this effect can be small provided the g-factor in the semiconductor is much larger than that in the superconductor as is often the case in 2D electron systems.

9. Discussion

Topologically non-trivial non-Abelian superconductivity can be realized in two different classes of systems. In class (a), superconductivity is proximity induced on a semiconductor (in the form of a film or a wire) which has a strong SO coupling. In class (b), superconductivity arises from intrinsic attractive pairing interaction in a system that also has a sizable SO coupling. In both cases, a firm requirement for the phase transition from an ordinary superconducting phase to a topologically non-trivial superconducting phase is an externally imposed Zeeman splitting. The Zeeman splitting creates a gap in the SO bands (figure 1). When this gap is large (Zeeman splitting is comparable to the chemical potential) so that the Fermi surface lies in only the lower band, it triggers a QPT at which the system goes from a regular superconducting phase (small Zeeman splitting) to a topological superconducting phase (large Zeeman splitting). This value of Zeeman splitting far exceeds the value at which an ordinary s-wave superconductor is known to lose superconductivity due to its inability to form spin–singlet zero-momentum Cooper pairs. As we have shown above, this is where the requirement of a sizable SO coupling is important to stabilize a topological superconducting phase. Below we recapitulate and discuss the main results first for the case where the superconductivity arises from an intrinsic pairing interaction and then for the much simpler case of superconductivity arising from proximity effect.

To discuss the various phases and the QPTs, we have divided the parameter space into two distinct regimes by the relative magnitude of μ with respect to all other energy scales in the problem. In the large-μ regime the underlying system always has two Fermi surfaces irrespective of the magnitude of the Zeeman splitting Γ. In the absence of the SO coupling α, with increasing the values of Γ it becomes increasingly difficult for the system to create spin-singlet s-wave pair potential at zero net momentum. Ignoring the possibility of Cooper pairs with non-zero net momentum, we find that when Γ crosses a critical value $\sim\Delta$ the system becomes non-superconducting at a first-order QPT. At this transition the pair potential drops discontinuously to zero. By including a non-zero α we find that, surprisingly, there is always a non-zero solution of the gap equation, equation (28). This is because with $\alpha \neq 0$ the individual bands can no longer be viewed as carrying a single spin component. Rather, both bands now carry a minority spin amplitude along with the majority component, which allows s-wave superconducting pairing even for large values of Γ. If α is small, $2\alpha k_{\mathrm{F}} \leqslant \Delta(0)$, where $\Delta(0)$ is the value of the order parameter for zero Zeeman splitting, there is still a precipitous drop in Δ at Zeeman splitting $\Gamma \sim \Delta(0)$ (figure 3). However, this is not a QPT, since, as already mentioned, Δ is never strictly zero in the presence of a non-zero α. When α itself crosses a threshold value, $2\alpha k_{\mathrm{F}} \geqslant \Delta(0)$, the first-order-like drop in Δ as a function of Γ turns into a slower continuous decay (black curve in figure 3). For high values of $\Gamma \geqslant 2\alpha k_{\mathrm{F}}$, Δ again decays exponentially with Γ. However, this high field scale, comparable to the SO strength at the Fermi surface, may not be attainable in real systems. Consequently, the s-wave superconducting gap may never vanish with a Zeeman coupling in the presence of strong SO coupling.

The regime of small μ is particularly important because of the possibility of a topological phase transition. In this case, the behavior of Δ with Γ for $\alpha = 0$ (first-order QPT) and small α (precipitous drop in Δ with Γ) remains unchanged from the case with large μ. For small μ, however, $\Delta(0)$ itself is small. Consequently α is always in the large SO coupling regime, $2\alpha k_{\rm F} > \Delta(0)$. Therefore, for realistic values of α, Δ falls only gradually with Γ and, strictly speaking, is never zero (figure 4). Let us now recall that for a TQPT from a regular s-wave superconductor to a topologically non-trivial superconductor the parameters need to satisfy the condition $\Gamma > \Gamma_{\rm c} = \sqrt{\Delta^2 + \mu^2}$. This implies that, for a robust non-Abelian phase, we require an appreciable Δ when Γ becomes $\geqslant \mu$. From the red curve in figure 4, we note that for $\Gamma \sim \mu$, Δ is still appreciable, $\Delta \sim 0.02\,\text{meV}$, and thus a stable non-Abelian phase is, in principle, allowed. Moreover, as shown in figure 5, the value of Δ for large Γ (i.e. Δ in the non-Abelian phase) is directly related to the SO strength α and increases appreciably if α can be increased (as in a cold fermion system). Conversely, there is no non-Abelian phase ($\Delta = 0$) if the system has no SO coupling.

From our self-consistent mean field theory, we find the TQPT at $\Gamma = \Gamma_{\rm c} = \sqrt{\Delta^2 + \mu^2}$ to be continuous. By this, we mean that the magnitude of Δ is continuous across this transition. At $\Gamma = \Gamma_{\rm c}$ the underlying system shifts from having two Fermi surfaces ($\Gamma < \Gamma_{\rm c}$) to just one in the lower band ($\Gamma > \Gamma_{\rm c}$). As shown in [1], for $\Gamma > \Gamma_{\rm c}$ a defect in the superconducting order parameter (e.g. vortex and sample edge) traps a unique zero-energy bound state Majorana mode. Such a non-degenerate bound state solution is absent for $\Gamma < \Gamma_{\rm c}$. The emergence of the topological bound state Majorana solution for $\Gamma > \Gamma_{\rm c}$ makes the transition a topological one. The exact location of the topological transition is indicated by the quasi-particle excitation energy $E_{\rm g}(\boldsymbol{k})$ (minimum of $E_{1(2)}(\boldsymbol{k})$ in equation (26)) passing through zero. This happens at $k = 0$ exactly when Γ passes through $\Gamma_{\rm c}$ (figure 6), indicating the existence of a QPT even though the superconducting order parameter Δ remains perfectly continuous.

When s-wave superconductivity is proximity induced on a semiconductor, there is no self-consistent gap equation to be satisfied in the semiconductor. Thus there is no self-consistency effects that suppress the pair potential with the Zeeman splitting as discussed above. In this case, the semiconductor simply 'inherits' the superconducting pair potential and its quasi-particle spectrum is modified accordingly. For weak tunneling between the semiconductor and the superconductor layers, the quasi-particles in the semiconductor cannot significantly influence the pair potential in the host superconductor. Therefore, the self-consistency requirement as in the discussions above can be neglected. If the Zeeman potential is also induced by the proximity effect of a magnetic insulator from the opposite side of the semiconductor, there will be minimal effect of the magnetic insulator on the s-wave superconductor. If the Zeeman potential is induced by a parallel magnetic field, then the effect on the host superconductor will again be minimal provided the g-factor in the semiconductor is larger than that in the superconductor.

10. Conclusion

To conclude, we have considered SO coupled systems with superconductivity arising from either intrinsic on-site s-wave pairing interactions or the proximity effect of an adjacent superconductor. In both cases, using BdG analysis of a postulated mean field Hamiltonian with an s-wave pair potential Δ, it has been shown [1, 2–5] that when an externally imposed Zeeman splitting crosses a critical value, there is a Majorana fermion mode at a vortex core. The required

Zeeman splitting, $\Gamma > \Gamma_c = \sqrt{\mu^2 + \Delta^2}$, seems to far exceed the value ($\Gamma \sim \Delta$) above which an s-wave pair potential Δ is known to vanish. This gives rise to the conceptual question of whether the postulated pair potential in [1] and all subsequent works on this system is spurious for $\Gamma > \Gamma_c$. If true, this will indicate that the BdG result of the Majorana fermion at a vortex core for $\Gamma > \Gamma_c$, based on the postulated mean field H [1, 2–5], is a spurious mathematical result with no physical connection. In this paper, we have resolved this question by showing that in the presence of SO coupling the s-wave pair potential can never be made strictly zero by the application of a Zeeman potential. This is in agreement with a similar result derived previously in a different context [7]. When the s-wave pair potential arises from an intrinsic local pairing interaction, our self-consistent analysis of the gap equation reveals that the decay of the pair potential with Zeeman splitting is more gradual in the presence of SO coupling, although for large enough Zeeman splitting the decay is exponential. Thus there can be a small but finite region in the parameter space (rhs of the arrow, which indicates a TQPT, in figure 4) where a topologically non-trivial superconducting phase can be realized. When the s-wave pair potential is proximity induced on a semiconductor, there is no need of satisfying the self-consistent gap equations. In this case, the pair potential is simply 'inherited' from the adjacent superconductor. Thus in this case the topologically non-trivial phase is much more robust than the other case where it is due to intrinsic pairing interactions.

Two final comments are in order here. For long- but finite-range pairing interactions (as opposed to local interactions as in this paper) it is well known that the SO interaction mixes s-wave and p-wave pair potentials [30]. In this case, it may appear that superconductivity can evade the CC limit merely because the p-wave part of the pair potential can survive the strong Zeeman field, even though the s-wave part cannot. It is, however, incorrect to ascribe the existence of the topological superconducting state at large Γ to this effect. As we have shown in detail in [3], the topological state owes its existence solely to the survival of the s-wave part of the pair potential. (The Pfaffian topological invariant discussed in [3] is completely insensitive to the p-wave part.) It is precisely to isolate and eliminate the effect of the mixed p-wave pair potential that in this paper we confined ourselves to a strictly local pairing interaction. The existence of the topological state at high Zeeman fields is strictly due to the survival of the s-wave pair potential, the physics of which is discussed in this paper and also summarized in the concluding paragraph of the introduction.

But this work is not just an academic resolution of the question of the survival of an s-wave pair potential in the presence of a strong Zeeman field. It also proves that all properties of the topological state when superconductivity is proximity induced continue to hold even when superconductivity is due to local s-wave pairing interactions. This result is directly relevant to the case of an s-wave Feshbach cold atom system. Note that in this case Δ cannot just be assumed in the BdG equations (as in the case of the proximity effect framework [34]), but has to be calculated from the gap equations as in the present paper.

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