Vortex Structures in Atomic Spin-1 Bose-Einstein Condensates

by

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This thesis is concerned with the structure and stability of vortices in spin-1 atomic Bose-Einstein Condensates (BECs) in rotating, optical traps. We numerically study these vortex structures using a classical mean-field theory which allows atomic interactions to change the local expectation value of the atomic spin. Initially applying a model in which the atoms interact only via scattering which does not conserve an initial longitudinal magnetisation, we identify the energetically stable configurations of singular and nonsingular vortices via propagation in imaginary time in a rotating frame of reference.

We find that the cores of singular vortices fill with atoms in the spinor BEC and show that this can be understood in terms of an energetic hierarchy of length scales. By refining the numerical model to explicitly conserve longitudinal magnetisation, we show that the conservation of a strong magnetisation can lead to a mixing of the two phases of the ground-state manifold (polar and ferromagnetic), which are characterised by the expectation value of the spin. This occurs as a result of the introduction of a new characteristic length scale determined by the longitudinal magnetisation. A surprising consequence is the stability of a ferromagnetic coreless vortex in the polar interaction regime, which otherwise is energetically unstable. We construct analytic spinor wavefunctions which parametrise the interpolation between the polar and ferromagnetic phases, exhibiting different vortex topologies in the respective phases.

Finally by identifying stationary states of the system, we show how nonlocal dipole-dipole interactions between atoms introduces an additional length scale determined by the strength of the dipolar interaction. The energetic hierarchy of length scales then determines whether the dipolar interactions have a significant effect on the stationary vortex structures. In particular we show how a BEC with polar interactions adopts the properties of a ferromagnetic condensate when the dipolar interactions dominate.
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Declaration of Authorship

I, Justin John Derek Lovegrove, declare that the thesis entitled Vortex Structures in Atomic Spin-1 Bose-Einstein Condensates and the work presented in the thesis are both my own, and have been generated by me as the result of my own original research. I confirm that:

- this work was done wholly or mainly while in candidature for a research degree at this University;
- where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated;
- where I have consulted the published work of others, this is always clearly attributed;
- where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work;
- I have acknowledged all main sources of help;
- where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;
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List of Abbreviations

1D - 1-Dimensional

2D - 2-Dimensional

3D - 3-Dimensional

ATC Texture - Anderson-Toulouse-Chechetkin Texture

BEC - Bose-Einstein Condensate

FM - Ferromagnetic

GPE - Gross-Pitaevskii Equation

MH Texture - Mermin-Ho Texture

SMA - Single-Mode Approximation

SOR - Successive Overrelaxation
Chapter 1

Introduction

When a gas of bosons is cooled to a sufficiently low temperature, it undergoes Bose-Einstein condensation — a transition from a large distribution of particle states to a system in which the majority of particles occupy the same quantum state, which is then much simpler to describe in certain limits (such as classical field treatments or exploiting similarities with crystalline lattices). The gas is then described as a Bose-Einstein condensate (BEC) [2, 3] and behaves as a superfluid, flowing without viscosity.

In this regime, one works with quantum mechanical wavefunctions, rather than point particles, and the behaviour of the BEC is strongly analogous to other wave systems such as electromagnetic waves. The wavefunction has an associated phase which varies in space and is not an observable per se, but it can lead to purely wavelike effects not seen in classical particles — the most well-known being interference. The BEC wavefunction then represents an order parameter [4] and quantised vortices may form as topological defects of this order parameter [See Secs. 3.1-3.2].

The study of the formation, stability and structure of vortices forms a cornerstone in the understanding of superfluid systems, as well as being of inherent interest as vortices represent macroscopically observable but inherently quantum-mechanical phenomena. This thesis is concerned with numerically studying both the energetically stable and stationary states of vortices in spin-1 atomic BECs, confined in rotating, optical traps.

When an atomic BEC is created in a purely optical trap [5], the absence of strong magnetic fields allows the atoms to retain their spin degree of freedom [6]. Spin rotations then combine with the condensate phase to form a multicomponent order parameter that supports several different types of vortices, both singular and nonsingular, as well as other topological defects and textures [7, 8]. This is similar to superfluid liquid $^3$He, where the non-zero spin and orbital angular momenta of the Cooper pairs similarly yield a multicomponent order parameter [9] supporting a large variety of vortex structures [9, 10, 11]. Parallels also exist between vortices in these systems and objects in early-universe cosmology [11, 12], quantum-field theory [13], liquid crystals [14, 15, 16, 17] and optics [18].
While the core of a singular vortex in a scalar BEC has vanishing density, the expanded order-parameter space of a spinor BEC enables a nontrivial vortex core structure to form. By exhibiting a spinor wavefunction orthogonal to the ground state of the uniform system, the zero-density vortex core may be avoided. Similar structures have been observed in superfluid liquid $^3$He [9]. It is therefore a nontrivial question to ask which of the permitted core structures forms the energetically stable configuration.

This thesis is structured as follows. The remainder of this Chapter briefly presents a qualitative review of the literature on topological defects in spinor BECs. Chapter 2 then presents the essential features of both scalar and spinor BECs, with no discussion of topological defects. Included in this Chapter is a piece of original work which calculates the characteristic length scale associated with the longitudinal magnetisation of a vortex-carrying spinor condensate in Sec. 2.7.2. A brief discussion of topological defects follows in Chapter 3, including a discussion of the experimental methods employed in the study of spinor BECs. Chapter 4 then presents the numerical methods employed in this study, also outlining the experimental quantities represented by the numerical parameters. With this background in place, we then consider the energetically stable vortex structures of the spin-1 spinor condensate, under different interaction models. With the exception of the calculation of magnetisation length scales, all original work in this thesis can be found in Chapters 5-7.

In Chapter 5 we consider only contact interactions between atoms. Although the dominant contact interaction conserves the longitudinal magnetisation [See Sec. 2.6], we neglect this conservation to study the energetic stability of singly-quantised and nonsingular vortices in spin-1 BECs in rotating optical traps. We identify the core structures of the energetically stable vortices, observing the filling of the vortex core with atoms which have been excited out of the ground state in both polar and ferromagnetic interaction regimes. We understand this filling of the vortex cores in terms of an energetic hierarchy of length scales. Additionally, we study the stability of these vortices, as well as the nonsingular vortex of the ferromagnetic phase, for varying rotation frequency, scattering length and linear and quadratic Zeeman splittings.

Chapter 6 then refines the numerical model to explicitly conserve an initial longitudinal magnetisation. This method is applied to the study of energetically stable vortices, demonstrating that a weakly-magnetised condensate exhibits vortex structures as identified in Chapter 5. However, the vortex core size required to produce a given magnetisation can violate the energetic hierarchy of length scales described above and so the previously-identified vortex structures are rendered unstable. The conserved magnetisation introduces a new length scale into the system, which determines the stable vortex core structures. We find that a strongly-magnetised polar condensate is forced to adopt properties of the ferromagnetic regime, enabling it to host a ferromagnetic coreless vortex which would otherwise be energetically unstable. This strong magnetisation also enables a nonsingular vortex of the polar phase, which is not usually energetically stable,
to be stabilised within the core of an outer, singular vortex of the ferromagnetic phase. By formulating an analytic parameterisation which can describe states which mix the polar and ferromagnetic phases, we demonstrate how the mixing of these phases can lead to highly nontrivial topological defect structures, including composite topological defects with disting small- and large-distance topology.

The magnetic dipole-dipole interaction, which is long-range and anisotropic in nature, is discussed in Chapter 7. This Chapter primarily presents an overview of the state of the literature, with the original material confined to Sec. 7.5 Since the dipole-dipole interaction does not conserve magnetisation, we do not enforce magnetisation conservation in the numerical process. For reasons of numerical efficiency, we identify stationary vortex states, which are not necessarily energetically stable. A sufficiently strong dipolar interaction is shown to cause a vortex to spontaneously form in a non-rotating condensate, as well as forcing a polar condensate to adopt properties of the ferromagnetic interaction regime. A strong dipolar interaction also renders the singular vortex unstable in the rotating ferromagnetic condensate. A brief conclusion and outlook is then presented in Chapter 8.

1.1 State of the Field: Vortices in Spinor BECs

In a spinor BEC, the combination of the condensate phase with spin rotations leads to a rich phenomenology of vortex states. As will be discussed in Sec. 2.4.1, the interactions between spin-1 atoms can energetically favour spin alignment or spin anti-alignment. These two interaction regimes—ferromagnetic (FM) and polar, respectively—can host different varieties of vortices as a result of the different symmetries broken by the atomic interactions. There has been much theoretical work demonstrating the variety of vortices one may construct but the existence of a vortex as predicted by the topology of the ground-state manifold [see Chapter 3] does not guarantee that such a vortex will be energetically stable—the criterion applied in this field to determine whether a state may be observed on experimental timescales. There have been numerical works in 2D which have demonstrated the energetic stability of singular and nonsingular vortex states in the FM interaction regime [19, 20, 21, 22], as well as of a singular vortex in the polar regime [19, 21, 23]. However, Chapter 5 presents the first fully 3D numerical study, which demonstrates a range of rotation frequencies and interaction regimes over which these vortices are energetically stable. Additionally, Chapter 6 is the first work to explicitly impose the conservation of magnetisation, which is observed on experimental timescales. Chapter 7 then presents the first treatment of vortices in an isotropically-trapped spinor dipolar BEC.

The first experimental creation of a vortex in an atomic BEC [24] was based upon the premise of mechanically imparting angular momentum upon the system, by rotating the
trap in which the condensate was held [25]. The vortex could not appear spontaneously and so a laser was applied, coupling the non-rotating condensate with a different internal state with unit angular momentum. In the experiment, rather than rotating the trap, the coupling laser was focused to only a small region. This was then rotated through a circular path in the condensate. This idea was further generalised in a subsequent theoretical work [26], such that rather than focusing the laser to a point, the amplitude of the laser would be allowed to vary spatially and this profile would then be rotated. By precisely placing one or more nodal lines in the coupling field, one could accurately specify the positions at which vortices would form.

Further advances in experimental techniques involved using an incident microwave field to induce a dipolar attraction within the condensate, causing the cloud to stretch in the direction of the applied microwave field. This enabled slight asymmetries to be induced in rotating traps, seeding vortex formation at the surface of the trap dynamically. This also did not require the coupling of two internal states, enabling vortices to be studied in single-component condensates. In the first reported experiment using these stirring lasers, four vortices were created [27] and subsequently, eleven vortices were formed [28]. The technique was soon able to produce arrays of over 100 vortices [29], demonstrating that, rather than forming one large vortex with higher angular momentum, BECs favour a regular lattice of singly-quantised vortices.

Subsequently, the transfer of angular momentum directly from Laguerre-Gaussian modes of incident lasers was achieved [30]. This was based upon the theoretical premise of utilising a two-photon transition, with one or both photons carrying angular momentum [31, 32], to produce a condensate of atoms in a different internal state but now carrying the angular momentum imparted by the photon(s).

Vortices in spinor condensates [see Secs. 3.3-3.4] are composed of vortex lines in the individual components of the spinor wavefunction [see Sec. 2.4]. The expanded order-parameter space of spinor BECs can lead to a rich phenomenology of vortices in these systems including the possibility of forming singular or nonsingular vortices and so it is not always obvious which vortex states would be nucleated by the application of stirring lasers. However, by phase-imprinting these vortex lines using Laguerre-Gaussian laser modes coupling the different Zeeman sublevels of the spinor condensate, it is possible to prepare both singular and nonsingular vortex states [33], although thus far only nonsingular vortices have been imprinted. Indeed, this experiment was performed using three Zeeman levels of a spin-2 BEC, which form only a pseudospin-1 system.

There have been many other suggestions for creating nonsingular vortices in spinor BECs, primarily making use of magnetic fields to manipulate the spin profile of the condensate [34, 35]. In Refs. [36, 37] nonsingular vortices were prepared using a time-dependent magnetic field to induce spin rotations, based upon the technique proposed by Ref. [35]. This technique has also been implemented experimentally to prepare singly
and doubly quantised vortices in a spin-polarised BEC [38, 39]. It was shown that the doubly-quantised vortex decays into two singly-quantised vortices [39]. By forming a doubly-quantised vortex in a two-component BEC in a toroidal trap, with singularity in the space in the middle of the torus, the decay of the doubly-quantised vortex was subsequently observed when the gap was removed [40]. The aforementioned magnetic field rotation methods have also been used to generate quadruply-quantised vortices [41, 42]. These quadruply-charged vortices also decay into four singly-quantised vortices [43, 44], supporting the result that multiple singly-quantised vortices are favourable to a single, multiply-quantised vortex.

Preparation of a spinor BEC to a range of predetermined magnetisations [see Sec. 2.6] has been realised in the vortex-free state in Ref. [45]. The phase-imprinting of a vortex state also leaves a controllable finite magnetisation in the condensate as a result of the preparation process yielding unequal populations of the Zeeman sublevels [see Sec. 3.4.1]. This is intuitive in the case of a FM coreless vortex, where the ‘fountain’ structure of the spin leaves a net positive magnetisation. By accurately creating specific spin textures, phase imprinting of coreless vortices therefore gives control over the longitudinal magnetisation of the cloud. This magnetisation is then conserved on experimentally relevant timescales, except in the presence of a magnetic field gradient [46], which causes spin rotations. A nonzero longitudinal magnetisation can stabilise a nonsingular FM vortex [22] and so an imprinted nonsingular vortex can be long-lived experimentally if prepared with an appropriate magnetisation.

It has been suggested that a spin-1 condensate initially prepared in the $m_F = 0$ state may be used to produce a vortex-antivortex superposition in the $m_F = \pm 1$ states [47]. The vortex-antivortex structure is induced via the application of a resonant magnetic field which points in the tangential direction in the $x$-$y$ plane and couples the $m_F = 0$ to the $m_F = \pm 1$ states. These resonant magnetic fields have been used recently to produce such a vortex-antivortex superposition, whose axisymmetry is broken by quantum fluctuations [48].

By using the quadratic Zeeman shift induced by a strong magnetic field to force a FM condensate into the polar phase [see Sec. 2.4.1], then decreasing the field strength, it is possible to study the spontaneous formation of spin domains [49, 50]. The domain walls then break down by forming vortex-antivortex pairs [51] or emitting spin waves [52]. An initially helical spin texture can also be used to form vortices [53] in the FM phase.

It has been argued that, in a pseudospin representation of the two-component condensate, a vortex in only one of the two components represents a nonsingular vortex [54]. Calculations of the density profiles of the two BEC components in such a coreless vortex system were presented in Ref. [55] as the inter- and intra-species scattering lengths varied. The ability to use magnetic rather than purely optical trapping makes two-component experiments much easier to perform than experiments on true spinor BECs.
Two-component experiments also have an advantage over single-component experiments in that the vortex core is larger when filled with the second component than when its density vanishes, making imaging the vortices much easier [56]. A singular pseudospin profile termed the \textit{spin monopole} has also been proposed [57].

The core of a singular topological defect [see Sec. 3.1] in a spinor BEC may either have vanishing density or have its spinor orthogonal to the ground-state manifold [58]. In the polar phase of a spin-1 condensate, the spinor orthogonal to the ground-state manifold is the FM spinor and vice versa. The energy required to force the density to zero in the defect core competes with the spin interaction energy to determine whether the defect will have vanishing density or fill with atoms of the alternate state. Such behaviour has been seen in superfluid $^3\text{He}$, in which the core of a singular vortex in the A-phase fills with the B-phase [10] and vice-versa [59, 60]. If there exists a continuous deformation between two singular defects with different spinors, the system is free to adopt the lowest-energy configuration, which is the state which would be realised in experiments. It is therefore of interest to theoretically study the energetic stability of vortex states, in order to determine whether a vortex may be studied experimentally.

A numerical study in 2D [23] showed that the singular vortex in polar BEC deforms to a nonaxisymmetric state with non-vanishing density. They successfully identified that the complicated structure of the spinor is easily understood in a preferred spinor basis, but did not recognise this as the spinor for a pair of half-quantum vortices [see Sec. 3.4]. A vortex phase diagram showed the energy-minimising vortex for varying $\Omega$ and magnetisation, via the application of an effective linear Zeeman splitting. Subsequently, a phase diagram for the magnetisation and quadratic Zeeman splitting was produced [61].

It was subsequently argued that some of the results of Ref. [23] were unphysical [19], though when one studies the result carefully, the argument of Ref. [19] is incorrect, as will be shown in Sec. 5.2 and Appendix D. Ref. [19] went on to argue that there are three possible vortices with winding numbers greater than zero and up to and including one. They are the half-quantum vortex in the polar phase, the singular vortex in both phases, the singular spin disgyration in the FM phase and the nematic coreless vortex in the polar phase [see Secs. 3.3-3.4]. All other vortex states with winding numbers between zero and one were shown to be equivalent to one of these three via basis transformations. Stability analysis in a non-rotating condensate as the magnetisation varied showed that magnetisations in excess of 0.9 are required to stabilise any of these vortices.

This was then extended to the rotating regime with assumed axisymmetry and the stability of these vortices as a function of magnetisation and rotation were plotted in Ref. [62]. The singular vortex states were also formulated in cylindrical symmetry in Ref. [63], though the imposed symmetry prevented any of the behaviours reported in Refs. [20, 23] from being observed. Further 2D simulation without imposed axisymmetry showed that in both the polar and FM phases, the singly-quantised vortex cores have
non-vanishing densities [20], though no analysis was made in terms of rotated bases. They inferred broken axisymmetry in both cases when, as will be shown in Sec. 5.1, the FM vortex exhibits an axisymmetric density profile in a suitable spinor basis.

An interesting consideration is the condensate whose atomic interactions are independent of the relative spins of the interacting atoms. This has been considered in a non-rotating frame with magnetic field in the angular direction in the $x$-$y$ plane and uniform in the $z$-direction [64]. The induced rotation of the spin vector forced the condensate to exhibit either the coreless or singular FM vortices despite the absence of rotation. The ratio between magnetic fields in the $z$-direction and in the $x$-$y$ plane determined which state was energetically favoured, as the associated spin texture should align with the magnetic field wherever possible.

A variational study showed that in the polar phase at high rotation frequencies, rather than one vortex with a large phase-winding, the system forms a lattice of half-quantum vortices [65], supporting the earlier result that the singly-quantised vortex is higher in energy than a pair of half-quantum vortices [23] (though the author did not explicitly recognise the lowest-energy state as a pair of half-quantum vortices). Ref. [65] also showed that in the FM phase at high rotation frequencies, a lattice of coreless vortices is favoured over a lattice of singular vortices, which is supported by the fact that the coreless vortex is lower in energy than the singular vortex [66, 67]. Both of these vortex lattice structures are also predicted to form when a rotating spinor condensate undergoes a rapid thermal quench [68, 69].

By tuning the scattering lengths of a spin-1 BEC in the two spin channels such that they vary with position, one may create a topological interface. The topology on one side of the interface is that of the polar phase, while on the other side of the interface the topology of the FM phase is formed. There have been recent theoretical proposals to study vortices which cross this topological interface, in order to observe which vortex topologies in the two phases of the ground-state manifold may be connected [70, 71].

As will be discussed in Sec. 2.5, the spin-2 condensate has three distinct phases: FM, polar and cyclic. The increased spin modifies the symmetry of the FM phase such that four classes of vortices exist, rather than the two classes in the spin-1 system [63], though the polar phase is precisely analogous to its spin-1 counterpart. The cyclic phase has a disconnected ground-state manifold. There are two regions, one of which hosts vortices which are classified by two winding numbers rather than one. The other region has a discrete symmetry much like the polar phase [63, 66, 72], such that it may host vortices with fractional winding numbers. This region of the cyclic phase can also exhibit non-Abelian vortices. When two such vortices cross, a vortex rung forms between them [73].

A recent proposal has been made to experimentally generate a fractional vortex in the cyclic phase using pulsed microwave lasers [74]. The authors then went on to study the stability of such vortices theoretically, for varying trap anisotropies and rotation
frequencies. A study of the stability of vortices in the polar and cyclic phases of the spin-2 condensate [75] calculated which vortices minimised the free energy in the absence of a magnetic field. Interestingly, they found that vortices with at least one spinor component containing no phase-winding were always the lowest-energy states, though they did not calculate the density profiles so it is possible that the cores may still have zero density. Neither of the cyclic phases permits point defects, though the non-connected ground-state manifold does permit the formation of domain walls [63].

In fact, the earlier point about the polar phase of spin-2 condensates is only correct in the mean-field treatment. It has been shown [76, 77, 78] that when quantum fluctuations are included, there is a first-order phase transition from the uniaxial nematic familiar from the spin-1 polar phase to a biaxial nematic for a certain set of scattering lengths. The biaxial nematic phase also permits non-Abelian vortices but again we emphasise that this state cannot be realised with mean-field calculations.

We briefly touch on the ground states of the spin-3 condensate in Sec. 2.5 but an analysis of the possible vortex states is far beyond the scope of this project and adds no further understanding to the vortices of a spin-1 condensate. We direct the interested reader to Ref. [79] for a detailed analysis.

The experimental condensation of chromium [80], dysprosium [81] and erbium [82], which have relatively large dipole moments, has caused studies of long-range dipole-dipole interactions to become a topic of keen interest in the spinor BEC community. Dipolar interactions also have nontrivial effects in superfluid $^3$He [9] and nematic liquid crystals [14]. We defer consideration of the effects of dipolar interactions upon vortex structures until Chapter 7. The dipolar interaction of spinor condensates can lead to the spontaneous formation of spin textures [83] and causes the vortex core profile to depend on the polarisation of the condensate [84]. When dipolar interactions are included, there is also a transition from a tangential to a radial spin profile for the lowest-energy coreless vortex structure as the rotation frequency increases [85]. It has also recently been shown that this long-range ordering causes the tangential spin disgyration to be the preferred singular FM vortex [86], as well as modifying the lattice structure of a many-vortex state [87, 88, 89].

Vortices are 1D topological defects — however, for an $N$-dimensional system, defects of dimension up to $N - 1$ may form. There are no 2D defects in the spin-1 system. However, there may be 0D defects, or point defects. In the FM phase, there are no stable point defects. For the polar condensate however, there are an infinite number of classes of point defects in this system, each of which may be labeled with an integer winding number, $Q$. The $Q = 1$ point defect is a monopole in the nematic axis [see Sec. 2.4.1].

The spinor order parameter for the $Q = 1$ monopole in the polar spin-1 BEC was presented in Ref. [90] and methods of generating such monopoles have since been put
forward [91]. However, it has been shown [58] that this monopole is unstable toward the formation of an *Alice ring* for a certain ratio of scattering lengths. The Alice ring is a half-quantum vortex which does not connect to the edge of the condensate but instead forms a closed ring, with the nematic axis rotating by $\pi$ in a closed loop which threads the ring. Such an object preserves the topology of the monopole but this deformation of the core merely recognises that the energy required to form a singular point is greater than that of the vortex ring. The possibility of a non-Abelian monopole in the two-component tripod system has also been suggested [92], although it was subsequently shown that this monopole has zero topological charge in the pseudospin representation [93].

As well as nonsingular vortices, there is also interest in nonsingular pointlike textures, which some in the literature term *Skyrmions* [13, 94], though the definition is somewhat ambiguous. For the purposes of this discussion, a Skyrmion is a nonsingular, pointlike texture. In a Skyrmion, all points on the surface of the condensate map to the same point in the order-parameter space [see Sec. 3.1]. Some references have been made to *singular Skyrmions*, alternatively called *monopoles*. Here, we have chosen to term these monopoles, so that the difference between these objects is explicit.

Although there are no stable monopoles or Skyrmions in the FM BEC [95], there are stable Skyrmions in two-component condensates [96, 97, 98]. There have been proposals to create a Skyrmion in such a system by enclosing a singly-quantised vortex in one component within a singly-quantised vortex ring in the other component [99]. This was then generalised to show that Skyrmions with winding numbers $W = n \times m$ could be generated by enclosing vortices totaling $n$ quanta of angular momentum in the first component, within vortex rings totaling $m$ quanta of angular momentum in the second component [100].

As has been stated, there is no true monopole which can be created in the FM condensate. However, there are proposals to create *Dirac monopoles* [101] in these systems [97]. A Dirac monopole takes the form of a vortex line with one end on the boundary of the medium and the other end somewhere inside the medium. Such objects have also been proposed for study in superfluid $^3$He [102, 103]. The Dirac monopole is not topologically stable and the vortex line will shrink, drawing the monopole out of the system. However, the timescales for such processes are sufficiently long that the monopole may be experimentally observed if it is imprinted on the system in a manner similar to the imprinting of vortices [104]. In precisely the same manner, a monopole-antimonopole pair, connected by a singular vortex, may also be created in the FM spin-1 BEC [97] or in superfluid $^3$He [105].
1.2 Publications Arising

Three publications have arisen from this work. Chapter 5 of this thesis has been published in Physical Review A as Ref. [1]. The work of Chapter 6 is currently being prepared for submission to Physical Review A, while Sec. 6.6 has been submitted to Physical Review Letters.
Chapter 2

Bose-Einstein Condensates

The purpose of this study is to identify the vortex structures which may be observed experimentally in spin-1 atomic BECs. In order to do this, we use fully 3D numerical algorithms to solve classical equations which approximately describe the BEC wavefunction. In the following, we first motivate the formulation of the equations governing which states may be observed experimentally. We then discuss the classical treatment of a BEC of spinless atoms, before generalising to spinor BECs. We then discuss the two phases of the ground-state manifold for a spin-1 BEC.

2.1 Energetic Stability

In a BEC, the mean occupation number $f(i)$ of a single-particle state $i$ is given by the Bose distribution

$$f(i) = \frac{1}{\exp[(E_i - \mu)/k_B T] - 1}$$  \hspace{1cm} (2.1)

where $T$ is the temperature, $\mu$ is the chemical potential and $E_i$ is the energy of the single-particle state $i$. Notice that $f(i)$ goes to infinity as $E_i$ approaches $\mu$. Therefore states with $E \sim \mu$ are of fundamental interest in the study of BECs. In order to identify the wavefunction of such a state, we minimise the energy of the system with respect to variations in the single-atom wavefunction $\psi$. That is,

$$\frac{\delta}{\delta \psi^*} (E - \mu N) = 0.$$  \hspace{1cm} (2.2)

The factor $\mu$ ensures that the number of atoms in the system, $N$, is preserved. Note that there may be multiple solutions to Eq. (2.2). Any of these states may be realised in a BEC, depending on the initial conditions of the system, which leads the solutions of Eq. (2.2) to be termed *energetically stable*. For a more complete treatment of this, see Chapter 2 of Ref. [106].
2.2 The Mean-Field Description

Typical experiments on atomic BECs consist of millions of atoms and so it will come as no surprise to the reader that some simplifications are generally made in the theoretical treatment of these systems. However, the fact that the condensed atoms are described by a single wavefunction does lead to one natural approximation. By treating the system as having zero temperature and assuming that all atoms have undergone condensation, we may approximate the BEC as being described a single-particle wavefunction $\psi(\mathbf{r})$. This approximation is valid in a sufficiently dilute gas, with $na^3 << 1$ where $a$ is the atomic scattering length and $n$ is the atom number density, as realised in current experiments.

In a system with $n\lambda^3 << 1$, where $\lambda$ is the de Broglie wavelength of the atoms, quantum fluctuations become negligible and so $\psi(\mathbf{r})$ may be treated as a classical field.

This energy functional in this mean-field approximation for $N$ condensate atoms reads

$$E = N \int d^3r \left[ \frac{1}{2m} |\hat{p}\psi(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{N-1}{2} U |\psi(\mathbf{r})|^4 \right],$$

(2.3)

where $\hat{p}$ is the momentum operator $\hat{p} = -i\hbar\nabla$, $V(\mathbf{r})$ is an external potential and $U_0$ is the energy associated with the interaction of two atoms. This interaction is treated as a delta-function but nonlocal interactions such as the atomic dipole-dipole interaction can also occur. We will consider the effects of dipolar interactions in Chapter 7 but defer them for the present discussion. The factor $(N-1)/2$ denotes the fact that each atom interacts with the $N-1$ other atoms in the system, with the factor 2 preventing double-counting. The nonlinear term forms an effective potential as the atoms interact with the mean field associated with the rest of the condensate atoms. Since $N >> 1$, we replace the $N-1 \rightarrow N$.

We then introduce the BEC wavefunction

$$\Psi(\mathbf{r}) = \sqrt{N}\psi(\mathbf{r}),$$

(2.4)

which may then be used to calculate the local number density of atoms via

$$n(\mathbf{r}) = |\Psi(\mathbf{r})|^2.$$  

(2.5)

The energy functional is then

$$E = \int d^3r \left[ \frac{1}{2m} |\hat{p}\Psi(\mathbf{r})|^2 + V(\mathbf{r}) |\Psi(\mathbf{r})|^2 + \frac{U}{2} |\Psi(\mathbf{r})|^4 \right].$$

(2.6)

Taking the functional derivative as in Eq. (2.2), one arrives at the Gross-Pitaevskii Equation (GPE),

$$\left( \frac{\hat{p}^2}{2m} + \hat{V} + U_0 |\Psi|^2 \right) \Psi = \mu \Psi.$$  

(2.7)
Here, we have defined the potential operator \( \hat{V} \) such that \( \Psi^*(r) \hat{V} \Psi(r) = V(r) |\Psi(r)|^2 \). Generally \( \hat{V} = V(r) \) but we retain this formalism to aid the extension of this treatment to spinor condensates.

The potential \( \hat{V} \) takes the form \( \hat{V}_{\text{opt}} + \hat{V}_{\text{mag}} \), where \( \hat{V}_{\text{opt}} \) is the optical trapping potential and \( \hat{V}_{\text{mag}} \) is the energy shift due to the particle’s spin in the presence of an external magnetic field. Throughout this study we assume a harmonic trap potential which can be arbitrarily isotropic or anisotropic

\[
\hat{V}_{\text{opt}} = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right),
\]  

(2.8)

where \( \omega_i \) is the trapping frequency in the \( i \) direction. If the trap is rotating with an angular velocity \( \Omega \), this then becomes

\[
\hat{V}_{\text{opt}} \Psi = \left( \frac{m \omega_x^2}{2} (x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) - \Omega \cdot \hat{L} \right) \Psi,
\]

(2.9)

in the rotating frame of reference, where \( \gamma_i = \omega_i / \omega_x \). \( \hat{L} \) is the angular momentum operator and the dot product indicates the fact that the angular momentum and the rotation axis are not necessarily aligned. The energy shift due to a magnetic field depends on the atomic spin, which will be discussed in Sec. 2.3.

Eq. (2.7) is in fact the time-independent GPE, while the time-dependent GPE reads

\[
i \hbar \frac{\partial \Psi}{\partial t} = \left( \frac{\hat{p}^2}{2m} + \hat{V} + U_0 |\Psi|^2 \right) \Psi,
\]

(2.10)

which we will tend to write in terms of the Hamiltonian operator,

\[
\hat{H} \Psi = i \hbar \frac{\partial \Psi}{\partial t},
\]

(2.11)

for brevity. The study of real-time dynamics of BECs is beyond the scope of this work, as our aim is simply to identify the energetically stable states, which would then be macroscopically occupied in experiments. We do, however, make use of the time-dependent GPE in a procedure to minimise the energy functional, which is described in Sec. 4.4. More detail on the derivation of the GPE can be found in Chapter 6 of Ref. [106] and in Sec. V of Ref. [3].

### 2.3 Spinor BECs

When the energy separations of multiple low-energy states of a system are small compared to the chemical potential, these different energy states become degenerate and so the condensate is no longer composed purely of atoms in one state but a combination of
Chapter 2 Bose-Einstein Condensates

the different states. While in early experiments, the condensed gas was held in a magnetic trap, forcing the atoms into a single Zeeman level, the use of purely optical traps enables the study of condensates with degenerate spin states \[107\]. Spin-1 condensates have been realised in, for example, sodium \[5, 6, 108\] and rubidium \[109, 110\]. Rubidium has also been used to create a spin-2 condensate \[110, 111, 112\], as has dysprosium \[81\]. Spin-3 condensates have also been realised in chromium \[80, 113, 114\]. These \textit{spinor} condensate experiments have observed novel behaviours, such as the formation of spin domains analogous to the magnetic domains in ferromagnets \[6, 115\].

A condensate of spin-\(F\) atoms exhibits a degeneracy of \(2F + 1\) states in the ground state in the presence of a sufficiently small (or zero) magnetic field, since the only energy difference between these states is due to the interaction of the atomic spin with the magnetic field. This degeneracy corresponds to the atomic spin having projections \(m_F = -F, 1 - F, ..., 0, ..., F - 1, F\) in the direction of the weak magnetic field. This degeneracy can be lifted by spin-dependent interactions between the atoms, as will be discussed in Secs. 2.4-2.5. As a result of this degeneracy of states, it is possible to have collisions between atoms which shift both atoms into different spin states. If the dominant process is \(s\)-wave scattering, as it is on experimental timescales, then both the total spin and the projection of the total spin in the direction of the magnetic field are conserved. This projection must be an integer for bosons, which restricts the possible scattering channels.

As a result of such collisions, the particle number in each state is no longer a conserved quantity and spinor notation \[116\] must be employed. In spinor notation, the particle wavefunction is replaced by a column vector, whose components are the wavefunctions of the different Zeeman sublevels. As a result, the order parameter is no longer a scalar but a normalised \(2F + 1\)-component spinor, \(\vec{\zeta}\), with each component being complex,

\[
\Psi = \sqrt{n}\vec{\zeta} = \sqrt{n}\begin{pmatrix} \zeta_F \\ \vdots \\ \zeta_0 \\ \vdots \\ \zeta_{-F} \end{pmatrix},
\]

(2.12)

where it is convenient to introduce \(\Psi_i = \sqrt{n}\zeta_i\).

The nonlinearity term \(U_0\) in the GPE [Eq. (2.7)] is replaced by a matrix \(\hat{C}\) which represents interactions between the different species. Adopting spinor notation, then, gives

\[
\hat{H}\Psi = \left(\frac{p^2}{2m} + \hat{V} + \Psi^\dagger\hat{C}\Psi\right)\Psi,
\]

(2.13)

where \(\Psi^\dagger = (\Psi^*)^T\) is the row vector of complex conjugates of \(\Psi\), such that

\[
\Psi^\dagger\Psi = \Sigma_m |\Psi_m|^2 = \Sigma_m n |\zeta_m|^2 = n.
\]

(2.14)
The term $U_0|\Psi|^2$ is replaced by $\Psi^\dagger \hat{C} \Psi$ since $\hat{C}$ is a matrix operator, with diagonal elements representing interactions between atoms in the same Zeeman level and off-diagonal elements representing interactions between different Zeeman levels. Expanding in terms of optical and magnetic potentials $\hat{V}_{\text{opt}}$ and $\hat{V}_{\text{mag}}$ respectively, we have

$$\hat{H} = \left( \frac{\hat{p}^2}{2m} + \hat{V}_{\text{opt}} + \hat{V}_{\text{mag}} + \Psi^\dagger \hat{C} \Psi \right) \Psi.$$  

These derivations are shown in more depth in Sec. VI. C. of Ref. [3] and Chapters 5, 6, 9 and 12 of Ref. [106].

## 2.4 Spin-1 Condensates

When a BEC of spin-1 atoms is trapped by purely optical means, the spinor wavefunction $\vec{\zeta}$ has three components. In the basis of spin projection onto the $z$ axis, we write

$$\Psi = \sqrt{n} \vec{\zeta} = \sqrt{n} \begin{pmatrix} \zeta_+ \\ \zeta_0 \\ \zeta_- \end{pmatrix}, \quad \vec{\zeta}^\dagger \vec{\zeta} = 1.$$  

Note that since there are only three spinor components, we only label the sign of the $m_F = \pm 1$ Zeeman levels. The 3-component spinor defines the local spin vector $\langle \vec{F} \rangle = \zeta_\alpha^\dagger \hat{F}_{\alpha\beta} \zeta_\beta$. The spin operator, $\hat{F}$, is the vector of spin-1 Pauli matrices,

$$\hat{F} = \hat{F}_x \hat{x} + \hat{F}_y \hat{y} + \hat{F}_z \hat{z}$$

$$\hat{F}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\hat{F}_y = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\hat{F}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Appendix A describes the origin of these matrices and how to generate Pauli matrices for any spin-$F$ system.

The Hamiltonian operator in the rotating frame of reference for the spin-1 BEC in mean-field theory is then

$$\hat{H} = \left[ \frac{\hat{p}^2}{2m} + \frac{m\omega_z^2}{2} \left( x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2 \right) - \vec{\Omega} \cdot \vec{L} + \hat{V}_{\text{mag}} + \Psi^\dagger \hat{C} \Psi \right] \Psi.$$  

(2.17)
The spins of colliding spin-1 atoms can combine to either 0 or 2. The $s$-wave scattering then proceeds via two spin channels with scattering lengths $a_0$ and $a_2$ respectively. The interaction term in the Hamiltonian is thus rewritten as

$$\hat{C} = \left( U_0 \hat{P}_0 + U_2 \hat{P}_2 \right), \quad (2.19)$$

where $U_0$ is the energy due to the interaction of two spin-antiparallel atoms (net spin zero) and $\hat{P}_0$ is the projection operator for the zero spin state. $\hat{P}_2$ and $U_2$ are the analogues of these for spin-parallel atoms (net spin 2). The $U_n$ represent the interaction energies of the two scattering channels with scattering lengths $a_n$. Substituting the definitions of the two projection operators, one may derive the relationship

$$\hat{C}_{\alpha\beta} = U_0 \delta_{\alpha\beta} + \frac{2U_2}{3} \hat{F}_{\alpha\gamma} \cdot \hat{F}_{\gamma\beta} = U_0 \delta_{\alpha\beta} + c_2 \hat{F}_{\alpha\gamma} \cdot \hat{F}_{\gamma\beta}. \quad (2.20)$$

We therefore have two interaction energies

$$c_0 = \frac{4\pi \hbar^2}{3m} (2a_2 + a_0), \quad c_2 = \frac{4\pi \hbar^2}{3m} (a_2 - a_0), \quad (2.21)$$

which are spin-independent and spin-dependent, respectively. Notice that if $c_0 + c_2 < 0$ (ie. $a_2 < 0$), having $|\langle \hat{F} \rangle| = 1$ causes increasing density to decrease the energy in the system and so the condensate becomes unstable towards collapse [117].

Although spinor condensates can only exist in weak or zero magnetic fields, this field must still be accounted for in the Hamiltonian. For a particle with spin $\langle \hat{F} \rangle$ in the presence of a magnetic field $B$,

$$\hat{V}_{\text{mag}} \Psi = g_1 B \cdot \hat{F} \Psi + g_2 (B \cdot \hat{F})^2 \Psi, \quad (2.22)$$

where $g_1$ and $g_2$ are coupling constants for the linear and quadratic Zeeman splittings, respectively [118]. This is only an approximation and breaks down when the above Zeeman energy approaches the hyperfine splitting. However, the system is no longer a spinor condensate in this regime and so we may consider only the linear and quadratic terms. Hence the effective rotating-frame potential becomes

$$\hat{V}_{\text{eff}} = \frac{m\omega_x^2}{2} \left( x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2 \right) - \Omega \cdot \hat{L} + g_1 B \cdot \hat{F} + g_2 (B \cdot \hat{F})^2 + c_0 \Psi^\dagger \Psi + c_2 [\Psi^\dagger \hat{F} \Psi] \cdot \hat{F}, \quad (2.23)$$

from which we also define the harmonic oscillator length $l = \sqrt{\hbar/m\omega_x}$. If an external magnetic field is applied, this fixes the spinor basis. We take the field to be in the $z$ direction, such that no modification is required in transforming to the rotating frame of reference. This yields a Gross-Pitaevskii type equation for each of the three spinor
components,

\[ \hat{H}\Psi_+ = \left( \frac{\hat{p}^2}{2m} + \frac{m\omega_z^2}{2} \left( x^2 + \gamma_0^2 y^2 + \gamma_z^2 z^2 \right) - \Omega \cdot \hat{L} + g_1 B_z + g_2 (B_z)^2 + c_0 \Psi^\dagger \Psi \right. \\
+ c_2 \left[ |\Psi_+|^2 + |\Psi_0|^2 - |\Psi_-|^2 \right] \right) \Psi_+ + c_2 \Psi_+^* \Psi_0^2, \]

\[ \hat{H}\Psi_0 = \left( \frac{\hat{p}^2}{2m} + \frac{m\omega_z^2}{2} \left( x^2 + \gamma_0^2 y^2 + \gamma_z^2 z^2 \right) - \Omega \cdot \hat{L} + c_0 \Psi^\dagger \Psi \right. \\
+ c_2 \left[ |\Psi_+|^2 + |\Psi_-|^2 \right] \right) \Psi_0 + 2c_2 \Psi_0^* \Psi_+ \Psi_- , \]

\[ \hat{H}\Psi_- = \left( \frac{\hat{p}^2}{2m} + \frac{m\omega_z^2}{2} \left( x^2 + \gamma_0^2 y^2 + \gamma_z^2 z^2 \right) - \Omega \cdot \hat{L} - g_1 B_z + g_2 (B_z)^2 + c_0 \Psi^\dagger \Psi \right. \\
+ c_2 \left[ |\Psi_-|^2 + |\Psi_0|^2 - |\Psi_+|^2 \right] \right) \Psi_- + c_2 \Psi_-^* \Psi_0^2. \]

Notice that if \( \zeta_0 \) is initially set to zero everywhere, it will remain zero at all subsequent times. Likewise if \( \zeta_\pm \) are both initially zero everywhere, they will remain zero. This puts an important constraint on the initial state; it must have non-vanishing densities in all three components in order to identify any stable state with non-zero populations of all three components. As will be shown in Section 2.4.1, a state with vanishing density in one or more components can be transformed into a state with non-vanishing densities in all three components via rotation of the quantisation axis.

### 2.4.1 The Ground-State Manifold

In order to predict which states may be observed in spinor BEC experiments, we wish to find the local minima of the energy functional. However, the solutions may not be unique if there is some symmetry in the Hamiltonian.

The GPE for a spin-1 atomic BEC with contact interactions is

\[ \hat{H}\Psi = \left( \frac{\hat{p}^2}{2m} + \frac{m\omega_z^2}{2} \left( x^2 + \gamma_0^2 y^2 + \gamma_z^2 z^2 \right) - \Omega \cdot \hat{L} + g_1 B \cdot \hat{F} + g_2 (B \cdot \hat{F})^2 + c_0 n \right. \\
+ c_2 \langle \hat{F} \cdot \hat{F} \rangle \right) \Psi. \]

The ground-state manifold is then the group of distinguishable, energetically degenerate spinors which minimise the energy of the system [see Sec. 3.1]. In the presence of a magnetic field \( B = B_z \hat{z} \) which is sufficiently strong, such that \( g_1 B_z \sim \mu \) or \( g_2 B_z \sim \mu \), where \( \mu \) is the chemical potential, the degeneracy of the \( m_F = 0, \pm 1 \) states is lifted and the remaining symmetry depends on the signs and relative magnitudes of \( g_1 B_z \) and \( g_2 B_z \).

In this study we focus only on weak magnetic fields so that the symmetry of the system is determined purely by \( c_2 \). While the present work is restricted to the spin-1 case, we shall also briefly discuss the symmetry for higher-spin and two-component condensates.

When atomic interactions and magnetic fields are neglected in the spin-1 GPE, the ground-state manifold is \( S^5 \) — all normalised spinors are degenerate [63]. This symmetry
arises from the fact that there are five independent free parameters which, together, must preserve the normalisation of the spinor $\vec{\zeta}$. There is no term in the Hamiltonian which distinguishes between the different spinors. When interactions are included and dominate over a weak magnetic field, the term which breaks the $S^5$ symmetry is the spin-dependent interaction. This term is left invariant under rotations of the spinor through three Euler angles $\alpha$, $\beta$ and $\gamma$, together with global phase rotations through $\phi$, such that

$$\vec{\zeta}_r = e^{i\phi} \exp \left( -i \vec{F}_\alpha \right) \exp \left( -i \vec{F}_y \beta \right) \exp \left( -i \vec{F}_z \gamma \right) \vec{\zeta}_i,$$  

$$ = e^{i\phi} \begin{pmatrix} e^{-i(\alpha+\gamma) \cos^2 \frac{\beta}{2}} & -e^{-i\alpha} \sin \beta & e^{-i(\alpha-\gamma) \sin^2 \frac{\beta}{2}} \\ \frac{e^{i\alpha}}{\sqrt{2}} \sin \beta & \cos \beta & -\frac{e^{-i\gamma}}{\sqrt{2}} \sin \beta \\ e^{i(\alpha-\gamma) \sin^2 \frac{\beta}{2}} & e^{i\alpha} \sin \beta & e^{i(\alpha+\gamma) \cos^2 \frac{\beta}{2}} \end{pmatrix} \vec{\zeta}_i,$$  

where $\vec{F}_i$ is the $i^{th}$ spin-1 Pauli matrix, $\vec{\zeta}_i$ is the initial spinor and $\vec{\zeta}_r$ is the spinor after rotation.

The spin-dependent interaction term in Eq. (2.25) gives rise to two separate phases of the ground-state manifold in a uniform, non-rotating spin-1 atomic BEC in the absence of magnetic fields. When $c_2 < 0$, as for $^{87}$Rb [119, 120], the ferromagnetic (FM) phase with $|\langle \vec{F} \rangle| = 1$ is energetically favourable [7]. This spinor’s ground-state manifold is the group of orientations of a triad of orthonormal vectors, $SO(3)$. These vectors may be defined in terms of the spinor basis vectors

$$\vec{\eta} + i\vec{\nu} = \frac{1}{\sqrt{2}} \begin{pmatrix} \zeta_- - \zeta_+ \\ -i(\zeta_+ + \zeta_-) \\ \sqrt{2}\zeta_0 \end{pmatrix}$$

$$\langle \vec{F} \rangle = \vec{\eta} \times \vec{\nu},$$

which can be defined regardless of $|\langle \vec{F} \rangle|$. From Eq. (2.29), it follows that in the FM phase, $\vec{\eta} \cdot \vec{\nu} = 0$.

By contrast, when $c_2 > 0$, as for $^{23}$Na [119, 121, 122], the polar phase with $|\langle \vec{F} \rangle| = 0$ is favoured. The ground-state manifold is the group of rotations of a nematic axis combined with global phase rotations, $(S^2 \times S^1)/\mathbb{Z}_2$. Ref. [7] initially classified the symmetry as $S^2 \times S^1$ and it was left for Ref. [123] to point out that the polar spinor can in fact be expressed in terms of the global condensate phase, $\phi$, and an unoriented axis, $\hat{d}$. Such unoriented axes are well studied in nematic liquid crystal systems and $\hat{d}$ is conventionally referred to as the nematic axis. The polar phase is realised when the spinor basis vectors, $\vec{\eta}$ and $\vec{\nu}$, are parallel or antiparallel. $\hat{d}$ then represents the axis on which $\vec{\eta}$ and $\vec{\nu}$ align or antialign and so $\hat{d}$ itself is unoriented. The unoriented nature of $\hat{d}$ leads it to be termed the nematic axis, and the polar phase has the property $\vec{\zeta}(\phi, \hat{d}) = \vec{\zeta}(\phi + \pi, -\hat{d})$, giving rise to the factorisation by $\mathbb{Z}_2$ which had originally not been recognised. This
property will be crucial in classifying the vortices in the polar phase. In the following we shall refer to \( c_2 < 0 \) (\( c_2 > 0 \)) as the FM (polar) regime, while a condensate whose wavefunction fulfills \( |\langle \hat{F} \rangle | = 1 \) (\( |\langle \hat{F} \rangle | = 0 \)) will be said to exhibit the FM (polar) phase. It should be noted that the ground-state manifolds specified above only hold when the magnetic field is absent or very weak. A phase diagram for varying quadratic Zeeman splittings is presented in Ref. [124].

### 2.5 Other Spinor Condensates

For the spin-2 condensate, the GPE takes the form [125]

\[
\hat{H} \Psi = \left( \frac{\hat{p}^2}{2m} + \frac{m \omega^2}{2} (x^2 + \gamma^2 y^2 + \gamma^2 z^2) \right) - \hat{\Omega} \cdot \hat{\mathbf{L}} + g_1 \mathbf{B} \cdot \hat{\mathbf{F}} + g_2 (\mathbf{B} \cdot \hat{\mathbf{F}})^2 + c_0 \Psi^\dagger \Psi \\
+ c_2 \left( \Psi^\dagger \hat{\mathbf{F}} \Psi \right) \cdot \hat{\mathbf{F}} + c_4 \Psi^\dagger \hat{P}_0 \Psi \right) \Psi,
\]

(2.30)

where \( \hat{P}_0 \) is the projection operator onto the spin-zero state. Note that this is not the notation generally adopted in the spin-2 condensate literature but has been adapted for comparison with the spin-1 case. The parameters \( c_0 \) and \( c_2 \) are modified by interactions in the spin-4 channel and so are not physically the same as those for the spin-1 case. The additional term \( c_4 \hat{P}_0 \) modifies the symmetry of this Hamiltonian such that there are now three possible ground states.

The ferromagnetic phase has \( |\langle \hat{F} \rangle | = 2, \langle \hat{P}_0 \rangle = 0 \) and is analogous to the spin-1 ferromagnetic phase, though the increased spin modifies the ground-state manifold to \( \text{SO}(3)/\mathbb{Z}_2 \) [63, 66]. The polar phase has \( |\langle \hat{F} \rangle | = 0, |\langle \hat{P}_0 \rangle | = 1 \) and is also analogous to its spin-1 counterpart [63]. The third phase, the cyclic phase, has no analogue in spin-1 BEC and is defined by \( |\langle \hat{F} \rangle | = 0, \langle \hat{P}_0 \rangle = 0 \). This phase has a non-connected ground-state manifold [63, 66, 125], consisting of two subgroups denoted the C0 and C1 phases.

Many of the experimental techniques for the study of spin-2 condensates are the same as those developed for spin-1 systems, such as the Stern-Gerlach splitting before measurement and the ability to use quadratic Zeeman splitting to prepare the initial state. However, the spin dynamics are sensitive to the choice of initial state [111]. Ref. [112] demonstrates the dependence of these dynamics on the strength of magnetic field applied, placing constraints on the level below which the background field must drop before its effects are negated. They infer a ground state for \( F = 2 \text{ }^{87}\text{Rb} \) that is either polar or cyclic in nature, in agreement with past experiments, which had indicated that the ground state should be polar but very close to the transition to the cyclic phase [111, 119]. Calculations of loss rates have also put limits on the timescales on which such experiments can be conducted [111, 112].
For a spin-3 condensate, such as $^{52}\text{Cr}$, an additional term appears in the Hamiltonian due to scattering of atoms in the spin-6 channel. We will not reproduce the Hamiltonian here but there are thorough treatments in Refs. [79, 126, 127, 128].

The ground state structure continues to grow richer as the spin increases [cf. Ref. [129] for spins up to 4], though an interesting suggestion is that the different ground states available to a spin-\(F\) condensate may be identified with \(2F\) points on a unit sphere, from which a polynomial may be derived and then minimised for the varying spin-dependent scattering lengths to identify the ground states [76]. This is well beyond the scope of this project and so we draw attention to one final variant of the spinor condensate; an effectively spin-1/2 system.

Shortly after the first experimental creation of an atomic BEC in 1995 [130, 131, 132] came the successful condensation of two separate atomic species [133]. In fact the first experimental creation of a BEC vortex came in a two-component condensate [24]. A two-component BEC may be achieved either using a single atomic isotope in two hyperfine spin states, two isotopes of the same atom or two entirely different atomic species.

One might at first expect this system to act like two independent order parameters, but interspecies interactions cause the system to adopt a single order parameter to describe both components. By assigning a pseudospin to each of the two components, an effectively spin-1/2 system is created, described by an effective spinor wavefunction

$$\Psi_{\text{eff}} = \sqrt{n}\zeta_{\text{eff}} = \left( \frac{\sqrt{n_a}e^{i\phi_a}}{\sqrt{n_b}e^{i\phi_b}} \right),$$

(2.31)

where $\sqrt{n_a}$ and $\phi_a$ are the number density of atoms and wavefunction phase for species a, and likewise for species b. Assigning pseudospin $+1/2$ to species a and $-1/2$ to species b, pseudospin textures will form as the relative densities and phases in the two components vary. In a true spin-1/2 system, the ground-state manifold is SU(2), though the inter-species interactions can break this symmetry.

The strength of the pseudospin analogy is also dependent on the nature of the two components which are trapped - if the populations of each individual component must be conserved, an effective magnetisation [See Sec. 2.6] of the system is induced, whereas if there is some coherent coupling between the two components enabling a transfer of atoms between them, such as the trapping of two hyperfine states of the same isotope, then the effective magnetisation may vary and much richer spin dynamics may be observed. An intriguing extension of this idea is to couple three low-level hyperfine spin states to one higher-energy state, which can be shown [92] to reduce to a two-component wavefunction. This specific system, known as the **tripod system** [92, 134], has the added benefit of being able to introduce synthetic gauge fields by varying spatially the relative strengths of the lasers coupling to the three low-energy states.
Prior to the recent surge in work on atomic BECs came a wealth of research on superfluid liquid $^3$He, which consists of pairs of fermionic atoms forming composite bosons, rather than bosonic atoms. As a result, $^3$He has a richer order-parameter space than spin-1 systems [See Sec. 2.4.1] in that both the spin and the orbital angular momentum of the pair are free to rotate, which, combined with global gauge symmetry, gives an overall ground-state manifold of $SO(3) \times SO(3) \times S^1$ when atomic interactions are neglected. The spin and orbital angular momentum are both equal to one and so many of the features of spin-1 atomic BECs were first seen in $^3$He.

As in the case of spinor BECs, with these added degrees of freedom come added terms in the energy functional, giving rise to a larger number of possible ground states dependent on the strength of angular momentum-dependent scattering, spin-dependent scattering, spin-orbit coupling, etc. $^3$He also has a large dipole moment compared to atomic BECs and so long-range interactions also play an important role. Although non-negligible dipolar effects are observed in, eg $^{52}$Cr [80, 135], in the majority of spinor BECs the dipolar interaction does not play a role on experimental timescales and so we defer its discussion until Chapter 7. In the absence of a magnetic field, only the so-called A and B phases of $^3$He are stable [10, 136, 137, 138], so we shall restrict our attention to these states. Within this treatment we will also focus on features which are relevant to spin-1 atomic BECs.

The order parameter of superfluid $^3$He is a $3 \times 3$ matrix $A_{m,l}$, with each component being complex. The components correspond to combinations of spin quantum numbers $m = 0, \pm 1$ and orbital angular momentum quantum numbers $l = 0, \pm 1$. The B-phase of $^3$He is that with the spin and angular momentum antiparallel [10], such that $m + l = 0$. With this relationship fixed, one can consider rotations of, say, the spin vector, in the knowledge that these rotations naturally determine the new orientation of the angular momentum. The order parameter reduces to three components, $A_{1,0}$, $A_{0,0}$ and $A_{-1,1}$.

The A-phase of $^3$He has unit orbital angular momentum and vanishing spin, though the spin and angular momentum axes are free to rotate with respect to one another when the dipole term is neglected. When the dipolar interactions become large, these axes align and two possibilities arise [10]: either $A_{1,0} = 1$ and all other components vanish or $A_{1,1} = A_{1,-1} = 1/\sqrt{2}$ and all other terms vanish. The spin quantisation axis is a nematic and so the ground-state manifold due to spin rotations is $S^2/Z_2$. That for rotations of the angular momentum is SO(3), giving a ground-state manifold for the A-phase of $(SO(3) \times S^2)/Z_2$ [10]. Many behaviours arising from the nematic axis seen in this system were later seen in the polar phase of the spin-1 BEC, though the additional SO(3) symmetry does introduce some effects which are not seen in the spin-1 polar BEC.

In regions where the superfluid or BEC leaves the ground state, such as in the cores of singular defects, the analogy between $^3$He and spin-1 condensates breaks down.
2.6 Longitudinal Magnetisation

The s-wave scattering preserves angular momentum, and therefore any spin-flip scattering arising from Eq. (2.20) must preserve the relative spin of colliding atoms [110, 139, 45]. The only allowed spin-flip processes in a spin-1 BEC are therefore

\[ 2 |m_F = 0 \rangle \leftrightarrow |m_F = +1 \rangle + |m_F = -1 \rangle. \tag{2.32} \]

Defining the local longitudinal magnetisation density as

\[ M(r) = \langle \hat{F}_z \rangle, \tag{2.33} \]

it follows from Eq. (2.32) that the total longitudinal magnetisation

\[ M = \frac{1}{N} \int n(r) M(r) d^3r = \frac{N_+ - N_-}{N} \tag{2.34} \]

is preserved by s-wave scattering. Here \( N \) is the total number of atoms and \( N_{\pm} \) are the populations of the \( m_F = \pm 1 \) Zeeman levels. Consequently, \( M \) is approximately conserved on time scales where s-wave scattering dominates over, e.g. dipolar interactions and collisions with high-temperature atoms. This is the relevant time scale in present experiments with spinor BECs of alkali-metal atoms [6, 45, 110] and its value can be experimentally controlled.

One may also define transversal magnetisations arising from the \( x \) and \( y \) components of the spin. However, a weak external magnetic field determines a preferred direction, which we will take to be the \( z \) axis, and only the longitudinal magnetisation in this direction is approximately conserved.

2.7 Characteristic Length Scales

As was discussed in Sec. 2.4.1, the ground state of a uniform spin-1 atomic BEC is the polar (FM) phase in when the spin-dependent interactions are polar (FM) in nature. However, in experiments the condensate is nonuniform — for example, there is a density gradient due to the harmonic trap. A system containing a topological defect is also inherently nonuniform, while a condensate with polar interactions and a nonzero magnetisation must necessarily exhibit regions of nonzero spin (i.e. non-polar phase) in order to produce the nonzero magnetisation. We therefore now discuss the length scales associated with spin and density perturbations. We also present an approximate calculation of length scales defined by the magnetisation in a spin-1 BEC containing a vortex. We calculate this from an analytical model in which the magnetisation is concentrated either entirely in the vortex core or entirely outside the core. We then present an analogous argument for a positively-magnetised bulk and negatively-magnetised vortex
core. These will enable us to understand the energetically stable vortex core structures of spin-1 atomic BECs, presented in Chapters 5-6.

2.7.1 Healing Lengths

A vortex core represents a singularity of the order parameter. On the singular line the order parameter must either vanish or be orthogonal to the ground-state manifold. However, if this deviation of the order parameter from its large-distance profile is only on the singular line itself, the gradient energy associated with the vortex will be infinite. Such a deviation from the background order-parameter profile, whether associated with a topological defect or some other physical effect, has an associated healing length, which constrains the size of any region over which the order parameter deviates from its large-distance behaviour.

Let us consider as an example a 1D BEC in a potential well of length \( L \). \( V(|x| < L/2) = 0 \) and \( V(|x| \geq L/2) \to \infty \). The order parameter must vanish at \( x = \pm L/2 \). For a noninteracting BEC, \( \Psi(x) \) would be a superposition of sine waves with wavelength 2\( L \). However, the inclusion of (repulsive) atomic scattering favours constant density where \( V(x) = 0 \). One then solves the simplified GPE

\[
-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) + U_0 |\Psi(x)|^2 \Psi(x) = \mu \Psi(x).
\] (2.35)

By solving this GPE numerically with the boundary conditions \( \Psi(x = \pm L/2) = 0 \), one finds that the density “heals” from zero at the edge of the well to a uniform value \( n \) inside the box. The healing occurs over the size given by the density healing length \( \xi_n \) [3]. This same argument may be applied to any externally-applied condition which forces the density to vanish at some point, to determine the healing of the density back to its bulk value. A density profile which approximately solves Eq. \( (2.35) \) is

\[
N(x) = \tan \left( \frac{x}{\sqrt{2\xi_n}} \right),
\] (2.36)

which is plotted in Fig. 2.1, showing that the density heals to its background value over a length scale \( \sim \xi_n \).

Rather than solving Eq. \( (2.35) \) numerically, one may instead consider the simplified problem

\[
-\frac{\hbar^2}{2m\xi_n^2} n + U_0 n^2 = 0 \quad (2.37)
\]

where the gradient has been replaced by \( \xi_n^{-1} \) as an approximation. The size of the density-depleted region is then approximately \( \xi_n \). By rearranging Eq. \( (2.37) \) and solving for \( \xi_n \), it follows that

\[
\xi_n = \frac{\hbar}{\sqrt{2mnU_0}}.
\] (2.38)
In the 3D harmonic trap we consider, the density profile is not uniform and nor is the potential. However, by adopting the local values of the potential and the density such that they are both effectively constant. The potential then does not play a role in the healing of the atomic density. In this system, the density healing length is calculated as

\[
\xi_n = l \left( \frac{\hbar \omega_x}{2 |c_0 n|} \right)^{1/2}. 
\]

(2.39)

Here, \( l \) is the harmonic oscillator length defined in Sec. 2.4. The spin-dependent interaction similarly yields a \textit{spin healing length},

\[
\xi_F = l \left( \frac{\hbar \omega_x}{2 |c_2| n} \right)^{1/2}, 
\]

(2.40)

which represents the characteristic length scale over which \(|\langle \hat{F} \rangle|\) is restored to its bulk value around a local perturbation. In spin-1 BECs of \(^{23}\text{Na}\) and \(^{87}\text{Rb}\), \( c_2 \sim 0.036c_0 \) \([119, 121, 122]\) and \( c_2 \sim -0.005c_0 \) \([119, 120]\), respectively, illustrating that usually \( \xi_F > \xi_n \) in experimentally relevant scenarios. Some example values of the healing lengths are presented in Table 2.1.

### 2.7.2 Magnetisation Lengths

The conservation of longitudinal magnetisation, which is the subject of Chapter 6, introduces a third length scale \( \eta_M^{(1)} \), which is the size required for a magnetised vortex
core in an otherwise unmagnetised condensate to give rise to a given magnetisation. In order to estimate the magnetisation length scale we represent the magnetised core by a cylinder of radius \( \eta_M^{(1)} \), with \( \langle \hat{F} \rangle = \hat{z} \) everywhere inside the core and \( |\langle \hat{F} \rangle| = 0 \) outside. The total magnetisation is then

\[
M(\eta_M^{(1)}) = \frac{1}{N} \int d^3r \, \Theta(\eta_M^{(1)} - \rho) n_{TF}(r),
\]

where \( \rho = (x^2 + y^2)^{1/2} \) and \( \Theta \) is the Heaviside function. We approximate the atomic-density profile by the Thomas-Fermi solution, which is valid when the kinetic energy is small compared to the other terms in the energy functional \([106]\). For large atom numbers, this approximation holds except at the edge of the trap. The Thomas-Fermi density profile is

\[
n_{TF}(r) = \frac{15N}{8\pi R_{TF}^3} \left(1 - \frac{r^2}{R_{TF}^2}\right), \quad r \leq R_{TF},
\]

where \( r = (\rho^2 + z^2)^{1/2} \), and

\[
R_{TF} = l \left(\frac{15 N c_{p,f}}{4\pi \hbar \omega l^3}\right)^{1/5}
\]

is the Thomas-Fermi radius. Here \( c_p = c_0 \) in a BEC with polar interactions, and \( c_f = c_0 + c_2 \) in the FM regime. Computing the integral in Eq. (2.41) and solving for \( \eta_M^{(1)} \) as a function of \( M \), we obtain

\[
\eta_M^{(1)} = R_{TF} \sqrt{1 - (1 - M)^{2/5}}.
\]

An analogous length scale \( \eta_M^{(2)} \) may be defined as the size required for an unmagnetised vortex core in an otherwise magnetised condensate to generate the requisite magnetisation. We represent the unmagnetised core by a cylinder of radius \( \eta_M^{(2)} \), with \( |\langle \hat{F} \rangle| = 0 \) inside the core and \( \langle \hat{F} \rangle = \hat{z} \) outside. The total magnetisation may then be calculated, again by approximating the density profile as the Thomas-Fermi solution, yielding

\[
M(\eta_M^{(2)}) = \frac{1}{N} \int d^3r \, \Theta(\rho - \eta_M^{(2)}) n_{TF}(r).
\]

Solving for \( \eta_M^{(2)} \) yields

\[
\eta_M^{(2)} = R_{TF} \sqrt{1 - M^{2/5}}.
\]

A recent topological analysis of vortex states in spin-1 BECs \([140]\) demonstrated the formation of a vortex with a highly nontrivial core structure, the details of which will be discussed in Sec. 6.5. The crucial features relevant to this treatment are that the outer bulk forms a domain of uniform spin, with the vortex core forming a domain of opposing spin. We may estimate the size of the inner spin domain for a given magnetisation by assuming a negatively-magnetised core enclosed by an outer, positively-magnetised bulk.
\[ Nc_0 / h \omega_x l^3 \quad Nc_2 / h \omega_x l^3 \quad M \quad \xi_n / l \quad \xi_F / l \quad \eta_M^{(1)} / l \quad \eta_M^{(2)} / l \quad \eta_M^{(3)} / l \quad R_{TF} / l \]

| 1000 | 640 | 0.1 | 0.24 | 0.30 | 0.84 | 3.2 | 1.9 | 4.1 |
| 1000 | 36  | 0.3 | 0.24 | 1.3  | 1.5  | 2.5 | 1.6 | 4.1 |
| 1000 | 5   | 0.5 | 0.24 | 3.4  | 2.0  | 2.0 | 1.4 | 4.1 |
| 1000 | −5  | 0.7 | 0.24 | 3.4  | 2.5  | 1.5 | 1.0 | 4.1 |
| 1000 | −36 | 0.9 | 0.24 | 1.3  | 3.2  | 0.84| 0.59| 4.1 |
| 1000 | −640| 0.1 | 0.30 | 0.22 | 0.69 | 2.6 | 1.6 | 3.4 |
| 10000| 360 | 0.1 | 0.15 | 0.81 | 1.3  | 5.0 | 3.0 | 6.5 |
| 10000| −50 | 0.5 | 0.15 | 2.2  | 3.2  | 3.2 | 2.1 | 6.5 |

Table 2.1: Example density and spin healing lengths \( \xi_n \) and \( \xi_F \) for varying \( c_2 \) and \( c_0 \), calculated using the peak of an isotropic Thomas-Fermi density profile. Magnetisation lengths \( \eta_M^{(i)} \) for different analytical models of the magnetisation density, which are all defined in terms of \( M \) and the Thomas-Fermi radius \( R_{TF} \), which is also listed. All length scales given in terms of harmonic oscillator length \( l \). Note the ratios \( c_2 / c_0 \sim 0.036 \) relevant for \( ^{23}\text{Na} \) and \( c_2 / c_0 \sim −0.005 \) for \( ^{87}\text{Rb} \).

The length scale of such a negatively-magnetised core, \( \eta_M^{(3)} \), is estimated by assuming a sharp transition between the outer FM phase with \( \langle \hat{F} \rangle = \hat{z} \) and the cylindrical core with \( \langle \hat{F} \rangle = −\hat{z} \). By again approximating the density profile by the Thomas-Fermi solution, we calculate the magnetisation

\[
M(\eta_M^{(3)}) = \frac{1}{N} \int d^3r \left[ \Theta(\rho − \eta_M^{(3)}) − \Theta(\eta_M^{(3)} − \rho) \right] n_{TF}(r). \tag{2.47}
\]

Solving for \( \eta_M^{(3)} \) yields

\[
\eta_M^{(3)} = R_{TF} \sqrt{1 − \left( \frac{1 + M}{2} \right)^{2/5}}. \tag{2.48}
\]

Some example values of the magnetisation length scales are presented in Table 2.1.
Chapter 3

Vortices and Defects

In the textbook examples of superfluids, liquid $^4$He [141] and BECs of spinless atoms [106], quantised vortices occur as quantised circulation around an empty vortex core whose size is determined by the density healing length. In a spinor BEC, spin rotations and condensate phase combine to form a larger set of physically distinguishable degenerate states, as discussed in Chapter 2. This is analogous to liquid $^3$He where superfluidity is formed by Cooper pairs of fermions exhibiting a nonzero spin and orbital angular momentum, resulting in a rich phenomenology of phases with different broken symmetries [9]. These give rise to nontrivial topological defects, as will be described in Sec. 3.1.

Atomic BECs offer the important advantage that vortices and other defects and textures may be prepared with great experimental control and observed in the laboratory. With the large phenomenology resulting from the multicomponent order parameter described in Secs. 2.4-2.5, spinor BECs thus emerge as highly suitable systems for the study of complex topological defects and textures, as will be discussed in Secs. 3.2-3.4. Experiments have already demonstrated controlled preparation of nonsingular vortices and related textures [33, 36, 37, 142], and out of equilibrium production of singular vortices in rapid phase transitions [51], as well as observations of spontaneously formed spin textures [53, 143]. Some details of these experiments are discussed in more detail in Sec. 3.4.1.

The set of physically distinguishable, energetically degenerate states which minimise the energy functional defines the ground-state manifold, the symmetry properties of which determine the families of topological defects one can construct in the spinor BEC. As discussed in Sec. 2.4.1, an atomic spin-1 BEC exhibits two phases of the order-parameter space, FM and polar, with distinct broken symmetries, and hence able to host different topological defects.

In a singular defect the singularity of the order parameter is contained by a defect core. Unlike scalar superfluids, in the spinor BEC this does not imply that the density
must vanish: it is also possible to accommodate the singularity by requiring the spinor wavefunction to be orthogonal to the ground-state manifold at the precise location of the singularity. The different possibilities for the defect core structure leads to an energetic hierarchy of different characteristic length scales [58]: Depending on the ratio of the spin and density healing lengths $\xi_F$ and $\xi_n$, respectively, associated with the two interaction strengths of spin-1 BEC, it can be energetically more favourable to force the order parameter to be orthogonal to the ground-state manifold at the defect singularity than to force the density to zero. This can lead to unexpected core structures. In Ref. [58] it was shown how in the polar phase of a spin-1 BEC a singular point defect with a vanishing density at the singularity can spontaneously deform to a ring defect with a FM core and a non-vanishing density. A stable nonaxisymmetric singular vortex with a nonzero superfluid density at the core has also been theoretically predicted [144, 145] and experimentally observed [146] in superfluid liquid $^3$He.

### 3.1 Topological Defects and Textures

For a given medium in a physical space $X$, one can define a space $M$ corresponding to the group of energetically degenerate internal states of the medium which minimise the energy. If one then defines a mapping $f(r)$ from all points $r$ in $X$ onto $M$, $f(r)$ is defined as an order parameter [147]. Examples of order parameters include the orientations of molecule axes in liquid crystals and magnetic moments in ferromagnets. The space $M$ is referred to as the order-parameter space or ground-state manifold. Any discontinuity in this order parameter which cannot be removed by continuous deformations of the system is referred to as a topological defect. In a $D$-dimensional system, defects of any dimension lower than $D$ may exist and the group of distinct classes of defects of dimension $D - (1 + N)$ is given by the $N^{th}$ homotopy group of the order-parameter space, $\pi_N(M)$.

A $(D - 1)$-dimensional defect takes the form of a wall separating two regions — for example, domain walls in ferromagnets. The characteristic of such a defect is that for any two points separated by the defect, there is no path between them along which the order parameter is continuous.

A $(D - 2)$-dimensional defect has the character of a string in a 3D medium, which we shall refer to as a line defect, in analogy with a 1D defect in 3D space. One example is a quantised vortex in a scalar superfluid. Line defects have the characteristic that there exist no deformations between paths enclosing the defect and paths not containing the defect, for which the order parameter is continuous for all intermediate deformations.

Finally we consider $(D - 3)$-dimensional defects, referred to henceforth as point defects. A point defect is much the same as a line defect but one must consider closed surfaces, rather than paths. Any closed surface containing the point defect cannot be continuously
deformed to a surface not enclosing the defect without encountering a discontinuity in the order parameter. For a more in-depth review on topological defects, see Refs. [4, 148].

It is also possible to have $D$-dimensional textures, which are nonsingular, nonuniform order parameter profiles in which the order parameter at the boundary of $X$ (the space occupied by the medium) is fixed to a single point in the order-parameter space. Only when this boundary condition is applied, is a texture topologically stable. When the boundary condition is not fixed, the texture may be removed by continuous deformation, although the texture may still be energetically stable. One example is the Skyrmion [94], which is a mapping from $S^3$ in $X$ onto $S^3$ in the order-parameter space.

### 3.2 Classification of Vortices

For a spin-$F$ condensate, the ground-state manifold in zero magnetic field is $S^{4F+1}$ when spin-dependent interactions are ignored [63]. This can be represented geometrically as the $4F + 2$-dimensional unit sphere. On such a sphere, any closed loop, surface or $D$-dimensional hypersurface with $D < 4F+1$ may be contracted continuously to a point and so the only nontrivial homotopy group is $\pi_F$. When $F \geq 1$, all relevant homotopy groups are trivial (since we are considering a 3D condensate and so only homotopy groups up to $\pi_3$ are considered) and so no topological defects are permitted. The change of symmetry resulting from spin interactions results in nontrivial homotopy groups and hence brings about the stability of defects. Before discussing such systems, we consider a scalar BEC ($F = 0$).

The order-parameter space for the scalar BEC is $S^1$, arising from the condensate phase. This has a first homotopy group homeomorphic to $\mathbb{Z}$ and so there are an infinite number of distinct topological classes of line defects. Consider a BEC in the absence of any trapping potential. Atomic wavefunctions can be engineered such that the phase depends on the azimuthal angle in cylindrical coordinates, $\varphi$, and has no dependence on distance from the $z$ axis. The requirement that the phase $\phi$ be specified at all points means that in a full circuit around the axis, the phase must change by an integer multiple of $2\pi$.

If the phase change is zero, any angular dependence of $\phi$ can be removed via a continuous deformation. If, however, the phase change is nonzero, such a change cannot be removed by continuous deformation. Now consider the phase on the $z$ axis. On the axis, $\varphi$ is undefined and so the phase is also undefined. This represents an irremovable discontinuity in the order parameter — a line defect.

Let us consider a scalar BEC with wavefunction $\Psi = fe^{i\phi}$ with $f$ independent of position. The superfluid velocity is then [2]

$$v = \frac{\hbar}{mn} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) = \frac{\hbar}{m} \nabla \phi. \quad (3.1)$$
Table 3.1: Example ground-state manifolds and associated homotopy groups for superfluid systems. The ground-state manifold of the cyclic phase of a spin-2 BEC is not well parameterised and so we omit it here. Note that the binary tetrahedral group $T^*$ is discrete and non-Abelian.

As a result, the velocity is irrotational unless there is a phase singularity in the condensate — as there is on the line considered above. Hence such objects are referred to as vortices.

Assuming the phase to depend only on $\phi$, it follows that at a distance $\rho$ from the vortex, the superfluid velocity is

$$v = -i \frac{\hbar}{m \rho} \frac{\partial \phi}{\partial \phi} \hat{\phi}. \quad (3.2)$$

One can clearly see from this that if the condensate density does not vanish on the $z$ axis, the velocity (and hence the kinetic energy) will diverge. Hence a zero-density vortex core forms on this axis, with a radial size given by the density healing length $(2.39)$ [2]. The vortex is classified in terms of its circulation

$$\nu = \oint v \cdot d\mathbf{r}. \quad (3.3)$$

Given a phase change of $2\pi b$ in one closed circuit around the $z$ axis, this becomes

$$\nu = \frac{hb}{m} \quad (3.4)$$

where $b$ must be an integer as discussed above and $m$ is the atomic mass. Recall the statement that there are an infinite number of distinguishable line defects in the scalar BEC. These are the vortices with different $b$. A review on vortices can be found in Ref. [149]. For the interested reader, Table 3.1 lists the ground-state manifolds and relevant homotopy groups for a number of relevant systems.

Prior to discussing the vortices of a spin-1 BEC, we first introduce a notational convention of the spinor BEC literature. It is often convenient (and instructive) to consider only the phase-windings in the spinor components, ignoring the relative populations of the Zeeman levels. The most usual notation for this in a spin-1 atomic BEC is to refer
to the \( (a - b, a, a + b) \) vortex, describing the spinor

\[
\zeta = e^{i\alpha \varphi} \left( \pm e^{-ib\varphi} \sqrt{n_+} \overline{\eta_0} e^{ib\varphi} \sqrt{n_-} \right),
\]

(3.5)

where \( a \) and \( b \) are integers. The spinor (3.5) is of the form of the generalised FM and polar spinors when the sign of \( \zeta_+ \) is positive or negative respectively. The spinor (3.5) also demonstrates an important property that both the FM and polar phases must satisfy. Denoting the phase of each component by \( \phi_i \), it follows that

\[
\begin{align*}
\phi_+ &= (a - b)\varphi - n\pi \\
\phi_0 &= a\varphi \\
\phi_- &= (a + b)\varphi \\
\therefore 2\phi_0 &= \phi_+ + \phi_- + n\pi,
\end{align*}
\]

(3.6) (3.7) (3.8) (3.9)

where odd \( n \) denotes the polar phase and even \( n \) denotes the FM phase [8, 19, 150]. Eq. (3.9) is the phase-matching condition and can be quickly applied to show which vortex states may be constructed from the generalised spinors of the FM and polar phases. There is a pitfall associated with this, though, as a \( \pi \) winding of the phase combined with a \( \pi \) discontinuity of the phase (a soliton plane) cannot be well described. As we will observe in Sec. 3.4, this scenario can occur in the polar phase, which can exhibit vortices with fractional winding numbers.

### 3.3 Vortices in Ferromagnetic Phase

We first consider vortices in the FM phase of a spin-1 BEC. The system becomes FM when the interaction term \( c_2 < 0 \) in the GPE (2.25); energetically it is then favourable to maximise the spin magnitude everywhere in space, so that \( |\langle \hat{F} \rangle| = 1 \). A general FM spinor wavefunction can be constructed from the representative spinor \( \zeta = (1, 0, 0)^T \) with \( \langle \hat{F} \rangle = \hat{z} \) by incorporating a macroscopic condensate phase \( \phi \) and a spin rotation 

\[
U(\alpha, \beta, \gamma) = \exp[-iF_z\alpha] \exp[-iF_y\beta] \exp[-iF_z\gamma],
\]

defined by three Euler angles. We obtain

\[
\zeta = e^{i\phi} U(\alpha, \beta, \gamma) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

\[
= \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} \sqrt{2}e^{-i\alpha} \cos^2 \frac{\beta}{2} \\ \sin \beta \sqrt{2}e^{i\alpha} \sin^2 \frac{\beta}{2} \end{pmatrix},
\]

(3.10)
where $\phi' = \phi - \gamma$. The local spin vector is then given by

$$\langle \hat{F} \rangle = \cos \alpha \sin \beta \hat{x} + \sin \alpha \sin \beta \hat{y} + \cos \beta \hat{z}. \quad (3.11)$$

The order-parameter space is the manifold of energetically degenerate spinors $\vec{\zeta}$. Degenerate FM spinors [Eq. (3.10)] differ only by rotations in spin-space given by the Euler angles $\alpha$, $\beta$ and $\phi'$. The order-parameter space therefore corresponds to the group of 3D rotations $SO(3)$.

The topological stability of line defects is characterised by the way closed contours encircling the defect map into order parameter space [4]. If the order-parameter space image of such a closed loop can be contracted to a point, the defect is not topologically stable. $SO(3)$ may be represented geometrically as $S^3$ (the unit sphere in four dimensions) with diametrically opposite points identified. The only closed loops that cannot be contracted to a point are those connecting such identified points an odd number of times. These loops can all be deformed into one another and there are therefore only two distinct classes of vortices: singular vortices corresponding to non-contractible loops, and nonsingular vortices corresponding to contractible loops [117, 7]. All the singular vortices with an odd-integer winding number are therefore topologically equivalent to a singly-quantised singular vortex and all singular vortices with an even-integer winding number are topologically equivalent to the nonsingular, vortex-free state. Mathematically, this is indicated by the first homotopy group of $SO(3)$ which has two elements $[\pi_1(SO(3)) = \mathbb{Z}_2]$, representing the two topological equivalence classes for the vortices.

The class of nontrivial vortices in the FM phase is formed by the singly-quantised vortices. The simplest way to construct a singly quantised singular vortex in the FM phase is as a $2\pi$ winding of the condensate phase $\phi$. By letting $\phi = \varphi$, where $\varphi$ is the azimuthal angle, the vortex can then be described by the spinor

$$\vec{\zeta}^S = \frac{e^{i\varphi}}{\sqrt{2}} \begin{pmatrix} \sqrt{2} \cos^2 \frac{\beta}{2} \\ \sin \beta \\ \sqrt{2} \sin^2 \frac{\beta}{2} \end{pmatrix}, \quad (3.12)$$

with the density required to vanish on the singular vortex line along the $z$ axis (where all the three spinor components are singular). The Euler angle $\beta$ is arbitrary but constant, giving a uniform spin distribution (which, without loss of generality, we assume to be in the $x$-$z$ plane such that $\alpha = 0$).

Vortices in the same equivalence class can be transformed into each other by local spin rotations. For example, $\langle \hat{F} \rangle$ may form a spin vortex represented by

$$\vec{\zeta}^{\nabla} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} e^{-i\varphi} \cos^2 \frac{\beta}{2} \\ \sin \beta \\ \sqrt{2} e^{i\varphi} \sin^2 \frac{\beta}{2} \end{pmatrix}. \quad (3.13)$$
For $\beta = \pi/2$ the spins lie in the $x$-$y$ plane, forming a radial spin disgyration. Two interesting equivalences emerge from Eq. (3.13). Setting $\beta = t\pi$, a continuous change in $t$ gives

$$\mathbf{\zeta}(t = 0) = \begin{pmatrix} 0 \\ 0 \\ e^{i\varphi} \end{pmatrix}, \quad (3.14)$$

$$\mathbf{\zeta}(t = 0.5) = \frac{1}{2} \begin{pmatrix} e^{-i\varphi} \\ \sqrt{2} \\ e^{i\varphi} \end{pmatrix}, \quad (3.15)$$

$$\mathbf{\zeta}(t = 1) = \begin{pmatrix} e^{-i\varphi} \\ 0 \\ 0 \end{pmatrix}. \quad (3.16)$$

The $t = 0$ spinor is a singly-quantised singular vortex. Hence a $2\pi$ winding in $\alpha$ lies in the same topological class as the same winding in $\phi$. The $2\pi$ phase winding is homotopic to the $2\pi$ rotation of the spin vector. Also, since the $t = 1$ spinor above is a singular vortex with negative winding of the phase, we infer that phase-windings of opposing sign are homotopic to one another. Following this method, the two topological classes are readily identified in terms of the global phase winding $e^{ia\varphi}$ and winding of the spin vector $F_x + iF_y = e^{ib\varphi}$ (integer $a$ and $b$), as

1. Odd $a + b$. These vortices are singular.

2. Even $a + b$. These are homotopic to the vortex free state and may be nonsingular.

It is possible for the core of a radial spin disgyration in a FM spin-1 BEC to have non-vanishing density, instead being filled with the polar phase [19, 150, 85]. It has been argued [63] that a vortex on the symmetry axis of a cylindrically symmetric FM condensate will have the lowest energy if it is a radial spin disgyration, via solution of the Euler-Lagrange equations. However, these symmetries are not imposed in experiments and so we consider the vortex core structure by solving the full 3D spinor GPEs in Sec. 5.1.

From the first homotopy group, there are only two classes of topologically distinct vortices: nonsingular vortices and singular vortices. Having classified the singly-quantised vortex as singular, it is now instructive to consider the doubly-quantised vortex. This may in fact be deformed to a nontrivial, nonsingular vortex—a coreless vortex—as follows. Let us construct a spinor which combines a $2\pi$ rotation of the spin vector with a simultaneous $2\pi$ winding of the condensate phase, corresponding to the choice $\alpha = \phi' = \varphi$,
Chapter 3 Vortices and Defects

In Eq. (3.10):

$$\vec{\zeta}_{\text{cl}}(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} \cos^2 \frac{\beta(\rho)}{2} \\ e^{i\varphi} \sin \beta(\rho) \\ \sqrt{2} e^{2i\varphi} \sin^2 \frac{\beta(\rho)}{2} \end{pmatrix}.$$  

(3.17)

In the limit $\beta = \pi$, this is simply

$$\vec{\zeta}(\beta = \pi) = \begin{pmatrix} 0 \\ 0 \\ e^{2i\varphi} \end{pmatrix},$$  

(3.18)

which is the doubly-quantised vortex. However, notice the opposite limit $\beta = 0$, which has spinor

$$\vec{\zeta}(\beta = \pi) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$  

(3.19)

corresponding to the vortex-free state. The doubly-quantised vortex and the coreless vortex are therefore in the trivial topological class. Let us now return to the coreless vortex with general $\beta$ in Eq. (3.17).

The angle $\beta$ describes how the spin vector tilts away from the $z$ axis. Since the spinor is nonsingular at $\beta = 0$, the coreless vortex exhibits $\langle \hat{\mathbf{F}} \rangle = \hat{z}$ on the vortex line itself, with $\beta$ smoothly increasing with the radial distance $\rho$. This results in a characteristic fountain-like spin texture that is continuous everywhere, with $\langle \hat{\mathbf{F}} \rangle = \hat{z}$ on the vortex line. The value of $\beta$ at the edge of the cloud is determined by the imposed rotation as increased $\beta$ increases the angular momentum of the system, reducing the total energy and stabilising the vortex against unwinding to the vortex-free state. In a non-rotating trap, there is no stabilising condition and correspondingly it has been shown [151] that in this case the coreless vortex is energetically unstable.

The coreless vortex is analogous to the nonsingular Anderson-Toulouse-Chechetkin (ATC) [152, 153] and Mermin-Ho (MH) [154] textures in superfluid liquid $^3$He. For a coreless texture, one may define a winding number similar to that of a point defect,

$$W = \frac{1}{8\pi} \int_{\mathcal{S}} d\Omega_i \epsilon_{ijk} \langle \hat{F} \rangle \cdot \left( \frac{\partial \langle \hat{F} \rangle}{\partial x_j} \times \frac{\partial \langle \hat{F} \rangle}{\partial x_k} \right),$$  

(3.20)

where $\mathcal{S}$ denotes the upper hemisphere. The charge $W$ counts the number of times $\langle \hat{F} \rangle$ wraps around the full order-parameter space. If the spin vector reaches a uniform asymptotic orientation everywhere away from the vortex (i.e., the bending angle $\beta(\rho)$ is an integer multiple of $\pi$), $W$ represents an integer-valued charge in the second homotopy group. The winding numbers are $1/2$ for an MH-like texture and $1$ for an ATC-like texture. This charge is topologically invariant whenever the boundary condition is fixed, e.g. by physical interaction or energetics, such that the unwinding process...
Figure 3.1: Schematic illustrations of FM vortex states. (a) The nonsingular, coreless vortex is formed as a combined disgyration of the spin vector (cones) and a spin rotation about the local spin vector (indicated by the orthogonal vectors). The vortex is nonsingular and the spin texture is continuous. (b) The singular FM spin vortex is formed as a radially-oriented disgyration of the spin vector around the singular core, which is filled by the polar phase. Figure reproduced from Ref. [1].

of Eq. (3.19) cannot proceed, as the coreless vortex is topologically protected by the topological charge (3.20) in the second homotopy group. If no boundary condition is imposed, the texture can unwind to the vortex-free state by purely local transformations of the wavefunction. The coreless vortex may be viewed as a 2D or baby Skyrmion, which maps from a 2D plane into $S^2$ [13, 99].

The superfluid velocity for a spin-1 BEC is defined as [7]

$$v = -\frac{i\hbar}{2m} \left[ \Psi^\dagger \nabla \Psi - \left( \nabla \Psi^\dagger \right) \Psi \right],$$

(3.21)

which for the coreless vortex becomes

$$v = \frac{\hbar}{m\rho} (1 - \cos \beta) \hat{\phi}.$$  (3.22)

This goes smoothly to zero at the centre of the vortex but increases away from it as $\beta$ increases. The spin-1 coreless vortex may therefore be stabilised by rotation as the bending angle $\beta(\rho)$ in Eq. (3.17), and therefore the superfluid circulation, adapts to the imposed rotation. Typical examples of a nonsingular coreless vortex forming a continuous spin texture and a singular spin vortex with a radial disgyration of the spin vector are schematically illustrated in Fig. 3.1.
3.4 Vortices in the Polar Phase

We now turn our attention to the polar phase of a spin-1 BEC. In this case the interaction term $c_2 > 0$ in the GPE (2.25), and it is energetically favourable to minimise the spin magnitude everywhere in space so that $|\langle \hat{F} \rangle| = 0$. We may construct the general spinor wavefunction of the polar phase by applying a spin rotation and global condensate phase to the representative spinor $\vec{\zeta} = (0, 1, 0)^T$. The general polar spinor in terms of the macroscopic condensate phase $\phi$ and the Euler angles $(\alpha, \beta, \gamma)$ is then

$$\vec{\zeta}^p = e^{i\phi}U(\alpha, \beta, \gamma) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} -e^{-i\alpha} \sin \beta \\ \sqrt{2} \cos \beta \\ e^{i\alpha} \sin \beta \end{pmatrix}.$$  (3.23)

Notice that $\gamma$ does not appear in the final spinor and that the condensate phase, $\phi$ is not coupled to the Euler angles $\alpha$ and $\beta$ defining the spin rotation. It is therefore beneficial to introduce the unit vector $\hat{d} = \cos \alpha \sin \beta \hat{x} + \sin \alpha \sin \beta \hat{y} + \cos \beta \hat{z}$, which parametrises the spin rotation relative to the prototype spinor. We may then write the spinor wavefunction in terms of $\hat{d}$ as [58]

$$\vec{\zeta}^p = \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} -d_x + id_y \\ \sqrt{2}d_z \\ d_x + id_y \end{pmatrix}.$$  (3.24)

The unit vector $\hat{d}$ takes values on a sphere and the condensate phase $\phi$ on a unit circle. The state of the spinor wavefunction, however, remains unchanged when a $\pi$ rotation of $\phi$ is combined with inversion of $\hat{d}$, so that the states $\vec{\zeta}^p(\phi, \hat{d}) = \vec{\zeta}^p(\phi + \pi, -\hat{d})$ are identical. These states must be identified to avoid double counting, and the order-parameter space is therefore $(S^2 \times S^1)/\mathbb{Z}_2$, from the condensate phase and rotations of $\hat{d}$, factorised by the discrete two-element group $\mathbb{Z}_2$ due to the identification. The vector $\hat{d}$ is thus taken to be unoriented and defines a nematic axis [155]. The first homotopy group of the polar phase of a spin-1 condensate is homeomorphic to $\mathbb{Z}$, so there are an infinite number of classes of vortices.

This nematic order also allows the formation of a vortex carrying half a quantum of circulation [123], constructed as a $\pi$ winding of the macroscopic condensate phase together with a $\hat{d} \to -\hat{d}$ rotation of the nematic axis around a closed loop encircling the vortex core. For example, we may have

$$\vec{\zeta}^{hq} = \frac{e^{i\varphi/2}}{\sqrt{2}} \begin{pmatrix} -e^{-i\varphi/2} \\ 0 \\ e^{i\varphi/2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ e^{i\varphi} \end{pmatrix}.$$  (3.25)
This half-quantum vortex has a singular core and is also well-known from, e.g., superfluid $^3$He-A [9, 10, 156], uniaxial liquid crystals and $d$-wave superconductors [157]. It has been suggested [123] that an incident laser could imprint a $\pi$ global phase-winding on a polar condensate with only $\zeta_{\pm}$ populated, while microwave radiation induces a $\pi$ phase shift between the two components, to experimentally generate a half-quantum vortex. An alternative suggestion is to start with the same state and apply a pulsed magnetic field and an oscillating trapping potential to nucleate half-quantum vortices either one at a time or in large numbers, via dynamical instabilities at the surface of the condensate [158]. As yet, half-quantum vortices have not been experimentally observed in the polar phase of a spinor BEC.

Next, consider the spinor

$$\tilde{\zeta}(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-ib\varphi} \sin [(1-t)\beta] \\ \sqrt{2} \cos [(1-t)\beta] \\ e^{ib\varphi} \sin [(1-t)\beta] \end{pmatrix}$$

(3.26)

$$\tilde{\zeta}(t = 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-ib\varphi} \sin \beta \\ \sqrt{2} \cos \beta \\ e^{ib\varphi} \sin \beta \end{pmatrix}$$

(3.27)

$$\tilde{\zeta}(t = 1) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$  

(3.28)

Hence any state with integer winding of the $\hat{d}$ vector can be continuously deformed into the uniform-$\hat{d}$ state. Unlike the FM phase, each vortex of the form

$$\tilde{\zeta} = e^{ia\varphi} \begin{pmatrix} -e^{-ib\varphi} \sin \beta \\ \sqrt{2} \cos \beta \\ e^{ib\varphi} \sin \beta \end{pmatrix}$$

(3.29)

lies in a topological class determined only by $a$, where $a$ and $b$ are integers. There are no continuous deformations between different values of $a$. Hence one can classify a vortex in the polar phase purely by looking at the global phase-winding.

A singly-quantised vortex in the polar phase can be formed as a $2\pi$ winding of the condensate phase $\phi$ around a closed loop encircling the vortex core. Choosing the vortex line along the $z$ axis, we obtain

$$\tilde{\zeta}^z = \frac{e^{i\varphi}}{\sqrt{2}} \begin{pmatrix} -e^{-ia} \sin \beta \\ \sqrt{2} \cos \beta \\ e^{ia} \sin \beta \end{pmatrix},$$

(3.30)

where $\alpha$ and $\beta$ may arbitrarily be constant or vary spatially. The topological class remains unchanged.
From Eqs. (3.23) & (3.21) one can show that the superfluid velocity in the polar phase is given by [7]

\[ \mathbf{v} = \frac{\hbar}{m} \nabla \phi, \] (3.31)

analogously to Eq. (3.1). It then follows by standard arguments [see, e.g. Ref. [8], Sec. 3.2] that circulation must be quantised. Due to the existence of the half-quantum vortex, circulation is thus quantised in units of \( \pi \), half the circulation of Eq. (3.30). This will be a crucial observation when we analyse possible deformations of the core of a singly-quantised vortex as energy is minimised.

Just as the FM phase may host a nonsingular texture, so, too, can the polar phase. The nematic coreless vortex displays a characteristic fountain texture analogous to the spin texture of the FM coreless vortex. To construct such a state, one must simply impose a \( 2\pi \) spin rotation, for example by the choice \( \alpha = \phi \),

\[ \vec{\zeta}_{nc} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \sin(\beta(\rho)) \\ \sqrt{2} \cos(\beta(\rho)) \\ -e^{i\varphi} \sin(\beta(\rho)) \end{pmatrix}. \] (3.32)

As in the FM coreless vortex, \( \beta(\rho) \) characterises the bending of \( \hat{d} \) away from the \( z \) axis, forming an analogous fountain texture in \( \hat{d} \) of

\[ \hat{d} = \sin \beta \hat{\rho} + \cos \beta \hat{z}, \] (3.33)

The angle \( \beta \) between \( \hat{d} \) and the \( z \) axis increases from \( \beta = 0 \) at \( \rho = 0 \) to \( \beta = \pi/2 \) (\( \beta = \pi \)) at the edge of the cloud for a MH-like (ATC-like) texture. The winding number \( W \) may be defined by replacing \( \langle \hat{F} \rangle \rightarrow \hat{d} \) in Eq. (3.20). The orientation of \( \hat{d} \) is not fixed at the boundary, and the coreless nematic texture may smoothly dissolve. Unlike the spin texture of the FM coreless vortex, it cannot be stabilised by rotation, due to its vanishing mass circulation [see Eqs. (3.3) & (3.31)].

A final consideration is the topological classification for a many-vortex state. This may be extrapolated from the classification of a pair of half-quantum vortices. Given such a pair with uniform \( \beta = \pi/2 \), with one half-quantum vortex at the centre of the trap and the other displaced by a distance \( x_0 \) in the \( x \) direction, one may construct a spinor which reproduces the phase behaviour of the half-quantum vortex pair as

\[ \vec{\zeta} = \frac{1}{\sqrt{2} \sqrt{(x-x_0)^2 + y^2}} \begin{pmatrix} -\sqrt{(x-x_0)^2 + y^2} \\ 0 \\ e^{i\varphi} (p e^{i\varphi} - x_0) \end{pmatrix}, \] (3.34)

where \( \rho^2 = x^2 + y^2 \). For the purposes of this discussion, we assume pure polar phase and consider only the phase behaviour of the spinor, since this may be used to classify
the vortex structure. Taking the $\rho >> x_0$ limit, this tends toward

$$\zeta \sim \frac{1}{\sqrt{2} \rho^2} \left( \begin{array}{c} -\sqrt{\rho^2} \\ 0 \\ e^{i\varphi} \cdot e^{i\varphi} \end{array} \right) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} -1 \\ 0 \\ e^{i2\varphi} \end{array} \right). \tag{3.35}$$

Since the topological class cannot change just by taking this limit, it follows that the pair of half-quantum vortices lie in the same topological class as the vortex

$$\zeta = e^{i\varphi} \left( \begin{array}{c} -e^{-i\varphi} \\ 0 \\ e^{i\varphi} \end{array} \right). \tag{3.36}$$

This is of the form of Eq. (3.30) with $\alpha = \varphi$, $\beta = \pi/2$. It can therefore be deformed continuously to $\beta = 0$ as previously, resulting in

$$\zeta = e^{i\varphi} \left( \begin{array}{c} 0 \\ 1 \\ 0 \end{array} \right). \tag{3.37}$$

A pair of half-quantum vortices therefore lies in the same topological class as the singly-quantised vortex. Following the same logic one readily finds that the combination of two vortices with phase-windings $c$ and $d$ lie in the same topological class as a single vortex with phase-winding $c + d$.

### 3.4.1 Experiments on Spin-1 BECs

Observing the spin dynamics of an optically-trapped BEC is a highly nontrivial problem. In order to study the relative populations of the Zeeman levels, the trap must be switched off and a Stern-Gerlach field applied to split the three components before they are separately measured. Ref. [110] used a periodic 1D optical lattice to generate coherent, effectively 2D BECs in neighbouring lattice sites and then attempted to measure the relative phases of each component through Stern-Gerlach splitting followed by interference. The relative phases of the spinor components define the transverse components of the spin vector and so recovering this phase information would allow the study of the full 3D dynamics of the spin vector. However, they were plagued by decoherence problems which they attributed to stray magnetic fields. They did, however, provide experimental evidence that the ground state of $F = 1^{87}$Rb is ferromagnetic, in agreement with past experiments [119]. They also demonstrated that the magnetisation is preserved throughout the spin dynamics in the weak-field limit. A magnetisation-dependent phase contrast imaging technique has also been developed, enabling experimentalists to probe the spin in a given direction in situ [159], although the full 3D spin vector cannot be
studied. In this work, nontrivial 3D spin textures are predicted to form in the energetically stable configurations of singular and nonsingular vortices, and so the method of Stern-Gerlach splitting followed by interference would be the most suitable to studying these structures. Even with the decoherence problems preventing phase information from being recovered, the density profiles in the three spinor components provide more information about the spin structure than magnetisation alone.

As well as further demonstrating the ferromagnetic nature of $F = 1$ $^{87}$Rb, Ref. [160] also measured the timescales for spin decoherence in this condensate. They prepared an initial state of atoms entirely in the $m_F = 1$ state via application of a negative quadratic Zeeman splitting. By applying an rf pulse, the spins were rotated by $\pi/2$ about a fixed axis, which we label $x$ for this discussion. After a variable amount of time, the rf pulse was applied again, rotating the spins by $\pi/2$ once more about the $x$-axis. By measuring the population of the $m_F = -1$ state, they were able to determine that the coherence breaks down on a timescale of milliseconds, which is the typical timescale for BEC experiments. With improved experimental control, it is possible that the coherence could be retained for appreciable experimental timescales and so this is a promising method for the imaging of spinor vortices.

The most studied method for creation of a coreless vortex in the spin-1 BEC begins with a condensate prepared in a fully spin-polarised state, which we take to be $\zeta_f = (1, 0, 0)^T$.

The condensate is subject to an external 3D magnetic quadrupole field [37]

$$B = B' \rho \hat{\rho} + \left[ B_z(t) - 2B'z \right] \hat{z}. \quad (3.38)$$

The zero-field point $z = B_z/2B'$ ($\rho = \varphi = 0$) of the quadrupole field is initially at large $z$ so that $B \parallel \hat{z}$ in the condensate.

The coreless-vortex structure is created by linearly sweeping $B_z(t)$ so that the zero-field point passes through the condensate. The changing $B_z$ causes the magnetic field away from the $z$ axis to rotate about $\hat{\varphi}$ from the $\hat{z}$ to the $-\hat{z}$ direction. The rate of change of the magnetic field decreases with the distance $\rho$ from the symmetry axis. Where the rate of change is sufficiently slow, the atomic spins adiabatically follow the magnetic field, corresponding to a complete transfer from $\zeta^+ \to \zeta^-$ in the laboratory frame. However, where the rate of change of the magnetic field is rapid, the atomic spin rotation is diabatic. In the laboratory frame, the spins thus rotate through an angle $\beta(\rho)$, given by the local adiabaticity of the magnetic-field sweep, which increases monotonically from zero on the symmetry axis. Linearly ramping $B_z(t)$ thus directly implements the spin rotation

$$\zeta^+(\mathbf{r}) = e^{-i\mathbf{F} \cdot \beta(\rho) \hat{\varphi}} \zeta^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} \cos^2 \frac{\beta}{2} \\ e^{i\varphi} \sin \beta \\ \sqrt{2} e^{i2\varphi} \sin^2 \frac{\beta}{2} \end{pmatrix}. \quad (3.39)$$

\footnote{The experiment in Ref. [37] actually starts from $\zeta = (0, 0, 1)^T$ and creates an “upside-down” coreless vortex.}
The resulting fountain-like spin texture

\[
\langle \hat{F} \rangle = \sin \beta \hat{\rho} + \cos \beta \hat{z}
\]  

(3.40)
defines the coreless vortex in the spinor BEC as described in Eq. (3.17).

The first controlled preparation of a nonsingular vortex \[36\] used a 2D quadrupole field together with an axial bias field. The magnetic field in the trap is then

\[
B(\rho, \phi, \theta) = B_z(t) \hat{z} + B' \rho \left[ \cos(2\phi) \hat{\rho} - \sin(2\phi) \hat{\phi} \right].
\]  

(3.41)

By the mechanism described above, ramping of \(B_z(t)\) then causes a spin rotation

\[
\vec{\zeta}_r(\mathbf{r}) = \exp \left[ -i \hat{F} \cdot \beta'(\rho) \hat{n} \right] \vec{\zeta}_0
\]

about an axis \(\hat{n}(\varphi) = \sin \varphi \hat{x} + \cos \varphi \hat{y}\). The rotation yields a nonsingular spin texture exhibiting a cross disgyration, instead of the fountain-like structure. The two are topologically equivalent.

The magnetic-field rotation technique used to phase-imprint the FM coreless vortex \[36, 37\] can also be applied to a BEC prepared in the polar state \(\vec{\zeta}_0 = (0, 1, 0)^T\) \[37, 142\], in which the nematic axis \(\hat{d} = \hat{z}\) and the longitudinal magnetisation \(M = 0\). The rotation \(\vec{\zeta}_r = \exp \left[ -i \hat{F} \cdot \beta'(\rho) \hat{n} \right] \vec{\zeta}_0\) induced by the magnetic-field sweep then leads to the nematic texture \(\hat{d} = \sin \beta' \hat{\rho} + \cos \beta' \hat{z}\), which defines a nematic coreless vortex. Owing to the magnetic field rotation, this always exhibits vanishing longitudinal magnetisation. In Ref. \[142\] an ATC-like (MH-like) texture was imprinted, with \(\beta'(\rho = 0) = 0\) and \(\beta' = \pi\) (\(\beta' = \pi/2\)) at the edge of the cloud. There are no boundary conditions on the \(\hat{d}\) texture and so it can continuously unwind. As was commented in Sec. 3.4 this nematic texture carries no mass circulation and so cannot be stabilised by rotation [See Eq. (3.31)].

Another technique for phase imprinting a coreless vortex was recently demonstrated in Ref. [33]. In this experiment, the coreless vortex was created in the \(m_F = \pm 2\) and \(m_F = 0\) magnetic sublevels of the spin-2 manifold of \(^{87}\text{Rb}\). The phase imprinting starts with a spin-polarised condensate in the \(m_F = 2\) level, with a magnetic field along the \(z\) axis. Collinear \(\sigma^-\) and \(\sigma^+\) polarised laser beams along the symmetry axis then couple \(m_F = 2\) to the \(m_F = 0\) and \(m_F = -2\) levels. The laser beams have Laguerre-Gaussian (LG) and Gaussian intensity profiles, respectively, so that the population transferred to the \(m_F = 0\) (\(m_F = -2\)) level pick up a \(2\pi\) (\(4\pi\)) phase winding. The intensity minimum of the LG beam leaves a remaining population in \(m_F = 2\) with no phase winding. The resulting five-component spinor represents a coreless vortex with the spin structure (3.40) when the three nonempty levels of the five-component spinor are regarded as a (pseudo)spin-1 system. The bending angle \(\beta\) is determined by the density profiles of the nonempty spinor components. The laser beams inducing the Raman coupling of the magnetic sublevels can be tailored with a high degree of control, and the vortex structure can therefore be precisely engineered. One further experiment using a laser to spatially vary the coupling between magnetic sublevels overcomes the rotation
frequency limit imposed on rotating-trap experiments and so should be able in the future to produce a much larger number of vortices than has previously been possible [161].

As was discussed in Sec. 2.6, the longitudinal magnetisation of a spinor BEC is approximately conserved on experimental timescales. The vortex-imprinting methods discussed above can leave a net magnetisation and so this will be conserved in the dynamics of the system. In the spin-2 coreless-vortex experiment [33], the resulting magnetisation in the spin-2 manifold is measured at $M = 0.64$ for an imprinted ATC-like spin texture, and at $M = 0.72$ for a MH-like texture. In the magnetic-field rotation experiment [36] the local magnetisation $\mathcal{M}(r) = [n_+(r) - n_-(r)]/n(r)$ is reported to be $\sim 0.7$ at the centre of the cloud and $\sim -0.5$ at the edge. Because of the lower density in the negatively magnetised region, this vortex can be estimated to also carry a positive, nonzero magnetisation $M$. 
Chapter 4

Numerical Treatment

The results presented in this thesis are obtained using purpose-built Fortran codes. Different algorithms were written to solve different problems—minimising the energy via propagation in imaginary time or identifying stationary states via a successive over-relaxation routine. Before briefly outlining the numerical methods underlying these algorithms, we also discuss the generation of figures.

In Chapter 5, every figure is produced in Matlab, usually reading in directly the data output by the aforementioned Fortran codes. However, for Chapters 6-7, we developed a new method of plotting the numerical data, which the reader may wish to reproduce. The numerical data is again read in Matlab, which is then used to write a file in the language of POV-Ray\(^1\). POV-Ray is a ray-tracing program and beautifully renders 3D scenes with large numbers of shapes. The positions and orientations of the cones indicating the spin vector are calculated from the data and used to produce lines of POV-Ray code. Likewise, a box or plane is created for every grid point, with the colour specified by RGB values determined by \(|\langle \hat{F} \rangle|\).

4.1 Calculation in Dimensionless Units

Rather than restricting ourselves to one particular experimental regime, we perform our numerical analysis using a dimensionless form of the spinor GPE, such that only the relative strengths of different contributions to the energy functional are relevant. The dimensionless, time-dependent GPE is calculated from

\[
\frac{i}{\omega} \frac{\partial}{\partial t} \psi = \left( \frac{\hat{p}^2}{2m\omega} + \frac{m\omega}{2\hbar} (x^2 + \gamma_y y^2 + \gamma_z z^2) \right) - \frac{\Omega}{\omega} \frac{\hat{L}}{\hbar} \cdot \hat{F} + \frac{g_1 \hat{B}}{\hbar \omega} \cdot \hat{F} + \frac{g_2 (\hat{B} \cdot \hat{F})^2}{\hbar \omega} + \frac{c_1 n}{\hbar \omega} + \frac{c_2 n}{\hbar \omega} |\langle \hat{F} \rangle| \psi.
\]  

\(^1\)http://www.povray.org/
where $\omega = \omega_x$. Denoting dimensionless parameters $P'$ in terms of their dimensionful counterparts $P$, one may immediately identify

$$t' = \omega t \quad (4.2)$$

$$g'_1 B' = \frac{g_1 B}{\hbar \omega} \quad (4.3)$$

$$g'_2 |B'|^2 = \frac{g_2 |B|^2}{\hbar \omega} \quad (4.4)$$

$$\Omega' = \frac{\Omega}{\omega} \quad (4.5)$$

$$\hat{L}' = \frac{\hat{L}}{\hbar}. \quad (4.6)$$

Since $\omega$ is the frequency of the harmonic trap, we define a corresponding trap length $l = (\hbar/m\omega)^{1/2}$ as in Sec. 2.4. By writing the momentum operator as $\hat{p} = -i\hbar \nabla$, we then have

$$i \frac{\partial}{\partial t'} \Psi = \left( -\frac{l^2 \nabla^2}{2} + \frac{x^2 + \gamma_2 y^2 + \gamma_2 z^2}{2l^2} - \Omega' \cdot \hat{L}' + g'_1 B' \cdot \hat{F} + g'_2 (B' \cdot \hat{F})^2 + c_0 n + \frac{c_2 n}{\hbar \omega} (\hat{F} \cdot \hat{F}) \right) \Psi. \quad (4.7)$$

From this we define the dimensionless parameters

$$x' = \frac{x}{l} \quad (4.8)$$

$$y' = \frac{y}{l} \quad (4.9)$$

$$z' = \frac{z}{l} \quad (4.10)$$

$$\nabla' = \frac{\nabla}{l}. \quad (4.11)$$

The treatment of the nonlinear terms in the dimensionless limit is less obvious but does follow from dimensional analysis. The number density, $n$, has units of length$^{-3}$ and so it is intuitive to set the dimensionless number density, $n' \sim nl^3$. However, this will leave our treatment sensitive to the total number of atoms in the trap. By instead defining

$$n' = \frac{nl^3}{N} \quad (4.12)$$

$$\Psi' = \sqrt{\frac{l^3}{N}} \Psi, \quad (4.13)$$

we then have a wavefunction normalised to

$$\int |\Psi'|^2 d^3 r = 1. \quad (4.14)$$

This has two key advantages; firstly, the dependence of the wavefunction on $N$ is removed, enabling us to describe a more general system. Additionally, we may explicitly
enforce this normalisation of the wavefunction in our numerical algorithm. The time-
derpendent GPE then becomes

\[ i \frac{\partial}{\partial t'} \Psi' = \left( \frac{-\nabla'^2}{2} + \frac{1}{2} \left( x'^2 + \gamma_y^2 y'^2 + \gamma_z^2 z'^2 \right) - \Omega' \cdot \hat{L}' + g_1' \mathbf{B}' \cdot \hat{F} + g_2' (\mathbf{B}' \cdot \hat{F})^2 \right. \]

\[ + \frac{N_c_0 n'}{\hbar \omega l^3} + \frac{N_c_2 n'}{\hbar \omega l^3} (\hat{F} \cdot \hat{F}) \bigg) \Psi'. \]  

(4.15)

From this one may define the dimensionless interaction parameters

\[ c'_0 = \frac{N_c_0}{\hbar \omega l^3} = \frac{4\pi N \hbar}{3m \omega l^3} (a_0 + 2a_2) \]  

(4.16)

\[ = \frac{4\pi N}{3l} (a_0 + 2a_2) \]  

(4.17)

\[ c'_2 = \frac{N_c_2}{\hbar \omega l^3} = \frac{4\pi N \hbar}{3m \omega l^3} (a_2 - a_0) \]  

(4.19)

\[ = \frac{4\pi N}{3l} (a_2 - a_0). \]  

(4.21)

Thus the dimensionless interaction strengths are defined similarly to the dimensionful
expressions, except in terms of dimensionless scattering lengths

\[ a'_{0,2} = \frac{a_{0,2}}{l}. \]  

(4.22)

The absorption of the total number of atoms, \( N \), into \( c'_{0,2} \) enables an increased nonlinearity in the numerics to represent either an increased atom number, an increased scattering
length or an increased trapping frequency, corresponding to tighter confinement of the
atoms.

The dimensionless time-dependent GPE reads

\[ i \frac{\partial}{\partial t'} \Psi' = \left( \frac{-\nabla'^2}{2} + \frac{1}{2} \left( x'^2 + \gamma_y^2 y'^2 + \gamma_z^2 z'^2 \right) - \Omega' \cdot \hat{L}' + g_1' \mathbf{B}' \cdot \hat{F} + g_2' (\mathbf{B}' \cdot \hat{F})^2 \right. \]

\[ + c'_0 n' + c'_2 n' (\hat{F} \cdot \hat{F}) \bigg) \Psi'. \]  

(4.23)

In future discussions, the \( ' \) notation will be retained to indicate where dimensionless
units are being used. This particular choice of units is know as harmonic oscillator
units, since they are defined in terms of the frequency of the harmonic trap. This choice
of units is beneficial as it removes the trapping frequency as a free parameter. Alternatively,
one might choose one of the condensate healing lengths as the unit of length
for dimensionless analysis, which would have a corresponding frequency. However, this
would vary depending on the scattering lengths \( a_0 \) and \( a_2 \) and the trapping frequencies
\( \omega_i \). For the purposes of this study, we adopt harmonic oscillator units both to simplify
the dimensionless trapping potential and to enable the units to be clearly fixed by a single parameter, which is itself determined by the experimental apparatus. In typical experiments, \( \omega \sim 10\text{Hz} \) and \( l \sim 10\mu\text{m} \).

4.2 The Split-Step Method

To compute the time evolution of an atomic wavefunction \( \Psi \), we return to the definition of the Hamiltonian operator

\[
\hat{H} \Psi = i\hbar \frac{\partial \Psi}{\partial t}.
\]  

(4.24)

Therefore, in a timestep \( t \to t + \delta t \) one may use the approximation

\[
\Psi(t + \delta t) = e^{-i\hat{H}\delta t/\hbar} \Psi(t),
\]  

(4.25)

where the Hamiltonian takes the form

\[
\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}_{\text{eff}}(r).
\]  

(4.26)

The effective potential contains every term of the Gross-Pitaevskii Hamiltonian except the kinetic energy term. One may use finite differences to calculate the angular momentum term in \( \hat{V}_{\text{eff}}(r) \) to ensure that \( \hat{V}_{\text{eff}} \) depends only on \( r \). Naively, one might expect that one can simply perform one timestep using the position-dependent term of the Hamiltonian followed by one using the momentum-dependent term. However, since \( \hat{V}_{\text{eff}} \) and \( \hat{p}^2 \) do not commute, reversing the order of these steps will give a different result, demonstrating that this method is incorrect. We avoid this by making use of a split-step method.

If the system is being evolved in timesteps of duration \( \delta t \), one begins by taking a timestep \( \delta t/2 \) using only the potential term in the wavefunction. Then a Fourier transform is performed to obtain the momentum representation of the wavefunction at this intermediate time. A full timestep \( \delta t \) is then carried out using only the momentum term in the Hamiltonian. Taking the inverse Fourier transform to recover the position-dependent form of the wavefunction, one then performs the final \( \delta t/2 \) timestep. That is,

\[
\Psi(t + \delta t) = e^{-i\hat{V}\delta t/2\hbar} \text{FT}^{-1} \left\{ e^{-i(\hat{p}^2/2m\hbar)\delta t} \text{FT} \left\{ e^{-i\hat{V}\delta t/2\hbar} \Psi(t) \right\} \right\},
\]  

(4.27)

where we have replaced \( \hat{V}_{\text{eff}} \to \hat{V} \) for visibility purposes. The error in such a calculation is of order \( (\delta t)^3 \). Ref. [162] gives symbolic techniques to minimise the error in such calculations by splitting each timestep into shorter timesteps. In this study, we utilise the above method with third-order accuracy.
4.3 Angular Momentum

We return now to the angular momentum term in the spin-one Hamiltonian. The angular momentum operator is defined as

\[ \hat{L} = r \times \hat{p}. \] (4.28)

Taking the rotation of the trap to be about the \( z \)-axis, one can set

\[ \Omega \cdot \hat{L} = \Omega \hat{L}_z = \Omega (x \hat{p}_y - y \hat{p}_x). \] (4.29)

Since \( x \) and \( \hat{p}_x \) do not commute, this again poses a problem when taking the exponent (4.25). The numerical method referred to in Sec. 4.2 calculates the gradient in each direction at each grid point and uses these gradients in the angular momentum but does not directly address the noncommuting nature of the angular momentum terms in the Hamiltonian. We find that such a method provides the level of accuracy required but for completeness shall now outline a method which is exact to third order in the timestep, consistent with the rest of the calculation.

First, the angular momentum term is extracted from the potential, so that the Hamiltonian may be written as

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}_{\text{eff}}^{(2)} - \Omega \cdot \hat{L}. \] (4.30)

Then Eq. (4.27) becomes

\[ \Psi(t + \delta t) = e^{-i\hat{V} \delta t/2\hbar} FT^{-1} \{ e^{-i(\hat{p}^2/2m\hbar)\delta t + i\Omega \cdot \hat{L}\delta t/\hbar} FT \{ e^{-i\hat{V} \delta t/2\hbar} \Psi(t) \} \}, \] (4.31)

which may be further expanded by noting that \( \hat{p}^2 \) commutes with \( \hat{L}_z \) so that the second step may be written as

\[ e^{-i(\hat{p}^2/2m\hbar)\delta t + i\Omega \cdot \hat{L}\delta t/\hbar} = e^{-i(\hat{p}^2/2m\hbar)\delta t} e^{i\Omega \cdot \hat{L}\delta t/\hbar}. \] (4.32)

One may then decompose the angular momentum exponent in the same split-step framework as before, namely

\[ e^{i\Omega \cdot \hat{L}\delta t/\hbar} = \exp \left[ -i\Omega y \hat{p}_x \frac{\delta t}{2\hbar} \right] \exp \left[ \frac{i\Omega x \hat{p}_y \delta t}{\hbar} \right] \exp \left[ -i\Omega y \hat{p}_x \frac{\delta t}{2\hbar} \right]. \] (4.33)

In order to apply this method one must take appropriate Fourier transforms to diagonalise the wavefunction in the respective positions and momenta at the three stages of the evolution. Though this method is the more accurate, the additional Fourier transforms required lead to a \( \sim 50\% \) increase in runtime and so we choose to use an 11-point finite-differencing calculation of the gradient in the angular momentum term. Comparison between results using this approach and the exact expression show minimal reduction in the error and so we do not further consider the exact representation of the angular momentum.
4.4 Energy Minimisation

In order to identify the energetically stable states of a spin-1 BEC, we minimise the free energy functional by propagating the spinor GPE in *imaginary* time. An intuitive way of understanding this is to return to Eq. (4.25). When this is propagated in imaginary rather than real time, we have

\[ \Psi'(\tau' + \delta\tau') = e^{-\hat{H}'\delta\tau'}\Psi'(\tau'), \tag{4.34} \]

where \( t' = -i\tau' \). As one can see, if this is expressed as a sum of energy eigenstates, we have

\[ \Psi' = \sum_{E} a_{E}\Psi'_{E} \tag{4.35} \]

which modifies Eq. (4.34) to

\[ \Psi'_{E}(\tau' + \delta\tau') = e^{-\hat{H}'\delta\tau'}\Psi'_{E}(\tau'), \tag{4.36} \]

such that the states with higher expectation values of the Hamiltonian (ie. higher energies) will decay more rapidly. By renormalising the wavefunction to

\[ \int |\Psi'|^2 d^3r = 1 \tag{4.37} \]

after each timestep \( \delta\tau \), this iterative process will return a state which minimises the energy functional with the constraint of constant \( N \), as in Eq. (2.2). If there are multiple energy minima, this method will return the nearest minimum and may be unable to overcome the energy barrier separating the nearest minimum from the absolute minimum. Hence in order to identify the absolute energy minimum, one must consider a variety of initial states and calculate the energy of each resulting state.

In this thesis we study the effects of varying different parameters the spinor GPE (2.25) on the structure and stability of vortices. Experimentally, such variation may be achieved as follows. Firstly, the harmonic oscillator frequency, \( \omega_x \), is simply the frequency of the optical trap in the \( x \)-direction. \( \gamma_y \) and \( \gamma_z \) may be fixed by controlling the trapping frequencies in the respective directions. The angular velocity, \( \Omega \), is the frequency at which the trap rotates, which may be controlled. The magnetic field, \( B \), is externally applied and again may be arbitrarily chosen. The coupling constants for linear and quadratic Zeeman splitting, \( g_1 \) and \( g_2 \) respectively, may be varied by applying an off-resonant microwave field [163] and each of the \( s \)-wave scattering lengths may be tuned using a laser with frequency near the resonance of a bound state of two condensate atoms [164, 165] with the appropriate total spin (known as an *optical Feshbach resonance*), which in turn sets the interaction energies \( c_0 \) and \( c_2 \).
4.5 Successive Overrelaxation

A numerically more efficient approach than evolution in imaginary time may be employed using a linearised version of the spinor Gross-Pitaevskii Equations. However, this approach does not identify energetic minima, but rather stationary states. Stationary states satisfy

\[ \hat{H} \Psi = \mu \Psi, \quad (4.38) \]

where \( \mu \) is the chemical potential. From the definition of the Hamiltonian operator,

\[ \hat{H} \Psi = i\hbar \frac{\partial}{\partial t} \Psi \quad (4.39) \]

and so the solutions of Eq. (4.38) do not evolve in time. Stationary states of atomic BECs are therefore solutions of the time-independent GPE.

Consider a system of linear equations written in matrix form

\[ Ax = y. \quad (4.40) \]

Such a problem may be solved by first splitting the matrix \( A \) into its diagonal (D) component and those below (L) and above (U) the diagonal. Eq. (4.40) then becomes

\[ (D + U + L)x = y. \quad (4.41) \]

It follows that

\[ (D + U + L)x = y \quad (4.42) \]
\[ Dx + Lx = Dx + [y - (D + U)x] \quad (4.43) \]
\[ (D + L)x = y - [U + (1 - 1)D]x \quad (4.44) \]
\[ x = (D + L)^{-1} \{ y - [U + (1 - 1)D]x \} , \quad (4.45) \]

where various factors such as \( 1 - 1 \) are left explicit to aid in a further expansion of the algorithm. Eq. (4.45) is called the Gauss-Seidel method of solving a system of linear equations. One can solve this iteratively by inserting \( x(t) \) on the right-hand side and \( x(t + \Delta t) \) on the left-hand side [166]. However, convergence is made much more rapid by identifying an overrelaxation parameter, \( \kappa \), which one may insert in Eq. (4.42) such that

\[ \kappa(D + U + L)x = \kappa y \quad (4.46) \]
\[ x = (D + \kappa L)^{-1} [\kappa y - [\kappa U + (\kappa - 1)D]x] . \quad (4.47) \]

\( \kappa \) takes some value between 1 and 2 but its optimal value is specific to the problem being solved. Choosing \( \kappa = 1 \) simply returns the Gauss-Seidel method outlined above.
Inserting $\kappa > 1$ gives a successive overrelaxation (SOR) algorithm. By taking each element of $\mathbf{x}$ in the above discussion to be the spinor wavefunction at a given spatial position, the source term $\mathbf{y}$ to be zero and specifying the matrix operator $A$ as $A = \hat{H} - \mu$, one may then use the SOR method to identify the stationary states of spinor BECs, which satisfy $(\hat{H} - \mu)\Psi = 0$.

Due to the way the SOR algorithm was formulated, it is no longer possible to evaluate the momentum terms via Fourier Transform. The matrices $U$ and $L$ are therefore used to calculate the gradient using finite differences for insertion into the momentum and angular momentum terms in the Hamiltonian, while $D$ contains the remaining terms. Note that the SOR algorithm applies to a linear system, while the Gross-Pitaevskii Equation is nonlinear. In order to employ SOR in this study, we must therefore linearise the system. We do this by calculating the matrix elements of $A$ after every iteration of the algorithm, such that the nonlinear terms and the chemical potential are correctly evaluated. We also renormalise the spinor wavefunction after every timestep, prior to calculating the matrix elements. Our matrix elements are then

$$
U_{ij} = \hbar^2 a_{ij} - \hbar \Omega x_j b_i + \hbar \Omega y_j b_i
$$

$$
L_{ij} = \hbar^2 a_{ij} - \hbar \Omega x_i b_j + \hbar \Omega y_i b_j
$$

$$
D_{ii} = m\omega x_i^2 \frac{\gamma_y y_i^2 + \gamma_z z_i^2}{2} + g_1 \mathbf{B} \cdot \hat{\mathbf{F}} + g_2 (\mathbf{B} \cdot \hat{\mathbf{F}})^2
$$

$$
+ c_0 n_i + c_2 n_i \langle \hat{\mathbf{F}} \rangle_i \cdot \hat{\mathbf{F}} - \mu,
$$

where $a_{ij}$ are the coefficients for calculating $\nabla^2$ via finite differences and $b_i$ are those for calculating $\nabla$. $x_i$, $y_i$ and $z_i$ are the $x$, $y$ and $z$ co-ordinates of the $i^{th}$ grid point from the origin, $n_i$ is the atom density at grid point $i$ and $\langle \hat{\mathbf{F}} \rangle_i$ is $\langle \hat{\mathbf{F}} \rangle$ evaluated at the $i^{th}$ grid point. The chemical potential is calculated after every iteration as

$$
\mu = \int d^3 \mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \Psi|^2 + nm\omega x_i^2 \frac{\gamma_y y_i^2 + \gamma_z z_i^2}{2} + g_1 \mathbf{B} \cdot \langle \hat{\mathbf{F}} \rangle + g_2 (\mathbf{B} \cdot \hat{\mathbf{F}})^2 \right]
$$

$$
+ c_0 n^2 + c_2 n^2 \left( \langle \hat{\mathbf{F}} \rangle \right)^2 - n\Omega \cdot \langle \hat{\mathbf{L}} \rangle.
$$

Since finite differences are used to calculate the gradient terms, rather than Fourier transforms, a finer grid is needed in the SOR algorithm than when using imaginary time evolution. However, by avoiding Fourier Transforms in the time evolution, the split-step method is no longer required for the iterative process. By avoiding the Fourier Transforms as well as being able to calculate every term in the Hamiltonian in a single timestep as opposed to the split-step formulation, a noticeable reduction in runtime is achieved compared to the imaginary time method for the same grid size. The price of this reduction in runtime is a reduction in accuracy, both from the use of finite differences.
to calculate the gradient and from the fact that we are solving a linearised version of the GPE, rather than the fully nonlinear problem.
Chapter 5

Vortex Core Deformation

Having discussed the topologies of the ground-state manifolds of spin-1 BECs, we now consider the energetic stability of vortices. Although vortices in different topological classes may be constructed, it is by no means guaranteed that there will be a parameter regime in which they are energetically stable. Where several vortex structures exist in the same topological class, it should also be asked which vortex from said topological class will be energetically stable, if any. In order to determine the energetic stability of the vortex configurations and stable vortex core structures, we numerically minimise the energy of specific vortex states belonging to distinct topological equivalence classes. We then classify the stable vortex core structures in terms of an energetic hierarchy of length scales.

In this Chapter, the energy relaxation is performed by numerically propagating the coupled set of GPEs in imaginary time using a split-step algorithm [162] [See Sec. 4.2]. We consider axially symmetric harmonic traps with \( \gamma_y \) = 1, though two different values of \( \gamma_z \) are investigated. \( \gamma_z = 1 \) describes an isotropic trap while \( \gamma_z = 10 \) describes an oblate trap. Since the trap is axially symmetric in all cases, we denote \( l \to l_\perp \) and \( \omega \to \omega_\perp \). We allow the magnetisation, \( M \) [Eq. (2.34)], to vary in the relaxation process and consider only contact interactions between atoms.

5.1 Stability and Core Deformation of Ferromagnetic Vortices

We begin by investigating the energetic stability of vortices in the FM regime. We consider an isotropic trap in a rotating frame with the nonlinearities \( Nc_0/\hbar\omega_\perp l_\perp^3 = 1000 \) and \(-640 \leq Nc_2/\hbar\omega_\perp l_\perp^4 \leq -10 \). As an initial state for a singular singly-quantised vortex we take the vortex of Eq. (3.12) in which case each spinor component exhibits a singly-quantised vortex line. These all perfectly overlap with a vanishing density at
Figure 5.1: Energetic stability of the (a) coreless and (b) core-deformed singular vortex in an isotropic trap for varying spin-dependent interaction strength $Nc_2/\hbar \omega \perp \ell_1^3 < 0$. The spin-independent interaction is fixed at $Nc_0/\hbar \omega \perp \ell_1^3 = 1000$. (●) initial vortex is energetically stable. (+) initial vortex leaves the cloud. (×) additional vortices nucleate due to rotation. A blue vertical line marks $c_0/c_2 \simeq -216$ relevant for $^{87}$Rb [120]. Note that with the parameters used here, this yields $N|c_2|/\hbar \omega \perp \ell_1^3 = 4.6$ and the line is very close to the vertical axis.

the core. We also perform an energy minimisation of the coreless, nonsingular vortex of Eq. (3.17). The coreless vortices have been shown to exist in the ground state of a sufficiently rapidly rotating FM spin-1 BEC [20, 65, 167, 168], such that increasing the rotation rate of a vortex-free cloud is predicted to result in nucleation of coreless vortices in the system.

We find a single coreless vortex to be energetically stable in a sufficiently rapidly rotating trap, as shown in the stability diagram of Fig. 5.1(a). Fig. 5.2(a) shows the characteristic fountain-like spin texture of the stable vortex. At slow rotation speeds the vortex exits the atom cloud and at faster rotation rates we observe nucleation of additional coreless vortices to the system. The threshold rotation frequency is increased for stronger spin-dependent interactions. Our findings are consistent with those in Ref. [167].

For the singular initial-state vortex the corresponding stability diagram is displayed in Fig. 5.1(b). Although its core structure is deformed during energy relaxation (as we will discuss below), we find that the singular vortex is energetically stable for a range of rotation frequencies at all investigated values of $c_2$. This energetic stability of the singular vortex seems surprising since there also exists a stable coreless vortex with lower energy at the same rotation frequencies and nonlinearities. Indeed, our numerics show that coreless vortices will nucleate due to rotation, whereas singular vortices will not. A comparison between the numerically calculated energies of a stable coreless vortex and a stable singular vortex as a function of the rotation frequency for $Nc_2/\hbar \omega \perp \ell_1^3 = -320$ is shown in Fig. 5.3. This value is chosen as it renders the coreless vortex stable for a large range of rotation frequencies. The energetics of coreless and singular vortices in FM
Figure 5.2: Numerically calculated spin textures of the stable FM vortex states in a rotating trap. The spin vector is shown in a cut perpendicular to the \( z \) axis (the axis of rotation). (a) The spin vector in the coreless vortex exhibits a characteristic fountain-like structure and maintains \(|\langle \hat{\mathbf{F}} \rangle| = 1\) everywhere. (b) In the relaxed singular vortex, the spin vector winds by \( 2\pi \) about the \( x \) axis on a path encircling the singular vortex core (indicated by the dot), in which \(|\langle \hat{\mathbf{F}} \rangle| \rightarrow 0\). The \( x \) axis is the orientation of the uniform spin far from the vortex. This texture can be continuously deformed into that shown in Fig. 3.1(b).

Figure 5.3: Numerically calculated energies of stable FM coreless (red) and singular (blue) vortices for varying rotation frequencies \( \Omega \). The coreless vortex is lower in energy for all parameter ranges investigated.

spin-1 atomic BECs may be contrasted with that in superfluid liquid \(^3\)He-\( A \), where the singular vortex has lower energy, but the energy barrier for nucleation of the singular core is higher than that for forming a coreless vortex [169]. Singular vortices can be created by cooling a rotating normal fluid through the superfluid transition.

The coreless and the singular vortices belong to distinct topological equivalence classes and they cannot be continuously deformed to each other. For the singular vortex to decay, the rotation frequency has to be sufficiently slow so that the vortex can exit the atom cloud and be replaced by a nucleating coreless vortex that enters from the edge of
the cloud. We find a range of frequencies and nonlinearities [Fig. 5.1(b)] for which the singular vortex remains in the atom cloud and no additional coreless vortices nucleate. A single, singly-quantised singular vortex thus represents a local minimum of the energy, topologically protected against decay to the lower-energy coreless vortex.

Having demonstrated that the singular singly-quantised vortex of Eq. (3.12) is energetically stable, we next study the vortex core structure of the relaxed state. The resulting vortex configuration with a stable vortex core is shown in Fig. 5.4(a). The vortex lines in the different spinor wavefunction components have moved apart and no longer spatially overlap. We show in Fig. 5.5(a) a 1D density cut along which the spatially separated vortices are aligned. The vortex line of the \( \zeta_0 \) component is located at the centre of the trap and the vortices of the \( \zeta_\pm \) components are symmetrically displaced from the centre. This split-core solution appears to break the explicit axial symmetry of the spinor component densities in Eq. (3.12). A similar core splitting has previously been demonstrated in 2D numerical simulations in Ref. [21]. We will show below how it is beneficial to analyse the vortex core using a spinor basis transformation. In particular, after an appropriate transformation we can easily identify the location of the vortex, non-vanishing atom density at the vortex line singularity, and axially symmetric density profiles of the spinor components in the new basis representation. In the vortex configuration displayed in Fig. 5.4(a) we may then identify the split-core vortex as spin winding around a core of non-vanishing atom density.

In order to analyse the vortex configuration of Fig. 5.4(a) we perform a basis transformation for the spinor wavefunction. We transform the split-core spinor to the basis where spin is quantised along the \( x \) axis as \( \vec{\zeta}(x) = U^{-1}(0, \pi/2, 0) \vec{\zeta}(z) \), explicitly indicating the spinor basis by superscripts. In \( \vec{\zeta}(x) \) the vortex appears as an opposite winding of the phase in the two components \( \zeta_\pm(x) \). These vortex lines again overlap as shown in Figs. 5.4(b) and 5.5(b). Crucially, there is no vortex line in \( \zeta_0(x) \), and this component therefore fills the vortex cores of the two other components so that the density is non-vanishing everywhere. The single vortex core, which is readily apparent from Fig. 5.7, is thus explicitly restored in \( \vec{\zeta}(x) \) by the transformation to the natural basis of the vortex. We identify the spinor wavefunction resulting from the basis transformation now as having the same structure as the singular vortex, defined in Eq. (3.13).

The spin structure of the stable vortex is shown in Fig. 5.2(b). The vortex line is oriented along the \( z \) direction—the axis about which the trap is rotating. However, the spinor takes the form of Eq. (3.13) in the basis defined along the (co-rotating) \( x \) axis. This vortex is singular, preserving the topology, and can be reached from Eq. (3.12) by local spin rotations and could similarly be continuously transformed into the singular spin vortex [Fig. 3.1(b)]. The stable vortex core Fig. 5.2(b) has a broken spatial parity (the spin profile has an antisymmetric spatial parity close to the vortex core). This spin profile is nonaxisymmetric. We also find a stable axisymmetric vortex core. This is achieved by starting energy relaxation from Eq. (3.13), such that the radial disgyration
of the spin vector is present already in the initial state. The spinor components and the resulting spin profile are shown in Fig. 5.6. The dependence of the final configuration on the initial state indicates a close energetic degeneracy of the two solutions.

To understand the vortex core deformation, it is also beneficial to compare the initial-state singular vortex of Eq. (3.12) to the vortex obtained in the energy minimisation. In Eq. (3.12) each spinor component exhibits a singly quantised vortex. These overlapping vortex lines imply that the total density $n(r)$ must be zero on the singular line in order to maintain single-valuedness of the order parameter. The size of the vortex core is determined by the healing length $\xi_n$. The density depletion can be avoided by splitting the vortex core such that the vortex lines in the spinor components no longer overlap. Since the total condensate density then does not vanish at the vortex line where the order parameter is singular, we must now require that the spinor wavefunction becomes orthogonal to the ground-state manifold at the vortex singularity. In the FM manifold $|\langle \hat{F} \rangle| = 1$, so at the vortex line we must have $|\langle \hat{F} \rangle| = 0$, which represents the spin magnitude of the polar phase.
Figure 5.5: (a) Densities in the three spinor components $\zeta_{\uparrow}^{(z)}$ (red line marked by +), $\zeta_{0}^{(z)}$ (green line marked by 0) and $\zeta_{\downarrow}^{(z)}$ (blue line marked by −) on the axis connecting the vortex lines in the spinor components [cf. Fig 5.4(a)]. (b) Densities in $\zeta_{\uparrow}^{(x)}$ (red line marked by +), $\zeta_{0}^{(x)}$ (green line marked by 0) and $\zeta_{\downarrow}^{(x)}$ (blue line marked by −) on the same spatial axis after spinor basis transformation. $|\langle \hat{F} \rangle|$ (black dash-dotted line) goes to zero in the vortex core (the apparent nonzero minimum is due to finite numerical resolution) which is filled by $\zeta_{0}^{(x)}$, keeping the density nonzero everywhere.

The spin magnitude of the numerically calculated singular vortex core is displayed in Figs. 5.5(b) and 5.7. We find that the value of the spin magnitude indeed rapidly approaches zero close to the vortex line singularity (the small deviations from zero are due to spatial resolution of the numerics). This indicates the formation of a polar vortex core, constituting a local violation of the spin condition for the ground-state FM manifold. An analytic description of the vortex solution is provided in Appendix C. The size of the vortex core is determined by the spin healing length $\xi_F$. The splitting is then energetically favourable when $\xi_F$ allows a larger core size (i.e., when $\xi_F \gtrsim \xi_n$) such that the energy cost of violating $|\langle \hat{F} \rangle| = 1$ is smaller than that of depleting the density.

We find that the region where the spin magnitude deviates from $|\langle \hat{F} \rangle| = 1$ extends over the entire core size, determined by the spin healing length $\xi_F$. Outside the core region of the vortex the symmetry of the spin-1 BEC is broken according to the FM energy condition of the spin-dependent interaction energy, so that we have $|\langle \hat{F} \rangle| = 1$. Close to the singular vortex however, the order-parameter bending energy restores the symmetry of the full spin-1 BEC wavefunction ($S^5$ determined by a normalised spinor wavefunction of three complex components), mixing the FM and polar phases. The bending energy is enhanced very close to the vortex singularity due to the large density gradient contributions that excite the system from the FM ground-state manifold. An analogous core deformation was previously found for a singular point defect in a polar spin-1 BEC in Ref. [58]. In that case an isotropic point defect with a vanishing density deformed to a ring defect with a FM core. This effect is closely related to the polar vortex core deformation described in Sec. 5.2.
Figure 5.6: Axially symmetric spin vortex. (a) Densities of the spinor components together with the spin magnitude along a radial cut (lines and labels as in Fig. 5.5(a)). The vortex lines in $\zeta^\pm$ overlap perfectly at the position of the vortex core. (b) Relaxed spin profile in the $x$-$y$ plane, showing the characteristic radial disgyration of the spin vector around the singular core. At large radii the spin vector bends out of the $x$-$y$ plane. The vortex line singularity is marked by a dot at the centre.

In experiments a stable singular vortex could be prepared in a controlled way by phase-imprinting the initial singular vortex state of Eq. (3.12) in a rotating trap, so that the parameter values of the system belong to the stable region of the stability diagram displayed in Fig. 5.1(b). The initial-state vortex [Eq. (3.12)] is composed by perfectly overlapping singly-quantised vortices in each of the spinor components. These could be phase-imprinted using previously realised experimental techniques [24, 30, 38]. The stability diagram also indicates the conditions under which a singular vortex created in a phase transition [51] could potentially be stabilised.

In the above analysis, we have allowed the magnetisation $M = N_+ - N_-$, where $N_\pm$ are the total populations of $\zeta_\pm$, to vary during the relaxation process. This in principle allows a spontaneous magnetisation to develop in the system. In experiments, dissipative relaxation of energy due to atomic collisions approximately conserves the magnetisation on relevant timescales. We will consider the effects of magnetisation-conserving relaxation in Chapter 6 but for now we simply note that the results presented in this Chapter will be modified in a sufficiently strongly-magnetised system.

Thus far we have considered an isotropic trap. We find that the results are qualitatively similar in an oblate trap with $\gamma_z = 10$. We find that also in this regime, the singular vortex represents a local energetic minimum and is stable for a range of $\Omega$, again despite the fact that a lower-energy coreless-vortex solution exists. The parameter regions allowing stable nonsingular coreless and singular split-core vortices in the oblate trap are shown in Fig. 5.8.
Applying a weak external magnetic field introduces a Zeeman shift between the spinor components according to Eq. (2.25). The spinor nature of the BEC is retained as long as the applied field is not too strong $g_1 |\mathbf{B}|, g_2 |\mathbf{B}|^2 \lesssim \mu$, where $\mu$ denotes the chemical potential. In the case of a small linear Zeeman splitting $g_1 |\mathbf{B}|$ (taking $\mathbf{B}$ along the $z$ axis) in the oblate trap, we find that the coreless and singular vortices are both stable, with the coreless vortex lower in energy. The Zeeman splitting will tend to align the
spins with the applied field. This causes the energy of the coreless vortex to increase as maintaining the fountain-like spin structure becomes energetically less favourable. Thus we find that for $g_1|B|/\hbar \omega_\perp \gtrsim 0.2$ the coreless vortex is no longer stable. The singular vortex, on the other hand, remains energetically stable for all $g_1|B|$ considered (up to 0.8), as shown in Figs. 5.9(a) and (b). For a sufficiently large linear Zeeman splitting the ideal spinor basis to analyse the singular vortex core becomes that defined by the magnetic field.

A quadratic Zeeman splitting, on the other hand, does not destroy the stability of the coreless vortex, but for $g_2|B|/\hbar \omega_\perp \lesssim -0.1$ the singular vortex is no longer energetically stable [Fig. 5.9(c) and (d)]. For a sufficiently large positive quadratic Zeeman splitting
the ideal spinor basis to analyse the singular vortex core is oriented perpendicular to the magnetic field.

5.2 Stability and Core Structure of a Polar Vortex

In order to investigate the energetic stability of a singly-quantised singular vortex in the polar phase of a spin-1 BEC we numerically minimise the energy of the system in a rotating frame. We follow the same procedure as in the FM case and this time take a singular polar vortex of Eq. (3.30) with $\beta = \pi/4$ and $\alpha = 0$ as the initial state of the numerical relaxation. Similarly to the FM case of Eq (3.12), the initial state is formed by overlapping vortex lines in all the three spinor components. Upon minimising the energy, the vortex cores of the individual spinor components separate. However, compared with the FM case, the splitting is now more complicated, as shown in Fig. 5.10. The result is highly deformed anisotropic vortex cores in the spinor components. The vortices in $\zeta_+$ and $\zeta_-$ overlap, but the one in $\zeta_0$ is displaced from the other two. There are no simultaneous density minima in all three spinor components, and the density is therefore nonzero everywhere. Similar split-core solutions found by numerical calculation in a rotating 2D system [23] have resulted in some controversy regarding the number vortices in the individual spinor components in the final configuration [21]. In the previous 2D studies the stable core structures were not classified. Here we show now how the split core in Fig. 5.10 can be identified as a topology-preserving splitting of the singly-quantised vortex into a pair of half-quantum vortices as illustrated schematically in Fig. 5.11. In Appendix D we demonstrate that the core structures of Refs. [21, 23] may be identified as the same structure viewed in different bases and that they are equivalent to the structures we identify in this Section. The structure and stability of a single half-quantum vortex is also briefly presented in Appendix E.

In the numerical simulations the initial state of a singly-quantised singular vortex in Eq. (3.30) is composed of three perfectly overlapping vortex lines in each of the three spinor components. The polar vortex consequently has a vanishing density at the line singularity of the polar order parameter of the spin-1 BEC. The singular vortex with zero density is energetically unstable with respect to core deformation. As the vortices of the individual spinor components move apart during energy relaxation, the density becomes non-vanishing everywhere in the vortex-core region. Similarly to the FM vortex case, we must therefore require that the spinor wavefunction becomes orthogonal to the ground-state manifold at the vortex singularity. This indicates that we must have $|\langle \hat{F} \rangle| = 1$ on the vortex line. We show in Fig. 5.12 the numerically calculated vortex core structure of a stable vortex whose initial state is the singular singly-quantised vortex of Eq. (3.30). The displayed spin magnitude exhibits two clearly separated cores in which the peak value increases to $|\langle \hat{F} \rangle| = 1$, indicating the emergence of a FM core region for the vortex.
Figure 5.10: Stable core structure of the singular vortex in the polar phase shown in the $x$-$y$ plane. (a) and (b): Densities in $\zeta_+^{(z)}$ and $\zeta_0^{(z)}$, respectively. (c) and (d): The corresponding phases. ($\zeta_-^{(z)}$ is identical to $\zeta_+^{(z)}$ up to a global $\pi$ phase shift.) The spinor wavefunction exhibits vortex lines with highly deformed anisotropic cores in the spinor components.
Figure 5.11: Schematic illustration of two vortex-core structures with the same topology for a singly-quantised singular vortex in the polar phase of a spin-1 condensate. In (a) the atom density vanishes at the vortex-line singularity with the core size determined by the characteristic length scale $\xi_n$ (healing length) associated with the spin-independent interaction strength. In (b) the atom density is non-vanishing in the core region whose size is determined by the characteristic length scale $\xi_F$ of the spin-dependent interaction strength. The vortex line singularity has now split into two half-quantum vortices with the atoms in the ferromagnetic phase at the precise location of the singularities. In both figures we show the nematic axis as a dashed line and the dotted line in (b) indicates a disclination plane for the nematic axis. Inside the core region (shaded area) of (b) the broken symmetry of the polar ground-state manifold is restored (as explained in the text). Outside the core the topological properties of the vortex are the same as those in (a).

The formation of the FM cores can be understood from the same argument used to understand the polar core of the singular FM vortex in Sec. 5.1 and is illustrated in Fig. 5.11: The singular polar vortex (3.30), which is used as an initial state in the energy relaxation, implies a density-depleted core whose size is determined by $\xi_n$. However, accommodating a singularity of the polar order parameter by requiring $|\langle \hat{F} \rangle| = 1$ at the vortex line means that the length scale, and thus the associated bending energy, is determined by $\xi_F$. The energy of Eq. (3.30) can thus be lowered by having a non-vanishing atom density and by extending the core size from $\xi_n$ to $\xi_F$. In the case of a polar vortex this is achieved by spontaneously breaking the axial symmetry and forming two FM cores by the mechanism sketched in Fig. 5.11. The separation between the cores is of the order of $\xi_F$, depending also on the angular momentum of the system when it adjusts to the rotation frequency and on the density gradient due to the trap.

We may analyse this symmetry breaking of the vortex core by means of a basis transformation. We write the spinor in the basis of spin projection onto the axis given by the spin vector in the FM core. For the case of Fig. 5.10(a), the spins in both cores
Figure 5.12: Splitting of the singly-quantised vortex into two half-quantum vortices. (a) Spin magnitude $|\langle \hat{F} \rangle|$, [colour map from white ($|\langle \hat{F} \rangle| = 0$) to red ($|\langle \hat{F} \rangle| = 1$)] together with the spin vector (arrows), showing the FM cores with non-vanishing density. The spins are antiparallel in the two cores. (b) Nematic axis $\hat{d}$ together with the vortex cores (indicated by green isosurfaces of $|\langle \hat{F} \rangle|$, with increasing spin magnitude indicated by the colour gradient inside). Away from the vortex cores the topology of the initial singly-quantised vortex is preserved. In the core region, $\hat{d}$ winds by $\pi$ about each half-quantum vortex core. For visualisation purposes, the unoriented $\hat{d}$-field is shown as cones. Here a quadratic Zeeman shift has been introduced to ensure that $\hat{d}$ lies in the x-y plane and the spins align with the z axis.

align/anti-align with the y axis and we calculate $\zeta^{(y)} = U^{-1}(\pi/2, \pi/2, 0)\zeta^{(z)}$. The resulting spinor then shows displaced vortex lines in $\zeta^{(y)}_\pm$ while the density vanishes in $\zeta^{(y)}_0$ [Fig. 5.13]. In the new spinor basis, the vortex lines in $\zeta^{(y)}_\pm$ coincide precisely with the spin maxima, as shown in Fig. 5.14

We can now identify the core structure emerging from the splitting of the singular vortex by comparing the spin-rotated state $\zeta^{(y)}$ with Eq. (3.25). We then find that each vortex line in $\zeta^{(y)}$ has exactly the form of a half-quantum vortex. The split-core configuration may thus be interpreted as a splitting of the singly-quantised vortex into a pair of half-quantum vortices with FM cores. The topological charges of vortices are additive in the polar phase as demonstrated in Sec. 3.4 and the topology is therefore preserved when the singly-quantised vortex splits into the pair of half-quantum vortices. This can also be inferred from the behaviour of the nematic axis $\hat{d}$. Figure 5.12(b) shows $\hat{d}$ in a numerical solution together with the FM cores of the half-quantum vortices. Away from the vortices, there is no net winding in $\hat{d}$ on a path enclosing the vortices. However on a path that encircles only one vortex core, $\hat{d}$ rotates by $\pi$, indicating the emergence of a disclination plane.

As in the case of a FM vortex, the core deformation can be explained in terms of the vortex topology and the energetic hierarchy of different length scales (see Fig. 5.11). Outside the vortex core region of size $\xi_F$, where the order parameter bending energy is not sufficient to excite the system away from the polar ground-state manifold, we
Figure 5.13: Spinor wavefunction of the stable singular vortex state from Fig. 5.10 after spinor basis transformation such that spin is quantised along the $y$ axis. (a) and (b): Densities in $\zeta^{(y)}_+$ and $\zeta^{(y)}_-$, respectively. (c) and (d): The corresponding phases. The component $\zeta^{(y)}_0$ (not shown) is unpopulated. The previously complex structure can now be identified as a pair of half-quantum vortices.
have $|\langle F \rangle| = 0$ and the topological properties of the initial singly-quantised singular vortex are preserved. This is indicated by the unit winding of the macroscopic condensate phase around any closed loop encircling the entire vortex core and by the nematic vector field outside the core region. It is only inside the core of size $\xi_F$ that the strong order parameter bending energy restores the symmetry of the full spin-1 condensate wavefunction by exciting the system out of the polar ground-state manifold and by allowing the complete range of spin values $|\langle F \rangle|$ from 0 to 1. The local deformation of the core is topologically possible due to the nematic order of the polar phase, where the axis $\hat{d}$ is unoriented, with the opposite orientations $\hat{d} \leftrightarrow -\hat{d}$ identified. The core deformation mechanism of the vortex line is related to the deformation of a point defect to a singular ring where the nematic order allows the spontaneous breaking of the spherical defect core symmetry [58]. In the $B$-phase of superfluid liquid $^3$He, a stable nonaxisymmetric singular vortex with a nonzero superfluid density at the core was theoretically predicted in Refs. [144, 145] and experimentally observed in Ref. [146]. The $^3$He $A$-phase core was explained to consist of two half-quantum vortices. In the high-pressure regime the axial symmetry of the vortex is restored but the core can still remain in the $A$-phase with a non-vanishing superfluid density [60].

We find that the singular vortex splits into a pair of half-quantum vortices by the mechanism described above for all investigated parameter regimes. However, we find a critical rotation frequency of $\Omega \simeq 0.3\omega_\perp$ below which the vortices start exiting the atom cloud. Figure 5.15 shows the energetic stability of the half-quantum vortex pair obtained from splitting of a singly-quantised vortex in both isotropic and oblate ($\gamma_z = 10$) traps. The energetic ground state of a rotating polar spin-1 BEC can consist of half-quantum

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**Figure 5.14**: (a) Density profiles of the spinor components on the axis connecting their density minima [cf. Fig. 5.10]. Lines labeled with spinor component index. Note that $|\zeta \pm|$ exactly overlap. (b) Spinor-component density profiles in $\zeta(y)$ after basis transformation [cf. Fig. 5.10] plotted along the axis connecting the half-quantum vortices. The spin magnitude $|\langle F \rangle|$ (black dash-dotted line) shows the FM cores. Unpopulated $\zeta(y)$ is not shown.
Figure 5.15: Energetic stability of the split-core singular vortex in the polar phase. (a) Stability in the isotropic trap for varying $c_2$ using $Nc_0/h\omega_\perp l_\perp^3 = 1000$. The vertical line marks the value $c_0/c_2 \simeq 28$ for $^{23}$Na [122]. (b) Stability in the oblate trap ($\gamma_z = 10$) for varying $Nc_2/h\omega_\perp l_\perp^3$ using $Nc_0/h\omega_\perp l_\perp^3 = 50$. (c) and (d): Stability of the split-core singular vortex in the presence of linear and quadratic Zeeman splitting, respectively. Increasing linear Zeeman splitting renders the singular vortex unstable, whereas the stability is robust against quadratic Zeeman splitting. In the slowly rotating region for all panels, the instability of the split-core singular vortex may be either towards the vortex-free state, or towards the state with a single half-quantum vortex. (Symbols as in Fig. 5.1.)

vortices [65, 168], so increasing the rotation frequency leads to nucleation of more half-quantum vortices in addition to the split core of the initial singular vortex.

The splitting mechanism of the singly-quantised vortex is qualitatively similar when a weak Zeeman splitting due to a magnetic field is introduced. However, as shown in Fig. 5.15(c), a linear Zeeman splitting of $g_1|B|/h\omega_\perp \gtrsim 0.4$ causes the resulting pair of half-quantum vortices to become energetically unstable at all rotational frequencies. By contrast, the vortex pair remains stable above $\Omega/\omega_\perp \simeq 0.3$ for the entire range of quadratic Zeeman splittings considered ($-0.8 \leq g_2|B|^2/h\omega_\perp \leq 0.8$) [Fig. 5.15(d)].
5.3 Conclusions

We have demonstrated that in the FM regime, both a singular, singly-quantised vortex and a nonsingular coreless vortex are stable. The singular vortex exists as a metastable state, with the coreless vortex forming the ground state.

The stable singular vortex core in the FM regime is formed by non-overlapping vortex lines in the three spinor components. We have demonstrated that this seemingly complex core structure can be understood in terms of the combination of the vortex topology and the energetics of characteristic length scales. By deforming the core of a singly-quantised, singular vortex in the FM regime so as to maintain a nonzero density everywhere, instead accommodating the singularity by forcing $|\langle \hat{F} \rangle| = 0$, the gradient contribution to the energy is lowered. The reason is that the size of the defect core is then determined by the spin healing length $\xi_F$ [Eq. (2.40)] which is in general larger than the characteristic size $\xi_n$ [Eq. (2.39)] of a defect core where the density goes to zero. In our numerics, $\xi_F > \xi_n$ [see Table 2.1]. In other words, in the larger core size case with a non-vanishing atom density, the gradient energy restores the full symmetry of the spin-1 condensate wavefunction within the core region. The system then simultaneously exhibits two different order parameter symmetries: maximal unbroken symmetry inside the core of size $\xi_F$ and a broken symmetry (of the FM phase) outside the vortex core.

The core deformation mechanism results in a singular vortex whose core is also filled with atoms in the polar phase. The spin vector winds by $2\pi$ as the core is encircled. The single vortex core can be explicitly restored in the spinor by judicious choice of spinor basis.

In the polar regime, we have shown that a singly-quantised vortex is stabilised by a spontaneous breaking of axial symmetry. The resulting stable defect is a pair of half-quantum vortices with FM cores, which is stable in a sufficiently rapidly rotating trap. The formation of the FM cores avoids depleting the density in the vortex core. This is energetically favourable by the same reasoning that was applied to explain the polar core of the singular vortex in the FM regime. The resulting spinor wavefunction is analysed and the vortex structure identified through a rotation of the spinor basis, so that in the rotated basis the half-quantum vortices appear as separate vortex lines in the $\zeta_{\pm}$ components.
Chapter 6

Magnetisation-Conserving Relaxation

In Chapter 5, we demonstrated the stability of singular and coreless vortices in spin-1 atomic BECs in rotating optical traps. However, during the relaxation process, the longitudinal magnetisation was not conserved. On experimentally relevant timescales, the longitudinal magnetisation is approximately conserved in spin-1 BECs and so the question must be asked: does this conserved magnetisation have any effect on the results of Chapter 5? We find that a sufficiently strong magnetisation cannot be accommodated by the previously-identified vortex cores, giving rise to novel vortex structures, including composite topological defects which exhibit different small- and large-distance topology. One particularly interesting consequence is the stability of a FM coreless vortex in a magnetised BEC with polar interactions, existing as the inner core of a composite topological defect with the large-distance topology of a singular polar vortex. The coreless vortex has been experimentally phase-imprinted upon a polar BEC [36, 37] and so its stability for a range of magnetisations and rotation frequencies provides the opportunity to study a composite topological defect using current experimental apparatus.

We demonstrate a method of constructing analytical spinors which can describe the filling of vortex cores with non-circulating states, by interpolating between the FM and polar ground-state manifolds. This methodology is also applied to describe composite topological defects such as the coreless vortex within the core of a singular polar vortex. In the composite defect structures, the small- and large-distance topologies are determined by the magnitude of the spin inside the outer core and far from the vortex core, respectively. From the construction of these analytic spinors, we also understand the stability of a nonsingular nematic coreless vortex of the polar phase, which may form the inner core of a composite topological defect with the large-distance topology of a singular FM vortex. A simple analytical model of a magnetised (unmagnetised) vortex core surrounded by an unmagnetised (magnetised) bulk is then applied to demonstrate
the emergence of a characteristic length scale associated with the conserved magnetisation. This magnetisation length scale then determines the energetic stability of vortex core structures.

6.1 Numerical Method

Here, we study the structure and stability of vortices subject to a conserved longitudinal magnetisation. We employ the imaginary time propagation technique with a small modification: after each timestep, when the system is renormalised, we also adjust the normalisations of the three spinor components to produce the required magnetisation. In this way, the magnetisation is then explicitly conserved in the relaxation process. For simplicity, we assume the quantisation axis (z axis) to coincide with the trap rotation axis. The value of the conserved magnetisation is determined by the initial state spinor-wavefunction. We therefore construct initial states by modifying the appropriate spinors representing the basic vortices in Sec. 3.2 to have the desired magnetisation.

When the magnetisation is not conserved, the renormalisation process is relatively straightforward. Suppose that after a timestep, the spinor populations are $N_i^{(0)}$ and they are to be renormalised to $N_i^{(r)}$. Defining

$$N_+^{(0)} + N_0^{(0)} + N_-^{(0)} = N^{(0)},$$

simply dividing all spinor components by $N^{(0)}$ will yield the appropriate normalisation

$$N_+^{(r)} + N_0^{(r)} + N_-^{(r)} = \frac{N_+^{(0)} + N_0^{(0)} + N_-^{(0)}}{N^{(0)}} = 1.$$  

When the magnetisation $M$ is conserved, the routine is modified to incorporate the magnetisation constraint, while still conserving the normalisation. The conserved magnetisation $M$ requires that

$$N_+^{(r)} - N_-^{(r)} = M.$$

In the renormalisation process, we may set

$$N_+^{(r)} = \frac{N_+^{(0)} + \Delta}{N^{(0)}},$$

$$N_0^{(r)} = \frac{N_0^{(0)}}{N^{(0)}},$$

$$N_-^{(r)} = \frac{N_-^{(0)} - \Delta}{N^{(0)}},$$

where

$$\Delta = M N^{(0)}.$$
which retains the normalisation. The magnetisation then becomes

\[ M^{(r)} = \frac{N_+^{(0)} - N_-^{(0)} + 2\Delta}{N^{(0)}}. \]  

(6.7)

By forcing \( M^{(r)} = M \), we then calculate the magnetisation correction factor

\[ \Delta = \frac{MN^{(0)} + N_-^{(0)} - N_+^{(0)}}{2}. \]  

(6.8)

This algorithm will then explicitly conserve both the magnetisation and the normalisation of the spinor. However, the algorithm is only valid if \(-N_+^{(0)} < \Delta < N_-^{(0)}\), which is violated when there are insufficient atoms in the combined \( \zeta_\pm \) components to produce the magnetisation. In this eventuality, we modify the normalisation procedure such that

\[ N_\pm^{(i)} = \pm M \]  

(6.9)

\[ N_0^{(i)} = 1 \mp M \]  

(6.10)

\[ N_\mp^{(i)} = 0, \]  

(6.11)

where the upper (lower) symbol indicates positive (negative) magnetisation. This mechanism does not have a strong effect on the duration of propagation in imaginary time which is required to produce a converged solution. However, shorter timesteps are required as the magnetisation constraint may be enforced only at the end of each timestep. Too long a timestep enables the magnetisation to deviate substantially from the value at which it should be conserved. This deviation in the magnetisation is contrary to the purpose of this study and so we must ensure that sufficiently short timesteps are used.

We consider a condensate in an isotropic, 3D harmonic trap with interaction strengths chosen such that \( Nc_0/\hbar\omega l^3 = 1000 \). The spin-dependent nonlinearity is kept fixed at \( Nc_2/\hbar\omega l^3 = -5 \) (\( Nc_2/\hbar\omega l^3 = 36 \)) in the FM (polar) regime, which is consistent with the experimentally measured ratio of \( c_2/c_0 \) for \( F = 1 \) \(^{87}\text{Rb}\) (\(^{23}\text{Na}\)).

### 6.2 Interpolation Between Vortex States

The two ground-state manifolds of the spin-1 BEC support different families of vortices as described in Secs. 3.3-3.4. However, when the energy of a vortex state relaxes, the FM and polar phases may in general mix as a result both of the filling of singular-vortex cores and of conservation of longitudinal magnetisation. In addition to the structureless filled cores of singular vortices identified in Chapter 5, it becomes possible to form composite topological defects which exhibit distinct small- and large-distance topology as the wavefunction interpolates between the FM and polar phases, such as the composite core structure of a singular FM vortex studied via homotopy sequences in Ref. [140]. These composite defects exhibit a hierarchical core structure. An outer vortex, representing
the large-distance topology, has within its core a nontrivial vortex structure representing the local topology. Composite defects exist in superfluid liquid $^3$He, in which case the hierarchy of different core structures can result from different interaction energies, owing, e.g. to spin-orbit or magnetic-field coupling [10, 169]. Here we explicitly construct spinor wavefunctions that smoothly interpolate between outer vortex states and inner, vortex-free states, as well as those which smoothly connect FM and polar vortex states to represent the basic composite topological defects. The analytic spinors presented are not solutions of the spinor GPEs, but serve to demonstrate how different vortex states may be connected via a transition between the polar and FM phases.

To this end, we derive a general spinor for a spin-1 atomic BEC where $|\langle \hat{F} \rangle| = F$ may take any value in $0 \leq F \leq 1$. We start from the representative spinor

$$\zeta_F = \frac{1}{\sqrt{2}} \begin{pmatrix} -f_+ \\
0 \\
f_- \end{pmatrix}, \quad (6.12)$$

where $f_\pm = \sqrt{1 \pm F}$. The $F = 1$ limit then corresponds to the representative FM spinor used in Sec. 3.3 up to a global phase factor. The limit $F = 0$, on the other hand, is a representative polar spinor with $\hat{d} = \hat{z}$ rather than that used in Sec. 3.4, which had $\hat{d} = \hat{x}$. For the trial spinor with arbitrary $F$, $\langle \hat{F} \rangle = F \hat{z}$ and $\hat{d} = \hat{x}$. In general, any $|\langle \hat{F} \rangle| = F$ order parameter may then be represented by spin rotations of the orthogonal vector triad ($\langle \hat{F} \rangle, \hat{d}, \langle \hat{F} \rangle \times \hat{d}$), together with the condensate phase. Hence, from $\zeta_F$ we form the general spinor

$$\zeta = \frac{e^{i\phi}}{2} \begin{pmatrix} \sqrt{2}e^{-i\alpha} \left( e^{i\gamma} \sin^2 \frac{\beta}{2} f_- - e^{-i\gamma} \cos^2 \frac{\beta}{2} f_+ \right) - \sin \beta \left( e^{i\gamma} f_- + e^{-i\gamma} f_+ \right) \\
\sqrt{2}e^{i\alpha} \left( e^{i\gamma} \cos^2 \frac{\beta}{2} f_- - e^{-i\gamma} \sin^2 \frac{\beta}{2} f_+ \right) \end{pmatrix} \quad (6.13)$$

with spin vector

$$\langle \hat{F} \rangle = F \cos \alpha \sin \beta \hat{x} + F \sin \alpha \sin \beta \hat{y} + F \cos \beta \hat{z}. \quad (6.14)$$

The nematic axis is found from the rotation of the orthogonal triad under the three Euler angles as

$$\hat{d} = (\cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma) \hat{x} + (\sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma) \hat{y} - \sin \beta \cos \gamma \hat{z}. \quad (6.15)$$

Here we note that the two angles $\alpha$ and $\beta$ specify the direction of $\langle \hat{F} \rangle$ according to Eq. (6.14). Therefore, since $\hat{d} \perp \langle \hat{F} \rangle$, the third Euler angle $\gamma$ describes additional rotation of $\hat{d}$ around the axis defined by $\langle \hat{F} \rangle$. This is only one possible parameterisation of the spinor order parameter but is useful in that it explicitly demonstrates the effects
Table 6.1: Table showing different vortex states constructed from Eq. (6.13) by setting \( \alpha \), \( \beta \), \( \gamma \) to be half-integer multiples of \( \varphi \). FM and polar limits are obtained by setting \( F = 1 \) and \( F = 0 \) respectively. The mass circulation \( \nu \) is calculated from Eqs. (3.3) & (3.21).

<table>
<thead>
<tr>
<th></th>
<th>Polar limit</th>
<th>( \phi/\varphi )</th>
<th>( \alpha/\varphi )</th>
<th>( \gamma/\varphi )</th>
<th>( m\nu/h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Vortex</td>
<td>Half-Quantum Vortex</td>
<td>1/2</td>
<td>0</td>
<td>1/2</td>
<td>((1 - F)/2)</td>
</tr>
<tr>
<td>No Vortex</td>
<td>Singular Vortex</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>(1 - F)</td>
</tr>
<tr>
<td>Coreless Vortex</td>
<td>Half-Quantum Vortex</td>
<td>1/2</td>
<td>1</td>
<td>(-1/2)</td>
<td>((1 + F)/2 - F \cos \beta)</td>
</tr>
<tr>
<td>Coreless Vortex</td>
<td>Singular Vortex</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>(1 - F \cos \beta)</td>
</tr>
<tr>
<td>Coreless Vortex</td>
<td>Nematic Coreless Vortex</td>
<td>0</td>
<td>1</td>
<td>(-1)</td>
<td>(F(1 - \cos \beta))</td>
</tr>
<tr>
<td>Spin Disgyration</td>
<td>Nematic Coreless Vortex</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>(-F \cos \beta)</td>
</tr>
<tr>
<td>Spin Disgyration</td>
<td>Half-Quantum Vortex</td>
<td>1/2</td>
<td>1</td>
<td>1/2</td>
<td>((1 - F)/2 - F \cos \beta)</td>
</tr>
<tr>
<td>Singular Vortex</td>
<td>Half-Quantum Vortex</td>
<td>1/2</td>
<td>0</td>
<td>(-1/2)</td>
<td>((1 + F)/2)</td>
</tr>
<tr>
<td>Singular Vortex</td>
<td>Singular Vortex</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

of phase and spin rotations as well as varying the magnitude of the spin expectation value.

In Appendix F, we demonstrate how having the Euler angles \( \alpha \), \( \gamma \) & \( \phi \) depend on \( \varphi \) and allowing \( \beta \) & \( F \) to vary with \( \rho \) enables one to construct vortices which interpolate between the polar and FM phases. The behaviours of \( \alpha \), \( \gamma \) & \( \phi \) then determine the topology in the polar and FM regions. In the Appendix we construct a number of interesting states including singular vortices with cores filled with nonsingular states as identified in Chapter 5 as well as composite topological defects. In Table 6.1 we list simple parametrisations of the states with winding numbers less than 1. A thorough investigation of the energetic stability of these states is beyond this work but several are shown to form as a consequence of energy minimisation from an initial vortex state. We observe the filling of the half-quantum vortex core with the vortex-free FM phase [see Sec. 6.3.2.2 and Appendix E], filling of the core of a singular polar vortex with an FM coreless vortex [see Sec. 6.6.1.2] and the filling of the core of a FM spin disgyration with the nematic coreless vortex [see Sec. 6.6.2]. We also observe the energetic stability of a composite topological defect with the large-distance topology of a singular FM vortex and the small-distance topology of the polar half-quantum vortex, although only in an effective two-component regime enforced by a quadratic Zeeman splitting [see Sec. 6.5]. Some of these structures are sketched in Fig. 6.1.

6.3 Singular Vortex Structures in the Weakly Magnetised BEC

In Sec. 5.1, we demonstrated the energetic stability of singly-quantised vortex structures in both phases of the spin-1 BEC. In that analysis, the magnetisation was allowed to vary
Figure 6.1: Schematic figures of vortices which mix the FM (blue) and polar (green) phases, yielding different vortex states depending on the combinations of Euler angles in Table 6.1.

during relaxation. We now analyse how these structures change if a weak longitudinal magnetisation is preserved throughout the relaxation procedure.
For this analysis, it is instructive first to review the central features of the state that results from energy minimisation if conservation of magnetisation is not imposed, identified in Sec. 5.1. A trial wavefunction representing a singly-quantised FM vortex is given by Eq. (3.12). The vortex is made up of overlapping vortex lines in the three spinor components, corresponding to a depletion of the atom density in the vortex core. The spin texture is uniform. As the energy is relaxed, these vortex lines move apart, such that the atom density is nonzero everywhere. The FM order parameter however, remains singular on a well-defined vortex line, on which the atoms adopt the polar phase.

The size of a density-depleted vortex core would be determined by the density-healing length $\xi_n$ [Eq. (2.39)]. By allowing the core to fill by perturbing $|\langle \hat{F} \rangle|$, the core can expand to the size of the spin healing length $\xi_F$ [Eq. (2.40)], thereby lowering its energy. The deformation of the vortex core corresponds to a local rotation of the spin vector in an extended core region. The result is a spin winding around a core with non-vanishing density and $|\langle \hat{F} \rangle| < 1$. Away from the vortex core the initial uniform spin texture is preserved.

In Sec. 5.1 we demonstrated how analysis and classification of the vortex core structure is facilitated by a basis transformation to a natural spinor basis for the vortex state. In the absence of external magnetic fields, we are free to choose the spinor basis.

By transforming to the basis of spin projection onto the axis defined by the uniform $\langle \hat{F} \rangle$ far from the vortex core, the spinor representing the relaxed core can be written in the form of an interpolation between an outer singular FM vortex and inner non-circulating polar phase, similar to Eq. (F.5). In this preferred basis, the spinor reads

$$\zeta^* = \frac{1}{2} \begin{pmatrix} \sqrt{2} e^{i\varphi} \left( \cos^2 \beta^* f_+ - \sin^2 \beta^* f_- \right) \\ \sin \beta^* (f_+ + f_-) \\ \sqrt{2} e^{-i\varphi} \left( \sin^2 \beta^* f_+ - \cos^2 \beta^* f_- \right) \end{pmatrix},$$

where the angle $\beta^*(\rho)$ describes the tilt of the spin away from the new quantisation axis. The vortex lines in $\zeta^*_\pm$ overlap and the core is filled by $\zeta_0^*$. The interpolation between the FM vortex and the polar core is described by $f_\pm(\rho) = \sqrt{1 - \hat{F}(\rho)}$ as defined in the construction of Eq. (6.13). In the numerically stabilised vortex, the FM phase exhibits a spin disgyration near the vortex core, bending to align uniformly with the preferred spinor basis at large radii, as in Sec. 5.1.

In this natural basis we may define a magnetisation

$$M^* = \frac{N^*_+ - N^*_-}{N},$$
where \( N^\pm_\star \) are the populations of the \( \zeta^\pm_\star \) spinor components. There is an associated magnetisation density in this basis,

\[
\mathcal{M}(\mathbf{r}) = |\zeta_+|^2 - |\zeta_-|^2 .
\] (6.18)

In the initial state, \( M^\star = 1 \). Owing to the rotation of the spin vector around the vortex core in the relaxed state, the contribution of the core region to the net magnetisation is canceled out. Therefore \( M^\star \) decreases during the relaxation. The spin then tends to point in the direction of the preferred spinor basis over a non-negligible distance from the vortex core, leading to a further reduction in \( M^\star \). In the relaxed state, \( M^\star \approx 0.5 \) at the lowest rotation frequency where the vortex becomes stable, increasing to \( M^\star \approx 0.7 \) at the upper limit of stability.

We are now in a position to understand how conserving an initial longitudinal magnetisation \( M \), defined by Eq. (2.34) in the basis of spin projection onto the \( z \) axis, changes the relaxed state. The trial wavefunction for the singular FM vortex is again given by Eq. (3.12), where the constant angle \( \beta_0 \) is now chosen to yield the desired \( M \). Energy relaxation under the condition that a sufficiently weak \( M \) is conserved now results in the spin texture shown in Fig. 6.2. Again relaxation results in a local rotation of the spin vector to allow the vortex core to avoid the density depletion and instead fill with atoms with \( |\langle \hat{F} \rangle| < 1 \). However, when the magnetisation is conserved, in addition to \( \xi_n \) and \( \xi_F \), also the magnetisation length scale \( \eta^{(2)}_M \) given by Eq. (2.46) may affect the core structure. The length \( \eta^{(2)}_M \) defines the upper limit on the size of the non-FM core for any given \( M \). As long as \( M \) is sufficiently weak that \( \eta^{(2)}_M \gtrsim \xi_F \), the core size after energy relaxation is determined by \( \xi_F \), and the filling of the vortex core may be understood from minimization of the gradient energy.

While the general understanding of the core-deformation mechanism is not qualitatively changed as long a \( M \) is sufficiently weak, the resulting spin texture must adapt to the conserved magnetisation. Compared with the result found when not accounting for conservation of magnetisation, the spins are everywhere tilted towards the \( z \) axis. This compensates for the amount of magnetisation that would otherwise be lost in the formation of the core region. Increasing \( M \) leads to a further local rotation of the spin vector everywhere towards the \( z \) axis, as shown in Fig. 6.2. We may then conclude that the effect of conserving a fixed longitudinal magnetisation is to fix the natural basis of the vortex as long as \( |M| \leq M^\star \). Greater longitudinal magnetisation cannot be achieved by tilting of the spin structure shown in Fig. 6.2. Our analysis thus immediately predicts a maximum magnetisation \( |M| = M^\star \) above which the vortex state has to change, as stronger magnetisation cannot be provided. At this magnetisation strength, also \( \eta^{(2)}_M \sim \xi_F \) in our simulations, implying that the size of the vortex core becomes determined by the magnetisation length scale rather than the spin healing length. The vortex structure arising from energy relaxation of a singular vortex in this strongly magnetised regime is described in Sec. 6.4.1.
6.3.2 Polar Regime

We now turn our attention to the core structures of singular polar vortices. Where in the FM phase there is only one class of singular vortices (which can all be transformed into each other by local operations), the polar phase supports topologically distinct singular vortices corresponding to multiples of half a quantum of circulation. We will examine the magnetisation dependence of the stable core structures of a half-quantum vortex and of a singly-quantised vortex. For the latter case we may compare with the Sec. 5.2, where magnetisation was not conserved.

The spin-1 BEC exists in the polar regime when $c_2 > 0$ in Eq. (2.25). Then the spin-dependent interaction is minimised for $|\langle \hat{\mathbf{F}} \rangle | = 0$, which defines the polar phase. However, this immediately implies that for a condensate entirely in the polar phase, $M = 0$. Nonzero magnetisation in the polar regime therefore means that regions with $|\langle \hat{\mathbf{F}} \rangle | > 0$ must form despite the polar interactions. Before analysing magnetised vortex states in a condensate with polar interactions, it is instructive to briefly consider how a finite $M$ is accommodated in a vortex-free BEC.
Chapter 6 Magnetisation-Conserving Relaxation

6.3.2.1 Magnetisation in the Polar Regime

Consider the spatially uniform spinor

$$\zeta = \frac{1}{2} \begin{pmatrix} -1 - M \\ \sqrt{2(1 - M^2)} \\ 1 - M \end{pmatrix}.$$  \hspace{1cm} (6.19)

This is a simple choice of spinor which has nonzero populations of all three spinor components for all values of $M$. It represents a BEC in the polar phase when $M = 0$, and otherwise yields uniform spin and $\hat{d}$ profiles such that the total magnetisation is $M$. Minimising the energy while conserving $M$ yields a nonuniform spin profile, with low magnetisation density at the centre of the cloud, where the atom density is large, and increasing $|\langle \hat{F} \rangle|$ towards the edges, as shown in Fig. 6.3.

This result may be understood in terms of the spin-dependent interaction energy density, $E_F = c_2 n^2 |\langle \hat{F} \rangle|^2/2$, which is proportional to the square of the atom density. The local contribution to the total magnetisation (2.34), on the other hand, is proportional to $n$. It is therefore energetically favourable to shift the regions of non-polar phase required to produce local magnetisation towards the edge of the cloud, where the density is small. This result, in the isotropic trap we consider here, is different from the approximately uniform spin structure found experimentally in tight confinement [45], where the condensate is smaller than the spin healing length. In the experiment, $\zeta_0$ is depleted. In the isotropic trap, we find a depopulation of $\zeta_-$ instead. The spin vector then carries a transverse component that does not contribute to the longitudinal magnetisation. The corresponding cost in interaction energy is offset by a smaller spin-gradient energy.
6.3.2.2 Half-Quantum Vortex

The analysis of the vortex-free state can immediately be applied to understand how a nonzero magnetisation is accommodated in the polar vortex states. We first consider a condensate with a single half-quantum vortex. It is again instructive first to ignore conservation of magnetisation and analyse the resulting relaxed state. A trial wavefunction carrying a half-quantum vortex may be constructed from Eq. (3.25) by applying a spin rotation such that all spinor components have a nonzero population.

The trial wavefunction corresponds to a vortex where the atomic density vanishes on the singularity. The size of the core is then determined by the density healing length \( \xi_n \) [Eq. (2.39)]. As energy relaxes, the vortex core is filled with atoms with \(|\langle \hat{F} \rangle| > 0\), reaching the FM phase on the singularity of the polar order parameter. The vortex core can then expand to the size of the spin healing length \( \xi_F \) [Eq. (2.40)]. In addition, a small region of nonzero \(|\langle \hat{F} \rangle|\), forms near the edge of the condensate, in which the spins anti-align with the spin inside the vortex core. This effect appears counter-intuitive, as exciting the wavefunction out of the polar phase costs interaction energy. However, this cost is relatively small in the low-density region of the cloud, and is offset by lowering the gradient energy arising from the filled vortex core. Increased magnetisation serves to expand this outer magnetised region as well as increasing \(|\langle \hat{F} \rangle|\) in this region.

Similarly to the analysis of the singular FM vortex, we may find a natural basis by transforming the wavefunction to the basis of spin quantisation along the axis defined by the spin vector on the vortex line. The spinor then reads [cf. Eq. (F.4) with \( \beta = 0 \)],

\[
\zeta_{\text{hq}} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} -\sqrt{1 + M^*(\rho)} \\ 0 \\ e^{i\varphi} \sqrt{1 - M^*(\rho)} \end{array} \right),
\]

where the local magnetisation density \( M^* \) [Eq. (6.18)] describes the filling of the vortex core and the magnetisation of the cloud edge. Far from the vortex core, this is recognised as a half-quantum vortex with nonzero magnetisation and the core is filled with the vortex-free FM phase.

The spinor in the preferred basis shows features of the composite topological defect of Eq. (F.12), with the large-distance topology of a singular FM vortex if the outer region is excited to the FM phase. The small-distance topology is that of a polar half-quantum vortex in the region with \( M = 0 \). The filling of the core with the vortex-free FM phase may then occur, as in Eq. (F.4). The composite topological defect then has the structure of a noncirculating inner FM core, a half-quantum vortex in the outer polar core and a region of \( 1 > F > 0 \) at the edge of the cloud, which tends toward the behavior of the singular FM vortex.
Chapter 6 Magnetisation-Conserving Relaxation

Figure 6.4: Spin vector (arrows) and magnitude (colour gradient) profiles in the $x$-$z$ plane for a half-quantum vortex with an initial magnetisation $M = 0.2$ which is (a) not conserved and (b) conserved. Arrow lengths scale with spin magnitude. The magnetisation arises from the outer regions, not the FM core.

With these observations in mind, we can now analyse the consequences of preserving a nonzero longitudinal magnetisation of the vortex-carrying condensate. In order to give the trial wavefunction representing the half-quantum vortex a nonzero magnetisation, we renormalise the occupations of the spinor components.

The relaxed half-quantum vortex state with fixed magnetisation is shown in Fig. 6.4. On the vortex line, $|\langle \hat{\mathbf{F}} \rangle| = 1$, and the core lowers its energy by expanding to the size allowed by the spin healing length. We also note that a significant region with nonzero $|\langle \hat{\mathbf{F}} \rangle|$ arises towards the edge of the cloud. From the spin texture we note that the longitudinal magnetisation $M > 0$ arises not from the vortex core, but from the magnetised edge regions. The spins in the edge regions remain nonzero to reduce spin gradients. However, the spins in the edge regions no longer anti-align with that inside the vortex core. This means that the treatment in terms of a natural spinor basis is no longer valid in a magnetised half-quantum vortex. The effect of fixing a weak longitudinal magnetisation is to increase the magnitude of the spin in the outer region and to orient the spin in this region towards the direction of the applied magnetic field.

We find that magnetisation of the edge region can only provide a total magnetisation of $|M| \sim 0.3$, beyond which the vortex is no longer energetically stable. At this magnetisation strength, the size of the polar region between the core of the half-quantum vortex and the magnetised edge region becomes comparable to $\xi_F$. Then the half-quantum vortex becomes unstable due to the large gradient energy. This mechanism and the resulting stable vortex state in the strong-magnetisation regime are described in Sec. 6.4.2.

The topology of the half-quantum vortex is unchanged by the conservation of this weak magnetisation, such that the large-distance topology tends toward that of the singular FM vortex. The magnetisation range which stabilised the half-quantum vortex is not sufficient to excite the condensate into the FM phase in the outer region. We note however, that the half-quantum vortex can be stabilised at greater magnetisation in the presence of a negative quadratic Zeeman splitting that is sufficiently strong to overcome
the gradient energy. With \( g_2B_2^2/\hbar\omega = -0.2 \) in Eq. (2.25) the half-quantum vortex remains stable up to \( |M| \sim 0.8 \). We discuss the topology of this vortex state in Sec. 6.5.

### 6.3.2.3 Singly-Quantised Vortex

The energetic stability and structure of a singly-quantised vortex in a polar spin-1 BEC were analysed in detail in Sec. 5.2. In that analysis, the initial state was entirely in the polar phase, and the magnetisation was allowed to vary during energy relaxation. Energy minimisation then resulted in a splitting of the singly-quantised vortex into a pair of half-quantum vortices with FM cores, whose spins anti-aligned. This splitting preserves the overall topology of the initial state, but forms an extended core region where the phases mix. The filling of the vortex cores with atoms with \( |\langle \hat{F} \rangle| \geq 0 \), and accommodating the singularities by requiring \( |\langle \hat{F} \rangle| = 1 \) on the singular lines, lowers the total energy by reducing the gradient energies.

Similarly to the cloud with a single half-quantum vortex, the gradient energies associated with the vortex cores are again lowered by the formation of two magnetised edge regions, illustrated in Fig. 6.5(a). The spins in the two edge regions anti-align with those in the nearest vortex core, immediately implying that the two edge regions exhibit spins pointing in opposite directions.

The formation of the magnetised edge regions is reminiscent of a composite topological defect such as those described by Eqs. (F.1) & (F.11). However, the breaking of axisymmetry renders the interpretation of this structure in terms of a hierarchical core structure prohibitively difficult.
This picture remains entirely unchanged as we account for a conserved magnetisation of zero. This is to be expected as the structure described above has zero net magnetisation. However, a conserved, weak, nonzero magnetisation does modify the structure somewhat. A magnetised singly-quantised vortex can be constructed from Eq. (3.30) by adjusting the populations of the spinor components to give the desired magnetisation. We now explicitly conserve this magnetisation throughout energy relaxation. The resulting relaxed states for conserved and non-conserved weak, nonzero magnetisations are shown in Fig. 6.5, and we note the splitting of the initial vortex into two singular lines in both cases, which may be identified as half-quantum vortices.

In contrast to the isolated half-quantum vortex, the nonzero magnetisation $M$ of the condensate is carried by the vortex cores rather than the edge regions. When the condensate contained only a single half-quantum vortex, the spin structure could adjust to a varying magnetisation $M$ by a simple rotation of the spins at the edge of the cloud. Because the spins in the two edge regions anti-align when magnetisation is not conserved, an equal rotation of spins can no longer increase the longitudinal magnetisation. The effect of preserving a nonzero $M$ throughout energy relaxation is to cause the spins in the two vortex cores to orient differently so that they no longer anti-align. This provides the required net magnetisation.

The gradient energy in the extended core region is reduced by this process and so the magnitude of the spin in the edge regions is not required to be as strong as in the case of zero magnetisation. However, the edge regions still exhibit non-vanishing spin and are no longer required to antialign as the spins in the FM vortex cores no longer antialign. A single magnetised edge region forms and so consideration of this state as a composite topological defect is now more natural than in the regime of non-conserved magnetisation. In the magnetised region, there is a unit phase-winding in each spinor component, corresponding to the behaviour of the composite topological defect (F.11) which represents a singular, singly-quantised vortex regardless of $|\langle \hat{F} \rangle|$. The composite-core structure consists approximately of an inner FM core with vanishing circulation, an outer polar core with unit circulation and an edge region with $1 > F > 0$ and unit circulation.

The core regions can only provide a weak magnetisation as their size is constrained by the spin healing length. The magnetisation length scale $\eta_{M}^{(1)}$ given by Eq. (2.44) described the smallest core size required to yield a given magnetisation $M$. Hence, when $M$ is sufficiently strong that $\eta_{M}^{(1)} \gtrsim \xi_F$, the magnetisation cannot be upheld by the vortex cores alone, leading to energetic instability of the state in Fig. 6.5. We find that this happens at $|M| \sim 0.3$. The relaxation of the vortex in this strong-magnetisation regime is described in Sec. 6.4.2. While a negative quadratic Zeeman splitting could restabilise a single half-quantum vortex at higher magnetisation, the same is not true for the split singly quantized vortex.
In conclusion, we find that also in the polar regime, the results of Sec. 5.2 remain qualitatively unchanged when accounting for conservation of an initial magnetisation $|M| \lesssim 0.3$. However, the required magnetisation in the relaxed state is produced by forcing the FM vortex cores to no longer exhibit the anti-aligning spins which were observed in the magnetisation non-conserving regime.

### 6.4 Singular Vortex Structures in the Strongly Magnetised BEC

Having established the effect of conserving a weak longitudinal magnetisation on the relaxed structure of singular vortices (compared with magnetisation non-conserving relaxation in Chapter 5), we now explore the more drastic consequences when a strong magnetisation is conserved. We consider first the more straightforward case of a singly-quantised vortex in a strongly magnetised FM condensate. We then show how strong magnetisation causes a condensate in the polar regime to adopt properties of the FM phase.

#### 6.4.1 FM Regime

We consider now a singly-quantised FM vortex with a magnetisation $M$ that is larger than that which can be accommodated by the vortex structure analysed in Sec. 6.3.1 and represented by Eq. (6.16). In other words, we choose $M > M^*$ as defined by Eq. (6.17). The natural magnetisation, $M^*$, increases with increasing rotation frequency as noted in Sec. 6.3.1. Here we consider a rotation frequency close to the slowest rotation that will still allow the singular vortex to be stable. At this rotation frequency, the strong-magnetisation regime corresponds to $M \gtrsim 0.5$.

From Sec. 6.3.1 we have that when $M = M^*$, the natural basis of the vortex structure coincides with the $z$ axis. The spinor describing this vortex state in the usual spinor basis of spin projection onto the $z$ axis is therefore of the form of Eq. (6.16). This vortex state consists of a magnetised outer region and a non-magnetised vortex core, a simplified version of which was described in Eq. (2.46). For $M > M^*$, the non-FM vortex core would have to shrink in size, increasing the associated gradient energy.

The size $\eta_M^{(2)}$ of a polar core in a FM condensate with given magnetisation $M$ can be estimated from Eq. (2.46). From $\eta_M^{(2)} \lesssim \xi_F$ we then get an estimate of $M \sim 0.6$ for the magnetisation at which the gradient energy associated with the small vortex core will exceed the interaction-energy cost of depleting $\zeta_-$ entirely, populating only $\zeta_+$ and $\zeta_0$. 
The singular FM vortex state is then described in an effective two-component regime by

$$\tilde{\zeta} = \begin{pmatrix} e^{i\phi} \sqrt{M(\rho)} \\ \sqrt{1 - M(\rho)} \\ 0 \end{pmatrix},$$

where $M(\rho)$ interpolates between the nonmagnetised polar phase in the singular core and the fully magnetised FM phase outside the vortex.

Numerically minimising the energy of a trial wavefunction constructed from Eq. (3.12) we find for the investigated parameters that depopulation of $\zeta_-$ happens already when a magnetisation $M \sim M^*$ is conserved. The spin magnitude and structure of the stable vortex state at $M = 0.8$ are shown in Fig. 6.6(a). Similar to the behaviour of the vortex when $M$ is small (Sec. 6.3.1), the spins in the core region rotate to allow the core to avoid depleting the atom density, instead filling with atoms with $|\langle \hat{\mathbf{F}} \rangle| < 1$, reaching the polar phase on the singular line. This is immediately clear from Eq. (6.21) and Fig. 6.6(c), which shows the spinor-component densities resulting from relaxation. The vortex-free $\zeta_0$ component fills the vortex in $\zeta_+$, and rapidly drops to zero outside the vortex core. The resulting spin structure forms a cross disgyration in the transition region between the polar core and the FM cloud. Away from the vortex line the density in $\zeta_0$ decreases, and the spins correspondingly bend rapidly towards the $z$ direction, aligning with it everywhere outside the core region to yield the required strong magnetisation.

As $M$ increases further, the size of the vortex core decreases, as does the core density. As the population of $\zeta_0$ is reduced by the increasing magnetisation, maintaining a core of the same size requires a lower density of $\zeta_0$ atoms inside the core region. The energetic cost of this is too great and so the core contracts. The system balances the gradient energy cost of a smaller core with that associated with a reduced density in the core region to settle at an equilibrium size.

We finally note briefly that the vortex structure is not qualitatively altered if a nonzero quadratic Zeeman energy $g_2B_z^2/\hbar \omega = \pm 0.2$ is included in the analysis.

6.4.2 Polar Regime

In Sec. 6.3.2 we found that singular half-quantum and singly-quantised vortices can remain stable in a BEC with polar interactions through spin textures arising in non-polar regions in the vortex cores and at the edge of the cloud. However, this requires that the conserved magnetisation does not exceed $M \sim 0.3$. Here we first explain the energetic instability at stronger magnetisation, and then show how instead the BEC takes on properties of the FM phase to form a stable vortex once more described by Eq. (6.21).
Figure 6.6: Numerically calculated spin magnitude (colour gradient) and vector (arrows) profile for the strongly-magnetised singular vortex in the $x$-$y$ plane, with arrow lengths scaled by spin magnitude in (a) the FM regime with $M = 0.6$ and (b) the polar regime with $M = 0.8$. Immediately outside the polar core, the spin is angled slightly out of the $x$-$y$ plane, bending very rapidly to the $z$ direction a short distance from the core. This is qualitatively similar to the low-$M$ FM singular vortex but the absence of planar spins near the vortex core is a crucial difference. Densities in $\zeta_+$ (red line marked with +) and $\zeta_0$ (green line marked with 0) together with the magnitude of the spin (black dashed line labeled $|\langle \hat{F} \rangle|$) on the $x$-axis for this vortex in (c) the FM regime and (d) the polar regime for the same respective magnetisations, showing the position of the polar vortex core and revealing its nature as a vortex in $\zeta_+$ filled with $\zeta_0$.

In the case of the singly-quantised polar vortex, energy relaxation at weak magnetisation results in a pair of half-quantum vortices whose non-polar cores of size $\sim \xi_F$ give rise to the required magnetisation (magnetisation arising from the edge regions is comparatively small). By approximating the non-polar cores as a single FM core region, we can get an estimate for the maximum magnetisation from Eq. (2.44). We find that the core size $\eta^{(1)}_M$ required at magnetisation $M$ is comparable to $\xi_F$ at $M \sim 0.3$. This prediction agrees well with our numerical results.

For a single half-quantum vortex, by contrast, we found in Sec. 6.3.2 that the magnetisation arises not from the non-polar core, but from the magnetised edge region. The size $\eta^{(2)}_M$ of the region that does not contribute to the magnetisation can then be estimated from Eq. (2.46) at a given $M$. However, we now recall that within this region, there is the non-polar core of the half-quantum vortex with size $\xi_F$. Hence the size of the polar...
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region must decrease below $\xi_F$ when $\eta^{(2)}_M \lesssim 2\xi_F$, at which point the associated gradient energy is greater than the cost of exciting the condensate out of the polar phase. This simplified model gives estimates the maximum magnetisation again at $M \sim 0.3$, in agreement with our numerical results.

If the magnetisation is sufficiently strong that neither of the cases described above are energetically stable, a new vortex structure must form. It was shown in the vortex-free polar phase (Sec. 6.3.2.1) that it is energetically more favourable to magnetise the edge of the cloud rather than the centre. We therefore expect the strongly-magnetised vortex state to have $F(\rho) \to 0$ for small $\rho$, while approaching the FM phase when $\rho$ is large. An outer magnetised region with the topology of a singular FM vortex is expected to form, while a nonsingular texture of the polar phase may fill the core region.

By numerical simulation we find that at strong magnetisation, the singly-quantised vortex, constructed as a $2\pi$ winding of the condensate phase, relaxes to an effective two-component regime where $\zeta_-$ is depopulated (Fig. 6.6). The vortex line remains in $\zeta_+$, while $\zeta_0$ loses the phase winding and fills the core. Hence despite the polar interaction regime, the condensate takes on a FM large-distance topology, representing the singular vortex. The polar phase is retained only on the vortex line. The energetically stable vortex state at strong magnetisation is thus also in the polar regime described by Eq. (6.21). The corresponding spin texture exhibits a radial disgyration close to the vortex core, bending towards $\hat{z}$ with increasing $\rho$. Note that, in contrast to the FM regime, the polar interactions now imply that $\xi_F$ does not restrain the size of the vortex core.

The effect of strong magnetisation, forcing the condensate to adopt the properties of the FM phase despite polar interactions, is robust against both positive and negative quadratic Zeeman splitting, $g_2B_2^2/h\omega = \pm 0.2$, although in the latter case a stronger magnetisation is required to stabilise this particular vortex structure, increasing as a function of $|g_2B_2^2|$.

6.5 Formation of Spin Domains

In Sec. 6.2 we derived spinor wavefunctions representing composite topological defects, including the nontrivial case of a polar half-quantum vortex forming the core of an outer singular FM vortex in Eqs. (F.12) & (F.13). As the energy relaxes, a hierarchical vortex core may form: The large-distance topology represents the singular FM vortex with spin $\langle \hat{F} \rangle = \sin \beta \hat{x} + \cos \beta \hat{z}$. Inside its core, $F(\rho)$ decreases to 0, displaying a half-quantum vortex with $\hat{d} = \cos \beta \cos(\varphi/2)\hat{x} + \sin(\varphi/2)\hat{y} - \sin \beta \cos(\varphi/2)\hat{z}$, as described by Eq. (F.13). To avoid depletion of the atom density, $F(\rho)$ may then increase back to $F(\rho \to 0) = 1$ inside the core of the half-quantum vortex, corresponding to the vortex-free FM phase.
We now ask whether this composite-vortex structure can form as the energy of the singular FM vortex relaxes, and whether it can be energetically stable. We consider the trial wavefunction for a singly-quantised FM vortex, constructed from Eq. (3.12) with magnetisation $0 \leq M \leq 0.8$, in a condensate with FM interactions. We find that in order for the composite-vortex structure to replace the vortex-free polar core in the stable state, a sufficiently strong negative quadratic Zeeman splitting is required. Here we take $g_2 B_z^2/\hbar \omega = -0.2$. The negative quadratic Zeeman effect favours occupation of the $m = \pm 1$ Zeeman levels. This causes the spin vector to align (anti-align) with the $z$ axis away from the vortex, and to anti-align (align) with it in the FM core. The two possible spin alignments are energetically degenerate (though conservation of magnetisation may only allow one).

The quadratic Zeeman splitting required to energetically stabilise the half-quantum vortex inside the core of a singular FM vortex is strong enough that $\beta$ is forced to adopt values of either $0$ or $\pi$, and the $\zeta_0$ spinor component is empty. In the resulting effective two-component limit, the spinor can be parametrised as

$$\zeta = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \sqrt{1 + M(\rho)} \\ 0 \\ \sqrt{1 - M(\rho)} \end{pmatrix},$$  

(6.22)

where $\langle \hat{F} \rangle = M \hat{z}$ with the local magnetisation density $M = -1$ in the inner core, and $M = 1$ away from the vortex. It is now readily apparent that the vortex line in $\zeta_+^c$ represents the overall topology of the singly-quantised FM vortex at sufficiently large $\rho$. Similarly in the inner core, $\zeta_-^c$ represents a vortex-free FM wavefunction. Where $F_z \to 0$ in the intermediate region, $\tilde{\zeta}$ takes the form of a half-quantum vortex similar to Eq. (3.25).

Due to the FM interaction, the thickness of the polar region is restricted by $\xi_F$. Hence the polar vortex takes on the character of a domain wall separating an outer spin domain from an inner domain with opposing spin. The size of the inner FM core is not constrained by the spin healing length, as it does not violate the FM spin condition.

However, in the atomic spinor BEC, magnetisation is conserved. The effect of this is to determine the size of the inner FM core, so that the antialigned spins in the FM regions yield the required magnetisation. This corresponds to a length scale $\eta_M^{(3)}$ associated with the conserved magnetisation. In a simplified model that ignores the thickness of the domain wall, an estimate for $\eta_M^{(3)}$ is given by Eq. (2.48). From this we can understand the upper limit on magnetisation for which the composite vortex is stable: The magnetisation must not cause the gradient energies associated with a small core to overcome the Zeeman energy. This happens when $\eta_M^{(3)} \lesssim \xi_Z = l(\hbar \omega/2|g_2|B_z^2)^{1/2}$, the healing length associated with the quadratic Zeeman energy, in agreement with our numerical results. The vortex structure at $M = 0.6$ is shown in Fig. 6.7, demonstrating
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Figure 6.7: (a) Numerically calculated spin texture (arrows) and magnitude (colour gradient) in the $x$-$y$ plane for the composite vortex in the FM regime with $M = 0.6$. Arrow lengths scale with spin magnitude. (b) Nematic axis profile (cylinders) and circulation (colour gradient) for the same, showing the non-circulating inner FM core and winding of $\hat{d}$ by $\pi$.

the formation of the composite core in which the innermost region exhibits the non-circulating FM phase.

It is interesting to note that the conservation of a nonzero magnetisation is required to stabilise this vortex in the FM regime. If the magnetisation is not conserved, or is conserved at zero, the gradient energy associated with the domain wall renders the vortex unstable.

In Sec. 6.3.2.2, we demonstrated that in the polar interaction regime, the energetically stable half-quantum vortex exhibits magnetised edge regions. In the absence of quadratic Zeeman splittings, these edge regions had $|\langle \hat{F} \rangle| < 1$ and so the composite topological defect with an outer singular FM vortex enclosing an inner half-quantum vortex was not realised. However, we find that a sufficiently strong magnetisation $|M| \gtrsim 0.3$ together with a quadratic Zeeman splitting $g_2 B_z/\hbar \omega = -0.2$ also allows this composite-vortex structure to be energetically stable in a BEC with polar interactions. The strong magnetisation is upheld by forcing the condensate away from the vortex line towards the FM phase, forming a singular vortex. Again the required Zeeman energy causes depopulation of $\zeta_0$. In contrast to the FM regime, the polar interactions now imply that that size of the FM core is determined by the spin healing length, while the thickness of the polar region is determined by the magnetisation. The quadratic Zeeman splitting is able to stabilise the composite vortex provided $\eta^{(3)}_M > \xi_Z$, corresponding to magnetisations of $M \sim 0.9$, which is supported by our numerics. When magnetisation is not conserved, both the half-quantum and singly-quantised vortices of the polar phase described in
Sec. 6.3.2 are stable under the influence of quadratic Zeeman splitting. For magnetisation \( M < 0.3 \), the half-quantum vortex remains stable. The stronger magnetisation serves to increase \( |\langle \hat{F} \rangle| \) near the edge of the trap, forming the FM phase.

### 6.6 Nonsingular Vortices and Textures

The two phases of the spin-1 BEC have different order-parameter symmetries, which in turn support different nonsingular textures, including the FM coreless vortex and the polar nematic coreless vortex, as outlined in Chapter 3. Such nonsingular textures have recently been experimentally phase-imprinted on spinor condensates \([36, 37, 142]\). While we have demonstrated the stability of an FM coreless vortex when magnetisation was not conserved in the relaxation process in Sec. 5.1, we now ask whether the coreless vortex is stable subject to the constraint of conserved magnetisation.

The phase-imprinting experiments of Refs. \([36, 37]\) were conducted in \(^{23}\text{Na}\), whose interactions are polar. As well as the FM interaction regime, we also therefore consider whether the conservation of magnetisation can cause the imprinted coreless vortex to be stable in the polar interaction regime, where energetic arguments alone would favour vanishing spin expectation value. Additionally, we investigate the conditions under which one may stabilise the nematic coreless vortex, which was also recently created in phase-imprinting experiments \([37, 142]\). The nematic coreless vortex has vanishing circulation and therefore cannot ordinarily be stabilised by rotation.

#### 6.6.1 Coreless Vortex

##### 6.6.1.1 FM Regime

Here we first study the stability of the coreless vortex with conserved magnetisation in the FM regime. We take as the initial state of our numerics the coreless vortex which is created in phase-imprinting experiments, with

\[
\zeta^{cl}(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} \cos^2 \frac{\beta(\rho)}{2} e^{i\varphi} \sin \beta(\rho) \\ \sqrt{2} e^{2i\varphi} \sin^2 \frac{\beta(\rho)}{2} \end{pmatrix},
\]

as in Eq. (3.17). The initial state is in the FM phase everywhere, with \( \beta(\rho) \) specifying the initial magnetisation. In the FM interaction regime, the FM phase with \( F = 1 \) is preserved everywhere during relaxation when magnetisation is not conserved. We find however that imposed weak magnetisation can lead to energetic instability of the coreless vortex, with a singular vortex then becoming the rotating ground state. This may seem surprising, since when the magnetisation is not conserved in energy relaxation, coreless
vortices are predicted to form the ground state at sufficiently rapid rotation [20, 65, 167, 168]; a singular vortex may then also be energetically (meta)stable, but always has a higher energy than the coreless vortex as noted in Sec. 5.1. To understand this instability of the coreless vortex, it is insightful to first consider the stable configuration of an FM coreless vortex when magnetisation is not explicitly conserved in the relaxation process.

When the magnetisation is not conserved, the fountain texture of the FM coreless vortex displays a characteristic radial profile of $\beta(\rho)$. As the rotation frequency increases, the angular momentum also increases. Since increased angular momentum requires a more rapid bending of $\beta(\rho)$, the result is that the magnetisation of the energetically stable configuration decreases as the rotation frequency increases, as illustrated in Fig. 6.8(f).

To understand this, we present a qualitative description of an axisymmetric vortex at the centre of the trap, described by the spinor,

$$\zeta = e^{ia\varphi} \left( \begin{array}{c} e^{-ib\varphi} |\zeta_+(\rho)| \\ |\zeta_0(\rho)| \\ e^{ib\varphi} |\zeta_-(\rho)| \end{array} \right),$$

(6.24)

where $|\zeta_i(\rho)|^2$ are the populations of the three spinor components as a function of radius, giving rise to the radial profile of $\beta$. $a$ and $b$ are integers representing the winding of the condensate phase and spin vector respectively. The expectation value of the angular momentum for such a vortex is [106],

$$\langle \hat{L}_z \rangle = (a - b)N_+ + aN_0 + (a + b)N_-, $$

(6.25)

which may be simplified via Eq. (2.34) to,

$$\langle \hat{L}_z \rangle = (a - bM)N.$$

(6.26)

In the case of the coreless vortex, $a = b = 1$ and so the angular momentum increases linearly with decreasing magnetisation. This illustrates why increasing the rotation frequency decreases the magnetisation when the magnetisation is not conserved—increased angular momentum acts to decrease the longitudinal magnetisation in the system. This qualitative description is also useful in understanding the behaviour of the coreless vortex subject to magnetisation-conserving relaxation.

Whereas in the study of singular vortices it was instructive to begin by considering a magnetisation of zero, the fountain texture of the coreless vortex energetically favours nonzero magnetisation. As a result, it is more instructive to first consider a conserved magnetisation $M \sim 0.5$ at a rotation frequency just above that which stabilises the coreless vortex and then reduce or increase $M$. Conserving $M \sim 0.5$ has little impact on the structure of the coreless vortex, as one would intuitively expect.
Figure 6.8: Numerically calculated spin textures in the $x$-$y$ plane for the coreless vortex in the FM regime with an initial magnetisation $M = 0.4$ (a) not conserved and (b) conserved throughout the relaxation process. (c) The same for a conserved magnetisation of $M = 0.2$, showing a displacement of the coreless vortex relative to the more strongly-magnetised case. (d) Displacement and (e) angular momentum of the coreless vortex in a trap rotating at $\Omega/\omega = 0.3$ for different values of the conserved magnetisation (black dots) compared with the angular momentum of an axisymmetric coreless vortex at the centre of the trap, for the same magnetisation (blue line). (f) Numerically calculated magnetisation of the energy-minimising coreless vortex in the FM regime as a function of rotation frequency, where magnetisation-conserving relaxation has not been enforced.

Reducing the value of the conserved magnetisation leads to a displacement of the coreless vortex from the trap center, as demonstrated in Fig. 6.8(d). This may be understood as reducing the contribution to the magnetisation arising from the centre of the vortex, by forcing the centre of the vortex to lie in a region of lower density. At the same time, the continuous bending of the spin vector ensures that an enlarged region of
negative magnetisation density forms at the edge of the trap farthest from the center of the vortex. The combination of these two effects results in a reduction of the total longitudinal magnetisation.

Decreasing the magnetisation further causes a greater displacement of the coreless vortex as illustrated in Fig. 6.8(a-d) until, at \( M \sim 0.2 \), the coreless vortex is unstable towards splitting into a pair of singular vortices. We note that the magnetisation at which this happens decreases as the rotation frequency increases and thus infer that it is the displacement of the coreless vortex that triggers this instability. Further displacement of the vortex would produce a vortex-free state, which for a range of rotation frequencies is higher in energy than the singular vortex. The coreless vortex therefore splits into a pair of singular vortices, one of which then exits the cloud. Contrary to the findings when magnetisation is not conserved, which showed that the coreless vortex is always the ground state, we find that the singular vortex is in fact the ground state for sufficiently weak magnetisations. The range of magnetisations for which this is true, decreases with increasing rotation frequency of the trap.

One additional consequence of this displacement of the coreless vortex due to a reduction of the conserved magnetisation, is that the angular momentum is approximately independent of the magnetisation provided that the coreless vortex remains stable, shown in Fig. 6.8(e). From the discussion of the axisymmetric coreless vortex at the centre of the trap, we saw that decreasing the magnetisation served to increase the angular momentum. However, the displacement of the vortex then reduces the angular momentum relative to the axisymmetric vortex at the center of the trap, canceling out the increased angular momentum due to the reduction in magnetisation.

The FM coreless vortex was found to be stable for magnetisations below \( M \sim 0.5 \). For stronger magnetisation we obtain an effective two-component coreless-vortex state, where \( \zeta_0 \) represents a singly-quantised vortex whose core is filled by \( \zeta_+ \). The transition to the two-component system occurs when the \( \beta(\rho) \) profile no longer allows the three-component vortex (3.17) to satisfy the magnetisation constraint, resulting in depopulated \( \zeta_- \). The threshold magnetisation value decreases with rotation until at \( \Omega \sim 0.35\omega \) the coreless vortex is stable only in the two-component regime. The polar phase is never exhibited in this vortex structure and so no composite defect is formed.

To see that, despite the non-FM regions, this remains a coreless vortex, it is beneficial to define a winding number for the coreless vortex with general \( F \)

\[
W = \frac{1}{8\pi} \int_S d\Omega \epsilon_{ijk} \hat{n}_F \cdot \left( \frac{\partial \hat{n}_F}{\partial x_j} \times \frac{\partial \hat{n}_F}{\partial x_k} \right),
\]

(6.27)

associated with the coreless spin texture, similar to Eq. (3.20). Here, \( \hat{n}_F = (\hat{F})/|\langle \hat{F} \rangle| \) is a unit vector in the direction of the local spin vector. The charge \( W \) defines a topological
invariant if the boundary condition on $\hat{n}_F$ away from the vortex is fixed. When the asymptotic texture is uniform, $W$ is an integer.

In the coreless vortex in the spinor BEC, the asymptotic behaviour of the spin texture is determined by rotation, as the bending of $\beta$ in Eq. (F.6), and therefore the circulation (F.3), adapts to minimise the energy. The spin texture away from the vortex line may also be determined by interactions with other vortices. We derive an expression for $W$ for the spin texture of a general coreless vortex by using $\hat{n}_F$ from the coreless vortex spin texture (3.40) and computing the integral in Eq. (6.27). Assuming cylindrical symmetry and taking $R$ to be the radial extent of the spin texture, we find

$$W = \frac{1 - \cos\beta(R)}{2},$$

(6.28)

where we have used $\beta = 0$ on the $z$ axis, such that $\hat{n}_F(\rho = 0) = \hat{z}$. The winding number now depends on the asymptotic value of $\beta(\rho)$, such that for $\beta(R) = \pi$ (ATC-like texture) $W = 1$, and for $\beta(R) = \pi/2$ (MH-like texture) $W = 1/2$.

It has been mentioned that the FM coreless vortex in the FM regime can be unstable against splitting into a pair of singular vortices when conservation of a weak magnetisation is imposed. One of these vortices then exits the cloud leaving a single, singular vortex where the coreless vortex had previously been found stable when the energy was relaxed without explicitly conserving magnetisation. As the magnetisation becomes increasingly negative, one might naturally expect this singular vortex to become unstable as $\zeta_+$ is depopulated. It may be expected that the resulting vortex structure is the strongly-magnetised singular vortex with a negative longitudinal magnetisation but, perhaps surprisingly, we find that a strongly-magnetised coreless vortex with negative magnetisation is stabilised in its place.

The coreless vortex first splits into the pair of singular vortices with polar cores, such that the doubly-quantised vortex in $\zeta_-$ splits into two singly-quantised vortices. As the energy relaxes, $\zeta_+$ is depopulated leaving a spinor with winding numbers 1 and 2 in $\zeta_0$ and $\zeta_-$ respectively. The vortices in $\zeta_-$ then exit the cloud, leaving a spinor of the same form as that for strong, positive magnetisation, with $\zeta_+$ interchanged. The structure is as described above with the spin rotated by $\pi$ about an arbitrary axis in the $x$-$y$ plane.

### 6.6.1.2 Polar Regime

We now study the energetic stability of a FM coreless vortex in the polar regime, which has been experimentally prepared via magnetic field rotation [36, 37]. As an initial state we take the experimentally phase-imprinted state [Eq. (6.23)] with $F = 1$ everywhere, for different $M$. The energetic stability and structure of the vortex is then determined by numerically minimising the free energy in a rotating trap (at the frequency $\Omega$).
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Figure 6.9: (a) Spin profile $\langle \hat{\mathbf{F}} \rangle$ (arrows) and $|\langle \hat{\mathbf{F}} \rangle|$ (colour gradient and arrow lengths) of the coreless vortex in the polar regime, interpolating between FM and polar phases and displaying the characteristic fountain texture inside the core of a singular polar vortex. (b) The corresponding superfluid velocity $\mathbf{v}$ and its magnitude (arrows) and circulation density $\mathcal{V} = \rho \mathbf{v} \cdot \hat{\phi}$ (colour gradient), continuously interpolating from nonsingular to singular circulation.

Figure 6.10: Stability of the coreless vortex in the (a) polar and (b) FM (right) interaction regimes; (■) stable coreless vortex; (□) stable effective two-component coreless vortex; (△) instability towards a half-quantum vortex, (○) pair of half-quantum vortices (polar regime) or singular vortex (FM regime), (+) vortex-free state; (×) nucleation of additional vortices;

The stable vortex state is shown in Fig. 6.9 and can be qualitatively described by the analytic model (3.17), which interpolates between an outer singular polar vortex exhibiting a $2\pi$ disgyration of $\hat{\mathbf{d}}$ and an inner FM coreless vortex. The spin texture of the coreless vortex remains in a non-polar core region, reaching maximum $\mathcal{F} = 1$. At the centre of the core, $\langle \hat{\mathbf{F}} \rangle \parallel \hat{z}$. As $\rho$ increases, the spin winds to $\langle \hat{\mathbf{F}} \rangle \simeq \hat{\rho}$ where minimisation of Eq. (2.25) causes $\mathcal{F} \to 0$ over a length scale $\sim \xi_F$. Away from the non-polar core, containing a nonsingular coreless vortex, the topology then corresponds to that of a singly-quantised, singular polar vortex.

In Sec. 2.7.2, we introduced the length scale $\eta_M^{(1)}$, which in the polar regime describes the size of a FM core needed to yield the required $M$. By considering a uniformly magnetised cylindrical core inside an otherwise polar density profile, we found by a straightforward integration the estimate $\eta_M^{(1)} = R_{TF} \sqrt{1 - (1 - M)^{2/5}}$, where $R_{TF}$ is the Thomas-Fermi radius [Eq. (2.43)].
As the energy of the imprinted coreless vortex relaxes, the singly-quantised vortex with $F \to 0$ forms in the outer region. At weak magnetisation, the vortex splits into two half-quantum vortices of size $\sim \xi_F$, similarly to the splitting of a singly-quantised vortex in Sec. 5.2, where magnetisation was not conserved. The fountain-like texture of the spin in the quantised vortex cores is then lost. Conservation of a sufficiently strong magnetisation can prevent the splitting, stabilising the composite vortex with the coreless vortex residing inside the singular vortex core of size $\eta_M^{(1)}$. Comparison of length scales suggests that this happens when $\eta_M^{(1)} \gtrsim \xi_F (> \xi_n)$. Numerically, we find the stability threshold at $M \simeq 0.2$ (Fig. 6.10), in qualitative agreement with the estimate $\eta_M^{(1)} \sim \xi_F$.

Note that it follows from the generalised circulation (F.3) that circulation alone is quantised only in the polar phase ($F = 0$). The relaxed composite-vortex state interpolates smoothly between the vanishing circulation at the centre of the nonsingular texture to the single quantum of circulation carried by the outer polar vortex. The composite defect therefore smoothly connects the small-distance topology, represented by the non-quantised circulation of the coreless vortex, with the large-distance topology, represented by the quantised circulation in the polar phase.

### 6.6.2 Nematic Coreless Vortex

When the magnetic-field rotation technique used to phase-imprint the FM coreless vortex [36, 37] is applied to a BEC prepared initially in the state $\hat{\zeta}^0 = (0, 1, 0)^T$, which represents the polar phase with $\hat{d} = \hat{z}$ and longitudinal magnetisation $M = 0$, a nematic coreless vortex is produced [37, 142], with $\hat{d} = \sin \beta' \hat{\rho} + \cos \beta' \hat{z}$. Since the condensate was unmagnetised prior to the magnetic-field rotation, the longitudinal magnetisation remains zero in the imprinted texture. Hence even if some regions of non-polar phase are produced in the imprinting process, the overall magnetisation of zero enables the system to relax to the polar phase everywhere. As was demonstrated in Sec. 3.4, this $\hat{d}$ texture can continuously unwind to the uniform state. Since the nematic coreless vortex has vanishing mass circulation, it cannot be stabilised by rotation as the coreless vortex can.

We ask instead whether the nematic coreless vortex can be stable inside the core of a composite topological defect when a conserved, nonzero magnetisation necessitates the formation of non-polar regions. A nematic coreless vortex with a nonzero magnetisation could be created by phase-imprinting via population transfer [24, 30, 33] that individually prepares the appropriate phase windings of $(-1, 0, 1)$ in the spinor components. In a magnetised BEC, $F$ will acquire a spatial structure interpolating between $F = 0$ at the centre of the cloud to $F > 0$ at the edge as energy relaxes. From $\hat{d} \perp \langle \hat{F} \rangle$, it follows that in order to have the fountain texture in $\hat{d}$ we must have $\beta = \pi/2$ at $\rho = 0$ and increasing monotonically. The corresponding mass circulation, $\oint d\mathbf{r} \cdot \mathbf{v} = -\frac{h F}{m} \cos \beta$,
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Figure 6.11: Stable nematic coreless vortex in a BEC with polar interactions. (a) The unoriented \( \hat{d} \)-vector (cylinders) exhibits the coreless fountain-like texture. The circulation density \( V = \rho v \cdot \hat{\phi} \) (colour gradient) shows the composite-vortex structure, interpolating between the non-circulating polar phase to the outer singly-quantised FM vortex. (b) Corresponding spin texture \( \langle \hat{F} \rangle \) (arrows) and spin magnitude \( |\langle \hat{F} \rangle| \) (colour gradient and arrow lengths), showing the core region. Conservation of magnetisation forces the BEC into the FM phase away from the vortex line.

interpolates from the non-circulating polar core to a nonzero circulation, in principle, allowing stabilisation by rotation.

For sufficiently strong magnetisation the condensate will reach \( F = 1 \) in an outer FM region. The vortex then represents a composite topological defect, described by Eq. (F.5). The outer, FM region represents the large-distance topology of a singular FM vortex. The nematic coreless vortex then forms the small-distance topology of the composite topological defect. However, our numerics demonstrate that the vortex is energetically stable only once magnetisation is strong enough to deplete \( \zeta_+ \), enforcing an effective two-component regime. We find this to occur at \( M \lesssim -0.2 \). The numerically computed, stable vortex state shown in Fig. 6.11 then exhibits a MH-like texture in \( \hat{d} \), and a corresponding bending of the spin vector from the \( \hat{\rho} \) direction at the centre to the \(-\hat{z}\) direction in the FM region. The core size is again determined by the magnetisation constraint. The instability at weaker magnetisation results from the existence of lower-energy singular vortices with FM cores.

For the nematic coreless vortex with general \( F \) we may define a winding number analogous to Eq. (6.27), associated with the fountain texture of the nematic axis \( \hat{d} \), by taking \( \hat{n}_F \rightarrow \hat{d} \). Note that due to the equivalence \( \hat{d} \leftrightarrow -\hat{d} \) the sign of \( W \) is no longer well defined. For the cylindrically symmetric fountain texture (3.33), the integral in Eq. (6.27) can be evaluated to yield

\[
W = \frac{1 - \cos \beta'(R)}{2} = \frac{1 - \sin \beta(R)}{2},
\]

(6.29)
where $\beta'$ is now the angle between $\hat{d}$ and the $z$ axis to account for the relative rotation of $\hat{d}$ in Eq. (6.12) compared with the prototypical polar spinor used to formulate Eq. (3.23). We have made use of $\beta' = 0$ on the symmetry axis where $\hat{d} = \hat{z}$. In the last step we have used the relation $\beta = \beta' + \pi/2$ to rewrite $W$ in terms of the Euler angle $\beta$ of Eq. (F.5). From Eq. (6.29), we find $W = 1$ for an ATC-like texture, and $W = 1/2$ for a MH-like texture such as that stabilised in the effective two-component regime (Fig. 6.11).

### 6.7 Conclusions

We have shown that the conservation of magnetisation in spinor BECs can lead to vortex core structures with distinct small and large-distance topology. The characteristic core size is then determined by the magnetisation constraint, instead of one of the healing lengths associated with the nonlinear interactions. In phase-imprinting experiments, the magnetisation of the initial vortex state can be controlled and the relaxation process of appropriately prepared initial states results in mixing of the different ground-state manifolds. In particular, a sufficiently strong magnetisation causes a condensate in the polar interaction regime to exhibit properties of the FM regime, including the stability of a nonsingular FM coreless vortex where simple energetic arguments alone would not predict its existence. The FM coreless vortex exists as a composite topological defect, with the large-distance topology of a singular vortex of the polar phase. Such a state may be prepared experimentally to the appropriate magnetisation via phase-imprinting and so spin-1 BECs present the interesting possibility of conducting laboratory studies of composite topological defects. A vortex with the overall topology of a singular FM vortex has also been shown to be stable for a strongly-magnetised polar condensate. Additionally, we have shown that the stable vortex configurations can be qualitatively understood by an analytic model for the spinor wavefunction which interpolates between the FM and polar phases, which may exhibit a vortex in one or both of the phases of the ground-state manifold. One may then construct analytic spinors describing composite topological defects.
Chapter 7

Dipole-Dipole Interactions

Any object with a nonzero electric or magnetic dipole moment produces an associated dipolar potential, which gives rise to non-local interactions. The effects of electric dipolar interactions are the focus of active studies in, for example, polar molecules [170] and Rydberg atoms [171]. Atoms with nonzero spin possess a finite magnetic dipole moment, such that the atoms can interact over long distances as well as via the contact interactions considered thus far in this study. The magnetic dipole-dipole interaction is considerably weaker than the electric equivalent and so dipolar effects in spinor or spin-polarised BECs play a smaller (although still nontrivial) role in their dynamics and energetics. The strongest currently realised spinor dipolar systems have dipolar energy on the order of \( \sim 10\% \) of the \( s \)-wave scattering energy. However, there are proposals to increase the relative strength of the dipolar interaction in experimental regimes [172, 173, 174, 175] and so it is natural to ask whether the dipolar interaction in spinor BECs can modify the structure or stability of vortices.

We begin by reviewing how the spinor GPEs are modified by the inclusion of dipolar interactions, before presenting the modifications required to our numerical method to account for this. We then review some of the key properties and behaviours of dipolar BECs before presenting the core structures of stationary states of vortices in spinor dipolar BECs.

7.1 Dipolar BEC Theory

The interaction energy of two electric or magnetic dipoles with dipole moments \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \) and separated by \( \mathbf{r} \) is given by

\[
V_{dd} = D_{dd} \left( \frac{\mathbf{e}_1 \cdot \mathbf{e}_2 - 3 (\mathbf{e}_1 \cdot \hat{\mathbf{r}}) (\mathbf{e}_2 \cdot \hat{\mathbf{r}})}{r^3} - \frac{\mathbf{e}_1 \cdot \mathbf{e}_2 \delta(r)}{3} \right),
\]

(7.1)
where \( r = |\mathbf{r}| \) and \( \mathbf{r} = \mathbf{r}/r \). The constant \( D_{dd} = 1/4\pi\epsilon_0 \) (\( D_{dd} = \mu_0/4\pi \)) for interacting electric (magnetic) dipoles. The dipole moment in an atomic spinor BEC is magnetic in origin, and is proportional to the expectation value of the atomic spin,

\[
e(\mathbf{r}) = d\langle \hat{\mathbf{F}}(\mathbf{r}) \rangle,
\]

where \( d \) is the magnitude of the magnetic dipole moment of the atom.

Since each atom interacts with every other atom in the system through their dipole moments, one must therefore include a nonlocal term in the energy functional of a spinor dipolar BEC, which in mean-field theory takes the form

\[
E_{dd} = E_{GP} + \int \int V_{dd}(\mathbf{r} - \mathbf{r}_1)d^3\mathbf{r}_1 d^3\mathbf{r}
\]

\[
V_{dd}(\mathbf{r} - \mathbf{r}_1) = \frac{c_{dd} n(\mathbf{r}_1) n(\mathbf{r})}{2} \left( \frac{\langle \hat{\mathbf{F}}(\mathbf{r}_1) \rangle \cdot \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle - 3 \frac{\langle \hat{\mathbf{F}}(\mathbf{r}_1) \rangle \cdot \hat{\mathbf{R}}}{|\mathbf{r} - \mathbf{r}_1|^3} \left[ \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle \cdot \hat{\mathbf{R}} \right] }{3} \right.
\]

where \( \hat{\mathbf{R}} \) is the unit vector in the direction of \( \mathbf{r} - \mathbf{r}_1 \), \( c_{dd} = D_{dd}d^2 \) and \( E_{GP} \) is the energy of the dipole-free spinor condensate [derived from Eq. (2.25), which gives the functional derivative of \( E_{GP} \)]. The GPE with dipolar interactions is obtained by taking the functional derivative of the energy functional as before, yielding

\[
\hat{H}\Psi(\mathbf{r}) = \left( \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \left( x^2 + \gamma_0^2 y^2 + \gamma_z^2 z^2 \right) - \mathbf{\Omega} \cdot \mathbf{\hat{L}} + g_1 \mathbf{B} \cdot \mathbf{\hat{F}} + g_2 (\mathbf{B} \cdot \mathbf{\hat{F}})^2 \right)
\]

\[
+ c_0 n(\mathbf{r}) + c_2 n(\mathbf{r}) \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle \cdot \hat{\mathbf{F}} + \mathbf{b}(\mathbf{r}) \cdot \hat{\mathbf{F}} \right) \Psi(\mathbf{r})
\]

\[
\mathbf{b}(\mathbf{r}) = \int d^3\mathbf{r}_1 \frac{c_{dd} n(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|^3} \left( \langle \hat{\mathbf{F}}(\mathbf{r}_1) \rangle - 3 \frac{\langle \hat{\mathbf{F}}(\mathbf{r}_1) \rangle \cdot \hat{\mathbf{R}}}{|\mathbf{r} - \mathbf{r}_1|^3} \right),
\]

where we have absorbed the contact terms from the dipolar interaction into \( c_0 \) and \( c_2 \). We define \( c'_{dd} = c_{dd} N m/\hbar^2 l \) when treating the spinor dipolar GPE in dimensionless units. The locally-defined vector \( \mathbf{b}(\mathbf{r}) \) can be thought of as an effective magnetic field generated by the dipole moments of all atoms in the condensate.

The divergence of the integrand in the definition of \( \mathbf{b}(\mathbf{r}) \) prevents the integral from being evaluated numerically. This divergence is avoided by making a cutoff for \( |\mathbf{r} - \mathbf{r}_1| \leq \epsilon \) and taking the limit \( \epsilon \to 0 \). By making use of the convolution theorem, one may rewrite the problem in momentum space as \([8, 176]\)

\[
\mathbf{b}(\mathbf{k}) = \frac{4\pi c_{dd} n(\mathbf{k})}{3} \left( 3 \left[ \langle \hat{\mathbf{F}}(\mathbf{k}) \rangle \cdot \hat{\mathbf{k}} \right] \hat{\mathbf{k}} - \langle \hat{\mathbf{F}}(\mathbf{k}) \rangle \right) \left[ \frac{\cos \left( \frac{\epsilon |\mathbf{k}|}{|\mathbf{k}|^2 - \frac{\sin \left( \frac{\epsilon |\mathbf{k}|}{|\mathbf{k}|^2} \right]}{\epsilon^3 |\mathbf{k}|^3} \right) \right],
\]
where we define $\hat{k}$ as the unit vector in the direction of $k$ and $\langle \hat{F}(k) \rangle = \zeta(k)\hat{F}\zeta(k)$, as in the position-dependent formalism. In the limit $\epsilon \to 0$, Eq. (7.5) becomes

$$b(k) = \frac{4\pi c_{\text{dd}} n(k)}{3} \left( 3 \left[ \langle \hat{F}(k) \rangle \cdot \hat{k} \right] \hat{k} - \langle \hat{F}(k) \rangle \right), \tag{7.6}$$

One may then evaluate $b(r)$ by first calculating $b(k)$ from the Fourier-transformed spinor wavefunction and then performing an inverse Fourier transform. This method does have an important problem—the dipolar interaction extends out to infinity, but our spatial grid is finite. As a result, when we take the Fourier transform we are treating a periodic system and therefore the dipolar interaction will cause the system to interact with an array of identical, regularly-spaced condensates. To avoid this, we modify the dipolar interaction to

$$V_{\text{dd}}(r - r_1) = c_{\text{dd}} n(r_1) n(r) \frac{1}{|r - r_1|^3} \left( \langle \hat{F}(r_1) \rangle \cdot \langle \hat{F}(r) \rangle - 3 \left[ \langle \hat{F}(r_1) \rangle \cdot \hat{R} \right] \left[ \langle \hat{F}(r) \rangle \cdot \hat{R} \right] \right) \Theta (R - |r_1|), \tag{7.7}$$

where $R > R_{TF}$ but $R$ is still within the spatial grid such that any spurious neighbouring condensates appearing in the Fourier transform are explicitly prevented from interacting with the condensate. In momentum space, this becomes [177]

$$b(k) = \frac{4\pi c_{\text{dd}} n(k)}{3} \left( 1 + 3 \frac{\cos R k}{R^2 k^2} - 3 \frac{\sin R k}{R^3 k^3} \right) \left( 3 \left[ \langle \hat{F}(k) \rangle \cdot \hat{k} \right] \hat{k} - \langle \hat{F}(k) \rangle \right), \tag{7.8}$$

such that the numerical efficiency of the momentum-space calculation is recovered but now the periodic terms of order $\sim 1/R$ are suppressed.

Just as the density and spin healing lengths, $\xi_n$ and $\xi_F$ respectively, define the size scales for deviations of the density and spin from their bulk values, so one can define the dipolar healing length

$$\xi_{\text{dd}} = l \left( \frac{\hbar \omega}{2 |c_{\text{dd}}| n} \right)^{1/2}, \tag{7.9}$$

which approximately constrains the size of regions where the spin texture deviates from that energetically favoured by the dipolar interaction. For $^{87}\text{Rb}$ ($^{23}\text{Na}$) in the spin-1 manifold, $c_{\text{dd}}/c_0 \sim 4 \times 10^{-4}$ ($2 \times 10^{-4}$) and so $\xi_{\text{dd}}/\xi_n = (c_{\text{dd}}/c_0)^{-1/2} \sim 50$ ($\sim 70$) [85]. For comparison, $c_{\text{dd}}/c_2 \sim 8 \times 10^{-2}$ ($c_{\text{dd}}/c_2 \sim \sim 7 \times 10^{-3}$) in $^{87}\text{Rb}$ ($^{23}\text{Na}$). The strongly-dipolar chromium condensate is usually realised in the $F = 3$ manifold of $^{52}\text{Cr}$, which has $c_{\text{dd}}/c_0 \sim 0.27$. However, we note that these ratios may be modified, for example by using optical Feshbach resonances to tune $c_0$ and $c_2$.

### 7.2 Numerical Implementation

The inclusion of nonlocal terms arising from the atomic dipolar interaction increases the convergence time of imaginary time routines by a prohibitive amount. Consequently, in
the study of dipolar systems we employ only the successive overrelaxation (SOR) algorithm. Since SOR identifies stationary states rather than minimising the free energy, we therefore aim to identify the stationary states rather than those which are energetically stable, due to the considerably faster convergence offered by SOR.

The matrices employed in the SOR algorithm for dipolar interactions are as specified in Eq. (4.48), with an additional term in the $D$ matrix:

$$D_{ii}^{\text{dipole}} = D_{ii} + b_{ii} \cdot \hat{F},$$ \hspace{1cm} (7.10)

where again the subscript $ii$ indicates that the $b$ vector must be evaluated at each point on the spatial grid. The effective field $b$ is evaluated in momentum space and then Fourier transformed to give the position-dependent form as described in Sec. 7.1. As with the contact interaction terms, $b$ must be recalculated after every iteration to ensure that the system is linearised. The chemical potential $\mu$ also includes the contribution from dipolar interactions.

While in principle a further increase in speed could be attained by calculating the dipolar interaction in the position representation rather than in momentum space, removing the need for any Fourier transforms, the divergence of the position-dependent form of the dipolar potential makes such an approach unfeasible.

### 7.3 Core Deformation in Dipole-Free SOR

Since we will be making use of the SOR algorithm to study vortices in spinor dipolar BECs, as a first test of the properties of the algorithm we verify that the results obtained from imaginary time evolution in the absence of dipolar interactions are correctly reproduced by SOR. Since SOR identifies stationary states rather than energetically stable ones, it does not necessarily follow that the results of the two algorithms will agree perfectly. Also, since dipolar interactions do not conserve magnetisation, we do not attempt to reproduce the results of the magnetisation-conserving relaxation method.

For a spin-1 BEC without dipolar interactions, we find stationary states representing each vortex described in Chapter 5. The core structures themselves are not modified but the stationary solutions are all found to be centred on the rotation axis of the trap; no displacement of the vortex is observed, which can happen in imaginary time. A consequence of this is that the $|\langle \hat{F} \rangle|$ profiles of almost all vortex structures identified by the SOR method are axially symmetric. The only exception is the core-deformed singular vortex of the polar phase, whose core splits into a pair of half-quantum vortices and therefore cannot be axisymmetric.

Since the vortices must occupy the centre of the trap to represent stationary states in the SOR method, the rotation frequency required to identify a vortex state is increased.
Intuitively, this arises as the increased rotation frequency in imaginary time causes the vortex to lie closer to the centre of the trap. These properties of the SOR algorithm must be kept in mind when interpreting the stationary vortex states in the presence of dipolar interactions. Unfortunately, the reason for this discrepancy between the SOR and imaginary time methods is unclear.

### 7.4 Literature Review: Dipolar BECs

#### 7.4.1 Motivation

The recent experimental condensation of chromium [80, 113, 114], and subsequently of dysprosium [81] and erbium [82], all of which have relatively large dipole moments [178], has motivated a surge in interest in the study of such long-range interactions. Here we consider the effects of dipolar interactions upon the cores of singular vortices in spin-1 atomic BECs. In current experiments on spin-1 atoms, the spin-dependent scattering term is an order of magnitude greater than the dipolar contribution to the energy functional. There have however, been proposals to use oscillating magnetic fields to effectively tune the strength of the dipolar interaction in a spinor condensate [172, 173, 174]. The ability to tune the strength of this effect, as the other terms in the Hamiltonian may also be tuned [175, 179], opens up a much wider parameter space for study. Therefore, while the dipole moments of $^{23}$Na and $^{87}$Rb may be used as prototypes for the polar and FM regimes respectively in our study of vortices in dipolar spin-1 BECs, there is a strong motivation for also considering stronger dipole moments.

#### 7.4.2 Spin-Polarised Dipolar BEC

In attempting to understand the properties of spinor dipolar systems, it is instructive first to consider a spin-polarised system, such that the dipole moment does not vary with position. If the polarisation is fixed externally, e.g. by applying a strong magnetic field to the system in a direction we will label $z$, this system can be described by a single-component GPE, rather than using the full spinor treatment. The dipolar interaction is anisotropic, causing repulsion in the $z$ direction and attraction in the $x$-$y$ plane, as may be seen from Eq. (7.1). As a result, increasing $c_{dd}$ has been predicted to cause the BEC to become more prolate subject to a fixed trap geometry [180]. Such behaviour has indeed been observed experimentally [181].

Subsequently, it was shown theoretically that dipolar interactions modify the critical frequency for vortex stability in a rotating, axisymmetric trap where the spins are polarised parallel to the rotation axis [182]. In a prolate trap, dipolar interactions reduce the critical frequency when compared to the dipole-free case, while in an oblate condensate the
critical frequency is increased. When the spins are polarised perpendicular to the axis of rotation, the dipolar interaction was subsequently shown theoretically to cause the cores of vortices to become asymmetric, deforming in the direction of the polarisation [183].

### 7.4.3 Single-Mode Approximation For Spinor Dipolar BECs

The single-mode approximation (SMA) for a spinor BEC assumes that the atomic spin does not vary spatially, describing a spin-polarised state where the direction of polarisation is not fixed externally. Applying the SMA to spinor dipolar systems predicts that the dipolar interaction can force a spin-1 BEC with polar interactions to exhibit nonzero spin, for sufficiently large $c_{dd}$ [184]. Additionally, the trap geometry lends a preferred direction to the spin, with a prolate trap favouring spin in the $z$ direction and an oblate trap favouring spins in the $x$-$y$ plane, where $z$ is the symmetry axis of the trap. The anisotropic nature of the dipolar interaction favours ‘head-to-tail’ alignment of spins [8], as may be seen from the $(e_1 \cdot r)(e_2 \cdot r)$ term in Eq. (7.1), and so it is unsurprising that the spin texture would align with the major axis of an anisotropic condensate.

### 7.4.4 Spontaneous Spin Texture Formation In Spinor Dipolar BECS

Although the SMA does not correspond to an experimentally realistic scenario, its predictions approximately hold for weak dipolar interactions, when the spin is allowed to vary with position [83]. However, the ground state for sufficiently strong dipolar interactions is a nonuniform spin texture representing the spontaneous formation of a vortex line. The SMA breaks down approximately when $R_{TF} \sim \xi_{dd}$, as now dipolar interactions can manifest themselves on length scales smaller than the size of the condensate [85].

In an oblate trap, for parameters consistent with spin-1 $^{87}$Rb, the ground state was shown to be a singular vortex aligned with the symmetry axis [83]. The core of this singular vortex is filled with the polar phase and outside of this core region, the spin forms a tangential disgyration [86]. In a prolate trap, the coreless vortex forms the ground state. The spin displays a chiral texture away from the vortex axis, which is again parallel to $\hat{z}$. In the isotropic trap, the ground state is again a singular vortex, though the symmetry of the trap means that there is no preferred orientation for the vortex line. The spin texture is as in the oblate trap.

In the isotropic trap it was subsequently shown that the ground state depends both on $R_{TF}/\xi_F$ and $R_{TF}/\xi_{dd}$. As has been mentioned, the SMA forms the ground state for $R_{TF} < \xi_{dd}$. The coreless vortex then becomes the ground state until, when $R_{TF} \gtrsim \xi_{dd}$, the ground state is the singular vortex. The precise ratio $R_{TF}/\xi_{dd}$ at which the transition occurs is weakly dependent on $\xi_F$, with smaller $\xi_F$ increasing the value of $\xi_{dd}$ at which the transition occurs.
These results may be understood in terms of the findings in the SMA; in an oblate trap, spins in the \(x\)-\(y\) plane are energetically preferred and so the planar spin texture has the lowest dipole-dipole interaction energy. Conversely, in the prolate trap, spin alignment with the \(z\) axis is preferred. In the coreless vortex, the highest-density region has \(\mathbf{F} = \mathbf{z}\), giving a considerable reduction in dipolar energy compared to the singular vortex with polar core. From this it may be inferred that sufficiently strong dipolar interactions will modify the structures of vortices to maximise spin alignment in the direction of the major axis of the condensate. Additionally, it is noteworthy that the coreless vortex formed in the non-rotating system carries angular momentum but the singular vortex does not. From this we may infer that the coreless vortex is likely to form the ground state of a rotating condensate as no modification to its structure is required to produce angular momentum. The fact that the dipolar interaction can determine the spin texture associated with either a singular or a coreless vortex also implies that the radial bending of the spin vector, observed in these vortices for a non-dipolar FM spin-1 BEC, should be modified by dipolar interactions.

In a prolate trap, the dipolar interaction has also been shown to cause the spontaneous formation of spin domains [176]. Two domains form, one with spin aligned with the symmetry axis and the other with anti-aligned spin. The symmetry axis is perpendicular to the domain wall separating the two spin domains. Application of a sufficiently strong positive quadratic Zeeman splitting with the field in the direction of the symmetry axis, causes the spin domains to dissolve into a helical spin texture with no domain wall.

### 7.4.5 Rotating Spinor Dipolar BECs

So far we have described the effects of dipolar interactions in spinor condensates only in a non-rotating trap. However, this study focuses on rotating traps and how including dipolar interactions changes the vortex structures identified in spin-1 condensates. To date, the only study of rotating spinor dipolar systems was restricted to an oblate trap [185]. A slowly rotating condensate behaves just as a non-rotating condensate does, with strong dipolar interactions causing the spontaneous formation of a vortex. As the rotation frequency increases in the FM regime, a coreless vortex, or lattice thereof, forms the ground state. In the polar regime, a lattice of half-quantum vortices forms when the dipolar interactions are weak just as it does in the dipole-free system. The spins in the FM cores of the half-quantum vortices display antiferromagnetic ordering — that is, the spin in each vortex core is antiparallel to that in the neighbouring vortex core. For increased \(c_{dd}\), a vortex sheet forms, while as \(c_{dd}\) is further increased, the system behaves as in the FM regime.

The dipolar interaction has also been shown theoretically to modify the lattice structure of a many-vortex state [87, 88, 89].
7.5 Singular Vortex Stability

The aim of this study is to determine the effect of dipolar interactions upon the vortex structures identified in the non-dipolar spin-1 BEC. We use the SOR algorithm to identify stationary states of the spinor dipolar GPEs. As a test of the numerical method, we first reproduce several key results from the literature.

The first test of the numerical implementation of the dipolar interaction is to reproduce the behaviour of a spin-polarised condensate. Our numerics show the expected change in condensate aspect ratio as the dipolar interaction strength is increased in a non-rotating trap \[180\]. In the rotating trap, the modified critical frequency for vortex stability is also well reproduced \[182\].

Having reproduced the behaviour of a spin-polarised condensate, we proceed to test whether our numerical method can spontaneously form spin textures from an initially uniform state. We observe the formation of coreless and singular vortices for varying trap geometries in both polar and FM regimes, in agreement with the literature \[83, 85\].

The final test of the numerical algorithm is to reproduce the phase diagram of a spinor dipolar BEC in a rotating, oblate trap \[185\]. All the states on the phase diagram are well reproduced.

With these numerical results successfully reproduced, we now apply the spinor dipolar SOR algorithm to a study of vortices in a rotating, isotropically-trapped spin-1 BEC with fixed \(Nc_0/\hbar \omega l^3 = 10^4\) and \(Nc_2/\hbar \omega l^3 = 300 (-50)\) in the polar (FM) regime. We present phase diagrams demonstrating the stationary states identified by this method in both polar and FM regimes with varying \(\Omega\) and \(c_{dd}\) in Fig. 7.1, which reproduce many of the features of the corresponding phase diagrams for an oblate trap [cf. Ref. 185]. These phase diagrams show the stationary states with minimal energy where multiple stationary states are identified. For example, in the weakly dipolar system with FM interactions, both coreless and singular FM vortices are identified as stationary states but the coreless vortex has lower energy. Sample spin textures are shown in Figs. 7.2-7.3 for the spin textures which form due to strong dipolar interactions in spin-1 condensates with FM and polar interactions, respectively. The only previously unreported feature observed is that the vortex sheet of the polar regime forms a chiral spin texture in the isotropic trap.

The formation of this spin texture may be intuitively understood from the formation of a similar texture in the FM regime, and also for larger \(c_{dd}\) in the polar regime in the oblate trap. The vortex sheet is stable for a very narrow range of \(c_{dd}\), which leads us to infer that the vortex sheet and the coreless vortex with chiral spin texture are in fact facets of the same texture in the isotropic trap, with the polar interaction overcoming the dipolar interaction over short distances and restoring the polar phase in small regions. The chiral spin texture of the coreless vortex is retained. The reason that this behaviour is
Figure 7.1: Energy-minimising stationary states of dipolar spin-1 (a) polar and (b) FM spin-1 BECs. (□) Polar regime: splitting into two half-quantum vortices, one of which exits the cloud. (■) In both regimes: stability of the singular vortex states found in the absence of dipolar interactions. (×) Polar regime: antiferromagnetic vortex lattice. FM regime: coreless vortex lattice. (○) Polar regime: vortex sheet. FM regime: coreless vortex. (△) Polar regime: coreless vortex lattice. Filled △ indicates additional singular vortices with polar cores. (+) FM regime: instability towards vortex-free state.

Figure 7.2: Example numerical spin texture formed in (a) the singular vortex and (b) the coreless vortex lattice of the FM regime.
Chapter 7 Dipole-Dipole Interactions

Figure 7.3: Example numerical spin texture formed in (a) the antiferromagnetic half-quantum vortex lattice and (b) the vortex sheet of the polar regime.

not observed in the oblate trap is that the chiral texture of the coreless vortex provides increased head-to-tail alignment as the trap becomes less oblate. Additionally, in the oblate trap, a greater number of polar regions are able to form since the size of the trap is increased in the $x$-$y$ plane. Thus, the vortex sheet behaviour is more prominent in the oblate trap. In the isotropic trap, the dipolar interaction favours the chiral spin texture, while the extent of the cloud in the $x$-$y$ plane is reduced compared to the oblate trap, such that the vortex sheet behaviour is suppressed in favour of the chiral texture.

For a strongly dipolar system in a non-rotating trap, we find that the tangential spin disgyration forms a stationary state. This represents a vortex with zero angular momentum. Since the trap is isotropic and non-rotating, there is no preferred orientation to the vortex line. As the rotation frequency is increased, one would intuitively expect the vortex line to orient with the rotation axis and perhaps to undergo some deformation to gain angular momentum. Recall that in the non-dipolar spinor BEC, the singular vortex of the FM regime displayed a radial bending of the spin vector to generate angular momentum. However, this is not the case for the spinor dipolar system. In the strongly dipolar FM condensate, no such radial bending of the spin is observed. Rather, the vortex line itself re-orientates to lie in the $x$-$y$ plane at slow rotation frequencies, eventually becoming unstable for increased $\Omega$ as additional vortices are nucleated. An intuitive way of understanding this is as follows.

In the absence of dipolar interactions, the singular FM vortex displays a radial bending of the spin to orient uniformly, far from the vortex core. All orientations are energetically degenerate in the absence of magnetic fields or dipolar interactions. There is also no energetic distinction between radial, tangential or cross disgyrations of the spin vector in the vicinity of the core. The inclusion of a dipole-dipole term in the Hamiltonian
however, has already been demonstrated to favour a tangential disgyration. This spin profile may still exhibit the radial bending required to produce aligned spins far from the core; however, the result is an increase in dipolar interaction energy.

As was commented in Sec. 7.4.4, the singular vortex exhibiting a tangential spin disgyration carries no angular momentum. It is the radial bending of the spin towards a uniform asymptotic orientation that gives rise to a nonzero angular momentum in the dipole-free system. It follows that in order for the singular vortex in a dipolar spin-1 BEC to carry angular momentum, it must exhibit a radial bending of the spin vector, thus increasing its dipolar energy as the preferred spin-alignment is broken. The increase in dipolar energy cannot be offset by the reduction in energy due to angular momentum. Instead, the first stable state with nonzero angular momentum is produced at sufficiently rapid rotation frequency to nucleate several vortices. This sudden nucleation of many vortices is a general feature of the numerics and is not a consequence of the dipolar interaction. The interpretation of the phase diagram is then that, for a strongly dipolar FM condensate, the tangential spin disgyration, which has zero angular momentum, plays the role of the vortex-free state in the weakly-dipolar limit. In this strongly-dipolar limit, the singular vortex with nonzero angular momentum is unstable.

In conclusion, a sufficiently strong dipolar interaction causes a spin-1 BEC with polar interactions to exhibit the behaviour of the FM condensate. While the anisotropic nature of the dipole-dipole interaction is sensitive to the trap geometry, we find that the stationary vortex states for an isotropic trap are primarily as previously identified in the oblate trap [185]. However, we have shown that the dipolar interaction causes a polar BEC to form a chiral spin texture in the isotropic trap, where a vortex sheet has been reported in the oblate trap. Additionally, we find that sufficiently strong dipolar interactions disrupt the metastability of the singular FM vortex with nonzero angular momentum, which was observed in the non-dipolar spinor BEC in Sec. 5.1.
Chapter 8

Concluding Remarks

This thesis has demonstrated numerically the energetically stable and stationary states of singular vortices in spin-1 atomic BECs in rotating, optical traps. In the absence of long-range dipole-dipole interactions, the energetically stable states were identified by the method of propagation in imaginary time. With dipolar interactions included, stationary states were identified via a successive overrelaxation algorithm. Stationary states are not necessarily energetically stable and so the energetic stability of singular vortices in spinor dipolar BECs remains an open question. In all scenarios studied, the cores of singular vortices exhibit non-vanishing density, in contrast to the vortices of single-component atomic BECs. This non-vanishing density arises due to the spin degrees of freedom in the system and can be understood in terms of an energetic hierarchy of length scales.

By numerically minimising the free energy functional without conserving longitudinal magnetisation, we have identified the energetically stable vortices of a spin-1 BEC. We have demonstrated that a singular, singly-quantised vortex can be energetically stable in the FM phase of a spin-1 BEC, despite the existence of a stable coreless vortex with lower energy. This implies that even though singular vortices would not be nucleated by rotation alone, a singly-quantised vortex created, for example, by phase-imprinting would remain stable in the rotating system. This provides an interesting opportunity for controlled studies of a singular vortex line in a ground-state manifold with a broken SO(3) symmetry. Such a system supports only two topological classes of vortices: those that can be locally deformed to a vortex-free configuration and those that are topologically equivalent to a singly-quantised singular vortex. Experimentally, one could phase-imprint overlapping vortex lines in each of the three spinor wavefunction components. The resulting structure represents a singular spin-1 vortex with a vanishing density at the vortex line. The core of such a vortex then deforms to an energy-minimised configuration within the same topological equivalence class.
The core of the stable singular vortex has non-vanishing density, instead having a spinor orthogonal to the FM ground-state manifold. The core of the vortex then fills with atoms in the polar phase. This core structure may be understood in terms of an energetic hierarchy of length scales as follows. The filling of the vortex core with the polar phase represents a perturbation of the spin magnitude and has a size scale constrained by the spin healing length, $\xi_F$, which for experimentally relevant interaction strengths is larger than the density healing length, $\xi_n$, which defines the size of a density-depleted core. The larger core has a reduced gradient energy and so is energetically favourable.

The spin texture associated with the stable, singular FM vortex continuously bends from a $2\pi$ winding about the vortex core to uniform spin alignment far from the vortex. This structure is a property of the SO(3) ground-state manifold, in which the $2\pi$ spin rotation and $2\pi$ phase-winding lie in the same topological class. As a result of this spin texture, the singular FM vortex appears to break axial symmetry. The vortex lines in the three spinor components, which overlap in the density-depleted vortex, are displaced from one another as a result of the spin texture. We have demonstrated that, by a suitable choice of spinor basis, axial symmetry of the densities of the spinor components can be restored.

We have also demonstrated the energetic stability of a singular, singly-quantised vortex in the polar phase in a sufficiently rapidly rotating trap. The singly-quantised vortex deforms into two half-quantum vortices, breaking axial symmetry. The two half-quantum vortices form an expanded vortex core region, outside of which the topology of the singly-quantised polar vortex is preserved. The cores of the half-quantum vortices fill with atoms in the FM phase by the same process as the filling of the singular FM vortex core with atoms in the polar phase. In the energetically stable configuration of the polar regime, the spins in the two half-quantum vortex cores anti-align to minimise the gradient energy. As in the FM phase, a suitable choice of basis can simplify the vortex structure and aid in understanding its classification, with the half-quantum vortices forming separate vortex lines in the $\zeta_{\pm}$ spinor components.

In both the polar and FM interaction regimes, it is energetically favourable to form vortex cores with non-vanishing density, such that they fill with atoms excited out of the ground-state manifold. The gradient energy restores the full symmetry of the spin-1 condensate wavefunction in the singular vortex core. The system then simultaneously exhibits two different order parameter symmetries: maximal unbroken symmetry inside the core of size $\xi_F$ and a broken symmetry outside the vortex core, corresponding to the FM (polar) phase for FM (polar) interactions.

On time scales where $s$-wave scattering dominates the interactions in a spin-1 BEC, the longitudinal magnetisation $M = (N_+ - N_-)/N$ is approximately conserved [45]. Magnetisation may change on longer time scales due to, for example, dipolar interactions,
atom loss, or spurious $p$-wave scattering with high-temperature atoms. We have determined the structure and stability of singular and nonsingular vortices by numerically relaxing the energy of trial wavefunctions, explicitly imposing conservation of magnetisation throughout the relaxation procedure. We demonstrated that the singular vortex structures identified in Chapter 5, which did not conserve magnetisation, are robust when the numerical model is refined to explicitly conserve a zero or weak magnetisation. However, the FM coreless vortex has an associated nonzero magnetisation arising from its characteristic fountain texture and so, if the conserved magnetisation is too weak, the coreless vortex cannot form and the singular vortex becomes the ground state.

We have also identified a characteristic vortex core size, which is determined by the magnetisation constraint as opposed to the atomic interactions. This magnetisation constraint must be obeyed and so any vortex structure which cannot produce the required magnetisation cannot form. When the magnetisation forces the vortex core to be larger than the spin healing length, novel vortex structures emerge which mix the two ground-state manifolds.

In addition, we have shown that the conservation of magnetisation in spinor BECs can lead to vortex core structures with distinct small and large-distance topology. In order to describe both the core-filling structures of Chapter 5 and these composite-core structures, we have constructed an analytic model of the spinor wavefunction which may interpolate between the polar and FM ground-state manifolds. We have used this to analyse the filled cores of singular vortices, demonstrating how the Euler angles associated with spin and phase rotations combine to yield a nonsingular state inside the vortex core. We have also applied this formalism to the study of composite topological defects, enabling us to classify the large- and small-distance topologies which may form in such a hierarchical core structure. In particular, we have shown that the singular vortex of the polar phase forms a structure akin to a composite topological defect, in which the large-distance topology would be that of the singular FM vortex if the FM phase were formed in the outer, magnetised region.

One especially interesting consequence of the mixing of FM and polar phases due to conserved nonzero magnetisation is the stability of a FM coreless vortex in the polar interaction regime, which has been phase-imprinted on a condensate of $^{23}$Na in recent experiments [36, 37]. Since the phase-imprinting process can be used to produce a specific magnetisation, our findings show that the FM coreless vortex may be studied in experimentally-viable regimes. The FM coreless vortex in the polar regime represents a composite topological defect, with the large-distance topology of a singular vortex of the polar phase.

We also demonstrate via our analytic construction how a nonsingular nematic coreless vortex vortex of the polar phase, which has also been experimentally phase-imprinted [37, 142], may exist within the core of a composite topological defect. Inside the composite
vortex core, the order-parameter remains in the polar phase, forming the fountain (or half-monopole) texture of the nematic axis which is the characteristic of the nematic coreless vortex. Far from the vortex, the condensate exhibits the FM phase with the large-distance topology of a singular FM vortex. The conservation of sufficiently strong magnetisation prevents the outer FM region from relaxing to the polar phase, rendering the nematic coreless vortex stable within the composite core when otherwise it would be unstable. In addition, we construct a composite topological defect with the small-distance topology of a polar half-quantum vortex and the large-distance topology of a singular FM vortex. However, the structure remains stable in a sufficiently rapidly rotating trap only in the presence of a negative quadratic Zeeman splitting.

The ability to experimentally control the magnetisation of a spin-1 BEC therefore presents the intriguing possibility of creating composite topological defects in the laboratory. By imprinting a vortex state with a specified magnetisation, otherwise unstable topological defects may be studied experimentally.

For all vortex states and interaction regimes considered, sufficiently strong magnetisation leads to the depopulation of the $m_F = -1$ Zeeman level, resulting in a mixing of polar and FM phases. In this regime, the magnetisation dominates over spin-dependent interactions, and the BEC exhibits regions of FM phase even if the interactions would favour the polar phase. The strong magnetisation then leads to two stable vortex structures. The magnetisation may be carried by formation of the FM phase away from the vortex core, inside which the spin magnitude drops to zero and a nematic coreless vortex forms. This is the only mechanism which can stabilise the nematic coreless vortex in the polar regime. The resulting vortex structure is then similar to the stable, filled core of a singular FM vortex. In this two-component limit we also find stable an analogue of the FM coreless vortex but with the magnitude of the spin diminishing away from the vortex line.

Additionally, by identifying the stationary states of the spin-1 spinor dipolar BEC, we have demonstrated that the inclusion of a weak dipolar interaction in a spin-1 BEC does not modify the stability or structures of vortices. A strongly dipolar spinor condensate, however, adopts the properties of the FM regime regardless of the sign of the spin-dependent contact interaction. In a non-rotating condensate, the dipolar interaction can cause the spontaneous formation of a singular FM vortex which does not carry any circulation. However, the coreless vortex emerges as the only stationary single-vortex state with nonzero angular momentum, as the spin texture associated with an angular-momentum-carrying singular FM vortex is disfavoured by the dipolar interaction. The dipolar interaction is anisotropic and so the trap geometry has a non-negligible effect on the stable spin textures. However, we have found that the vortex phase diagram of a rotating dipolar condensate is approximately the same in an isotropic trap as that previously reported in a rotating oblate trap [185], with one modification. The isotropic
trap favours the formation of a FM coreless vortex with chiral spin texture in the polar interaction regime where in the oblate trap, a vortex sheet was found to form.

8.1 Future Work

The stability of composite topological defects presents a surprising and intriguing consequence of the conservation of magnetisation. While we have demonstrated the stability of several such composite defects, it is natural to ask whether a suitable combination of parameters may stabilise other composite defects.

The energetic stability of singular vortices in a non-dipolar spin-1 BEC has been demonstrated. However, only the stationary states have been studied in the dipolar condensate. It is natural to extend this work to a study of energetically stable vortices in a spinor dipolar BEC. By beginning with a stationary vortex state and conducting evolution in imaginary time, the convergence times of such studies will be greatly reduced. Additionally, one may then consider vortex dynamics in the spinor dipolar system and in particular how two or more vortices interact in the spinor dipolar system, via their associated spin textures.

The energetic stability of vortices in higher-spin systems may also be studied, although this requires solving a system of $2F + 1$ coupled GPEs for a spin-$F$ system. In a spin-2 condensate, the existence of three phases of the ground-state manifold opens up a rich phenomenology of possible core structures, which one may study numerically or by constructing analytical spinors, as we have for the spin-1 condensate in Sec. 6.2. However, since the spin-2 order parameter has 9 free parameters, any such analytical constructions will be extremely complex. The effects of conserved magnetisation can also be studied in the spin-2 system, although the five-component order parameter cannot be treated with our numerical algorithm for controlling the magnetisation explicitly. While one can induce a magnetisation via a linear Zeeman-type term in the spinor GPE, this does not predetermine or fix the magnetisation and so a trial-and-error approach must first be employed to determine the magnetisation induced by a given linear Zeeman splitting. In principle one could consider the simplified case of a spin-2 system with two spinor components emptied, such as in the experiment of Ref. [33]. However, the scattering processes of a spin-2 condensate may then populate the spinor components which are initially empty and so such a treatment would be tenuous.
Appendix A

Generating Pauli Matrices for Arbitrary F

In a BEC of spin-$F$ atoms, the spin operator $\hat{F}$ determines the local expectation value of the atomic spin, via

$$\langle \hat{F} \rangle = \zeta^* \delta_{\alpha \beta} \hat{F}_{\alpha \beta},$$  \hspace{1cm} (A.1)

where $\zeta$ is the normalised $2F + 1$-component spinor order parameter. $\hat{F}$ is the vector of Pauli matrices,

$$\hat{F} = \hat{F}_x \hat{x} + \hat{F}_y \hat{y} + \hat{F}_z \hat{z}. $$ \hspace{1cm} (A.2)

The three $(2F + 1) \times (2F + 1)$ Pauli matrices, familiar from undergraduate physics in the case of $F = 1/2$, satisfy the commutation relations

$$[\hat{F}_x, \hat{F}_y] = i \hat{F}_z,$$
$$[\hat{F}_y, \hat{F}_z] = i \hat{F}_x,$$
$$[\hat{F}_z, \hat{F}_x] = i \hat{F}_y.$$ \hspace{1cm} (A.3)

Additionally, the vector of Pauli matrices satisfies

$$\hat{F} \cdot \hat{F} = F(F + 1)I,$$ \hspace{1cm} (A.4)

where $I$ is the $(2F + 1) \times (2F + 1)$ identity matrix. In order to uniquely specify the three Pauli matrices, a third relationship is required. This third relationship arises naturally
from the choice of spinor basis:

\[
\begin{pmatrix}
F & 0 & 0 & \cdots & 0 & 0 \\
0 & F - 1 & 0 & \cdots & 0 & 0 \\
0 & 0 & F - 2 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 - F & 0 \\
0 & 0 & 0 & \cdots & 0 & -F
\end{pmatrix}
\]  

(A.5)

Operating with this on a spinor \( \vec{\zeta} \) simply returns the spinor with each component \( \zeta_i \) multiplied by its projection in the \( z \) direction, \( i \). This relationship is the reason that the spinor is written in terms of Zeeman levels rather than in terms of the cartesian components of the spin vector.

Given the definition of \( \hat{F}_z \) and the commutation relations, along with the modulus squared of the Pauli vector, one may then calculate the Pauli matrices for arbitrary \( F \).
Appendix B

Homotopy Groups and Homeomorphisms

In Chapter 3, topological defect structures are discussed in terms of the homotopy groups of the ground-state manifold. The homotopy groups of the ground-state manifold classify which topological defects may exist and whether they may be continuously deformed into one another. Here we briefly review the meaning of a homotopy group before demonstrating how the homotopy groups may be used to classify topological defects. In Chapter 3, the homotopy groups are presented in terms of groups to which they are homeomorphic. To clarify this discussion, we also briefly discuss the meaning of this. For further detail see Ref. [148] [in particular Chapters 1, 3 & 5] and Chapter 3.3 of Ref. [12].

The origin of the word *homeomorphic* stems from the Greek words *homoios*, meaning ‘similar’, and *morphe*, meaning ‘shape’. Two shapes are homeomorphic if there is a continuous mapping between the two, with a continuous inverse. For example, a square is homeomorphic to a circle. One might expect such shapes to be termed *homomorphic*, meaning ‘same shape’, but this term is reserved for shapes which are genuinely identical, as opposed to being related by some mapping. The mapping between homeomorphic shapes is called a homeomorphism. This concept will be used in the discussion of the different homotopy groups.

We now describe the construction of a homotopy group. For simplicity, we will discuss the formulation for the zeroth and first homotopy groups, before discussing the higher homotopy groups in a more generalised manner. We begin with the zeroth homotopy group or *fundamental group* of a manifold.

We consider two points $x$ and $y$ on a manifold $M$. If $x$ may be transformed into $y$ by a series of infinitesimal deformations, with the point remaining in $M$ at all intermediate stages of the deformation, then $x$ and $y$ are said to be in the same *conjugacy class*. 
That is to say, two points lie in the same conjugacy class if they may be connected by a continuous line on the manifold. If, however, \( x \) cannot be transformed into \( y \) by a series of infinitesimal, continuous deformations, then they are not in the same conjugacy class. Each conjugacy class of points on the manifold \( M \) is therefore a collection of points which may be continuously deformed into one another. The zeroth homotopy group of the manifold, \( \pi_0(M) \), is the group of conjugacy classes of points on the manifold. The zeroth homotopy group is trivial if all points on the manifold may be continuously deformed into one another, such as in the complex plane or on the surface of a sphere. The manifold is then said to be connected.

The definition of the first homotopy group is similar, with the points replaced with closed loops. We consider two closed loops \( A \) and \( B \). If there exist a series of continuous, infinitesimal deformations of \( A \) which will transform it into \( B \), with the loop remaining on the manifold at all intermediate stages of the deformation, then \( A \) and \( B \) are in the same conjugacy class of loops on the manifold. If \( A \) cannot be continuously deformed into \( B \) then they are in different conjugacy classes. The first homotopy group of the manifold, \( \pi_1(M) \), is then the group of conjugacy classes of loops on the manifold. The first homotopy group is trivial if all closed loops may be continuously deformed into one another, again such as in the complex plane or on the surface of a sphere. The manifold is then said to be simply connected.

Homotopy groups of higher order are analogously defined: the \( n^{th} \) homotopy group, \( \pi_n(M) \) is the group of conjugacy classes of closed \( n \)-dimensional surfaces on the manifold. If all closed \( n \)-dimensional surfaces may be continuously deformed into one another, the \( n^{th} \) homotopy group is trivial.

Rather than considering the specific conjugacy classes of the manifold \( M \), it is generally more useful to consider the group structure of the various homotopy groups. For example, the group \( \text{SO}(3) \) may be represented geometrically as the solid ball in 3 dimensions with antipodal points identified. Any loop which connects antipodal points an odd number of times, lies in the same conjugacy class as every other such loop. Any loop which connects antipodal points an even number of times lies in another conjugacy class. Therefore there are only two conjugacy classes. By considering how these loops add and subtract, one may then construct a group algebra for the conjugacy classes. With only two conjugacy classes this is simple but for most manifolds this is a nontrivial calculation. It is then insightful to identify a well-known group with the same number of elements and same algebra, in order to turn difficult problems involving large numbers of surfaces or an unintuitive number of dimensions, into problems well-studied in group theory. It is sufficient simply to show that there exists a homeomorphism between the relevant homotopy group and the representative group being invoked. In the case of \( \text{SO}(3) \) discussed here, the first homotopy group is homeomorphic to \( \mathbb{Z}_2 \).
Continuing with the example of closed loops, an intuitive picture emerges of how the homotopy groups classify the topological defects of the manifold \( M \). Suppose that we have two line defects in a 3D system. A loop enclosing one defect maps to a loop in order-parameter space. A loop enclosing the other defect also maps to a loop in order-parameter space. If the two loops in order-parameter space can be continuously deformed into one another (i.e. the loops are in the same conjugacy class), then the two defects are topologically the same. They correspond to the same group element of the first homotopy group. If the loops in order-parameter space cannot be continuously deformed into one another (the loops are in different conjugacy classes), the two defects correspond to different elements of the first homotopy group. Let us call these two loops \( A \) and \( B \) and consider the case where \( A \) and \( B \) both pass through a point \( y \). If we imagine a loop \( C \) which starts at \( y \), travels around \( A \) and returns to \( y \), then travels around \( B \), returning again to \( y \). This is a closed loop enclosing both defects. The conjugacy class of \( C \) is determined by the algebra of the first homotopy group: \( C = A + B \). This tells us the overall topology far from the location of the line defects. This large-distance topology must be preserved, but the local topology may change, for example as the system relaxes its energy or as two defects collide.
Appendix C

Basis Transformation for Singular FM Vortex

In the numerical simulations of Sec. 5.1 we found that the singular FM vortex relaxes to a stable configuration formed by non-overlapping vortex lines in the three spinor components, as shown in Fig. 5.4(a). By an appropriately chosen basis transformation we showed that this seemingly complex vortex structure can be identified as a single, singular vortex with the line singularity populated by atoms in the polar phase [Fig. 5.4(b)]. In this Appendix we demonstrate this basis transformation through a qualitative analytic treatment and show how the core structure of the singular FM vortex may be identified.

For simplicity, we implement the basis transformation by starting from the final configuration of the singular vortex with a single vortex line as in Figs. 5.4(b) and 5.6 and rotating to the configuration of non-overlapping vortex lines in the three spinor components [see, e.g. Fig. 5.4(a)]. The analytic expressions become notably simpler in the case of the axisymmetric vortex of Fig. 5.6 than the one displaying a more complex spin rotation in Figs. 5.4(b) and 5.4, but the basic principle of the transformation is the same in both cases. In order to describe the vortex of Fig. 5.6 we rewrite the singular vortex displaying a radial disgyration of the spin vector $\vec{\zeta}^{sv}$ of Eq. (3.13) in the following form

$$\vec{\zeta} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}(\cos \varphi - i \sin \varphi) \cos^2 \frac{\beta}{2} \\ \sin \beta \\ \sqrt{2}(\cos \varphi + i \sin \varphi) \sin^2 \frac{\beta}{2} \end{pmatrix}. \quad (C.1)$$

Here we have neglected the filling of the vortex core with polar phase. Although this is an important physical effect, it is not required to observe the splitting of the vortex lines in the rotated basis. For $\beta \neq \pi$ we obtain a radial spin disgyration and for $\beta = \pi$ and we recover a vortex with zero density at the singularity. For the numerically minimized
stable solution of Fig. 5.6 the parameter $\beta$ is not constant; close to the vortex core we have $\beta \simeq \pi/2$ and far away from the vortex $\beta \to \pi$.

When we perform the rotation of Eq. (C.1) by the angle $-\pi/2$ about the $y$ axis, we obtain the spinor wavefunction

$$\begin{pmatrix}
\cos \varphi - i \sin \varphi \cos \beta + \sin \beta \\
\sqrt{2} (- \cos \varphi \cos \beta + i \sin \varphi) \\
\cos \varphi - i \sin \varphi \cos \beta - \sin \beta
\end{pmatrix}. \tag{C.2}
$$

The spinor wavefunctions are of the form $(x - x_0) + i \eta(y - y_0)$, indicating that a singly quantised vortex line is located at $(x_0, y_0)$. The anisotropy of the vortex core is described by the parameter $\eta$. The singularity in $\zeta_0^{(-x)}$ is therefore on the $z$ axis, while those in $\zeta_\pm^{(-x)}$ are displaced to $(\mp x_0, y_0 = 0)$. Here $x_0$ is determined as the point at which $\sin \beta < 1$, in other words the position at which the spin begins to bend away from the $x$-$y$ plane. The vortex configuration of Eq. (C.2) with three spatially separated vortex lines is analogous to that shown in Fig. 5.4(a). The filling of the vortex core with the polar phase does modify the positions of $(x_0, y_0)$ but the qualitative behaviour is unchanged.
Appendix D

Phase-Matching in the Singular Polar Vortex

In the spin-1 BEC literature, there has been controversy as to the winding numbers associated with the singular vortex of the polar phase. Ref. [23] presented a vortex structure with broken axisymmetry, which we term here the A vortex. Subsequently, it was argued [19] that this result violated the phase-matching condition. A later study of singular polar vortices identified a seemingly different structure [21], though no analysis of the core structure was performed. We term this second vortex the B vortex. In this Appendix, we demonstrate that a suitable basis transformation shows the A and B vortices to be identical and that the A vortex obeys the phase-matching condition.

D.1 The A Vortex

The A vortex has densities and phase-windings in the $x$-$y$ plane as shown in Fig. D.1. They identified that with spin quantised in the $y$-direction ($y$-quantisation), the spinor may be expressed as

$$\zeta(y) \propto \begin{pmatrix} -e^{i\varphi} \\ 0 \\ x_1 + e^{i\varphi} \end{pmatrix},$$  \hspace{1cm} (D.1)

as shown in Fig. D.2, although in different notation. If one studies the winding number in the original basis, one might interpret this state as a $\langle 2, 1, 2 \rangle$ vortex, as the original authors did. However, such a classification clearly violates the phase-matching condition, leading to the assertion and therefore that this vortex state is not permissible [19]. However, by recognising that the winding structure is in fact of the form of two windings each of $\pi$ accompanied by a $\pi$ discontinuity of the phase, the correct classification is obtained. $\zeta_0$ also displays such a phase-winding structure but the $\pi$ discontinuity is on a soliton plane connecting the FM vortex cores and so the overall $2\pi$ phase-winding
Appendix D Phase-Matching in the Singular Polar Vortex

Figure D.1: Density (red: high density, blue: low density, logarithmic scale) and phase (red: $\phi \sim \pi$, blue: $\phi \sim -\pi$) in the A vortex in the initial basis.

Figure D.2: Density and phase for the A vortex in the rotated basis, for (left panels) $\zeta_+^{(y)}$ and (right panels) $\zeta_-^{(y)}$.

Figure D.3: Density and phase in the B vortex in the original basis.

is more clearly evident. In the rotated basis, the A vortex may be seen as a pair of half-quantum vortices, either by inspection of the spinor in Eq. (D.1), or by comparison of the densities and phases in Fig. D.2. Note that $\zeta_0^{(y)}$ is not plotted as its density is zero everywhere. In Eq. (D.1), the quantity $x_1$ denotes the separation between the half-quantum vortices.

D.2 The B Vortex

The B vortex is more explicit in preserving the winding number in each component. The vortex in $\zeta_0$ detaches from those in $\zeta_{\pm}$, as shown in Fig. D.3. Unlike the A vortex, there are no discontinuities in the phase. The vortices in $\zeta_{\pm}$ overlap perfectly. This deformation is precisely as seen in 2D [21], though we now expand upon this result by rotating the basis. In $y$-quantisation, one again clearly sees the pair of half-quantum vortices, as demonstrated by Fig. D.4, where again we have omitted the spin-zero component as it has zero density. The vortex lines in the spinor components in the initial basis become
asymmetric. They are in fact splitting into soliton planes, as the vortex in $\zeta_0$ does for the A vortex. Each soliton plane terminates on the boundaries of the FM half-quantum vortex cores.

The A and B vortices are both pairs of half-quantum vortices, though it is not clear from these arguments alone that they represent the same state. Sec. D.3 will demonstrate analytically this equivalence via basis transformation.

### D.3 Vortex Core Positions in Rotated Bases

Let us now apply a spin rotation to the A vortex. We rotate the spin through an angle $\gamma$ about the direction of the spin in one of the FM cores. The spin in the FM cores is therefore left invariant under this rotation, while the $\hat{d}$ texture is modified. $\hat{d}$ rotates through the angle $\gamma$ everywhere. The result is for the soliton planes in the three spinor components to be displaced from their initial positions as presented in the A vortex. The soliton plane position in $\zeta_0$ is plotted for varying $\gamma$ in Fig. D.5(a). Notice that for a particular range of $\gamma$, a structure similar to the B vortex is formed [cf. Fig. D.5(b)].

The key outcome of this analysis is that the A and B vortices are two instances of the same phenomenon, as opposed to being two separate vortex structures. The positions of the soliton planes and phase-windings in each component are determined entirely by the positions of the two half-quantum vortices and the radii of their FM cores.
Figure D.5: (a) Soliton plane positions in $\zeta_0$ as $\gamma$ is varied, where the soliton planes emerge from the centres of the two half-quantum vortices. (b) Positions of soliton planes (blue lines) in each spinor component for the A and B vortices. Dark grey regions represent the FM cores of the half-quantum vortices.
Appendix E

Energetic Stability and Core Deformation of a Half-Quantum Vortex

The half-quantum vortex has a singular core but is not in the same topological class as the singly-quantised vortex. However, its study does help to understand the results for the singly-quantised vortex and so we shall discuss it briefly in this Appendix. We numerically minimise the energy of an initial half-quantum vortex with polar interactions as in Chapter 5, such that the magnetisation is not conserved in the relaxation process. The prototypical half-quantum vortex spinor,

\[ \zeta = e^{i\frac{\phi}{2}} \begin{pmatrix} -e^{-i\frac{\phi}{2}} \\ 0 \\ e^{i\frac{\phi}{2}} \end{pmatrix}, \]  

(E.1)

shows intuitively that, as \( \zeta_+ \) displays no phase-winding behaviour, the core may fill with this spinor component, exhibiting the FM phase. In order to demonstrate this numerically, we first rotate the spinor basis by \( \alpha = \beta = \pi/2 \) to ensure nonzero populations of all three spinor components. We apply a \( \pi \) phase factor for convenience, producing the initial state for our numerics,

\[ \zeta = e^{i\frac{\phi}{2}} \begin{pmatrix} -\sin\frac{\phi}{2} \\ \sqrt{2} \cos\frac{\phi}{2} \\ \sin\frac{\phi}{2} \end{pmatrix}. \]  

(E.2)

Evolution in imaginary time results in a filling of the vortex core with atoms in the FM phase, with the spin vector \( \langle \hat{F} \rangle = \hat{y} \), as one might expect from the form of the spinor in the initial state. The edge of the condensate also exhibits nonzero spin antialigned
Appendix E Energetic Stability and Core Deformation of a Half-Quantum Vortex

Figure E.1: Stability of the half-quantum vortex in (a) the isotropic trap with $c_0 = 1000$ and (b) the oblate trap with $c_0 = 50$ in the absence of Zeeman splittings. Stability with respect to (c) linear and (d) quadratic Zeeman splittings in the oblate trap with $c_0 = 50$, $c_2 = 10$. (+) vortex exits cloud. (●) vortex stable. (×) nucleation of additional vortices. The half-quantum vortex is stable at slower rotation frequencies than the singly-quantised polar vortex, though the minimum rotation frequency now increases noticeably with increased $c_2$ (the stable region is approximately indicated by the shaded grey region). The stability of the half-quantum vortex is unaffected by linear Zeeman splittings but a positive quadratic Zeeman splitting does disrupt the stability. Note that panel (a) has a logarithmic scale in $c_2$ to enable a wider range of parameters to be studied than in the oblate trap.

We find that a positive quadratic Zeeman splitting has no effect on the stability of the half-quantum vortex, serving only to fix the orientation of the spin in the FM vortex core. Negative quadratic Zeeman splittings however, reduce the energy threshold for nucleating additional vortices while a positive quadratic Zeeman splitting $g_2 B_z^2/\hbar \omega_{\perp} \geq 0.4$ renders the half-quantum vortex unstable.
Appendix F

Construction of Defect Structures From Generalised Spinor

From Eq. (6.13) we can now construct spinor wavefunctions that describe how the wavefunction connects an outer vortex structure to a vortex-free core, as well as interpolating between the small- and large distance topology in the composite topological defects. We assume the two Euler angles $\alpha$ and $\gamma$, as well as the condensate phase $\phi$, to be half-integer multiples of the azimuthal angle $\varphi$ unless otherwise stated. These choices of parametrisation are the most general whilst ensuring the single-valuedness of the spinor order parameter. The Euler angle $\beta = \beta(\rho)$ and the spin magnitude $F = F(\rho)$ are taken to be a functions of the radial distance only. $F(\rho)$ then parametrises the interpolation between polar and FM vortices. This will enable us to describe not only core-deformed vortices such as those identified in Chapter 5 but also composite topological defects with distinct small- and large-distance topology.

F.1 Vortex Core Filling

For simplicity, we first construct the spinors representing the filling of the cores of singular vortices with non-circulating states, such as those identified in Chapter 5. These states are not solutions of the GPE but serve to illustrate the underlying physics of the filling of vortex cores. We begin with a singly-quantised polar vortex. The wavefunction must then reach the FM phase on the singularity of the polar order parameter. Consider the choice $\phi = \gamma = \varphi$ and $\alpha = 0$, with constant $\beta = \beta_0$. Eq. (6.13) then yields

$$\zeta = \frac{e^{i \varphi}}{\sqrt{2}} \begin{pmatrix} \sqrt{2} \left( e^{i \varphi} \sin^2 \frac{\beta_0}{2} f_- - e^{-i \varphi} \cos^2 \frac{\beta_0}{2} f_+ \right) \\ \sin \beta_0 \left( e^{i \varphi} f_- + e^{-i \varphi} f_+ \right) \\ \sqrt{2} \left( e^{i \varphi} \cos^2 \frac{\beta_0}{2} f_- - e^{-i \varphi} \sin^2 \frac{\beta_0}{2} f_+ \right) \end{pmatrix}, \quad (F.1)$$
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which reduces to Eq. (3.30) with \( \alpha = \varphi \) in the \( F = 0 \) limit, representing a singly-quantised polar vortex with a \( 2\pi \) winding in \( \hat{d} \). In the limit \( F = 1 \), on the other hand, Eq. (F.1) represents the vortex-free FM phase. By allowing \( F(\rho) \) to decrease monotonically from \( F(\rho \to 0) = 1 \) to \( F = 0 \), we find the spinor representing a polar vortex with a FM core.

We can confirm this interpretation by studying the superfluid circulation. A general expression for the superfluid velocity may be derived from Eq. (6.13) as

\[
\mathbf{v} = \frac{\hbar}{m \rho} (\nabla \phi - F \nabla \gamma - F \cos \beta \nabla \alpha).
\]

Since we here assume axial symmetry, we consider the mass circulation on a path at constant \( \rho \),

\[
\nu = \oint d\mathbf{r} \cdot \mathbf{v} = \frac{\hbar}{2m} (l - qF - pF \cos \beta),
\]

where in our construction \( l = 2d\phi/d\varphi \), \( p = 2d\gamma/d\varphi \), and \( q = 2d\alpha/d\varphi \) are integers. For the vortex (F.1), we then obtain \( \nu = h(1 - F)/m \), and we see that this interpolates smoothly between the non-circulating FM core (\( F = 1 \)) and the single quantum of circulation in the polar phase (\( F = 0 \)).

It follows from Eq. (3.25) that the polar phase also exhibits a half-quantum vortex, with half the circulation of the singly-quantised vortex (3.30). The half-quantum vortex is likewise singular, and its core may fill with the FM phase. This state is described by \( \phi = \varphi/2, \gamma = \pi + \varphi/2 \) and \( \alpha = 0 \) with constant \( \beta = \beta_0 \) to yield

\[
\zeta = \frac{e^{i\pi/2}}{2} \begin{pmatrix}
\sqrt{2} \left( e^{-i\pi/2} \cos^2 \frac{\beta_0}{2} f_+ - e^{i\pi/2} \sin^2 \frac{\beta_0}{2} f_- \right) \\
\sin \beta_0 \left( e^{-i\pi/2} f_+ + e^{i\pi/2} f_- \right) \\
\sqrt{2} \left( e^{-i\pi/2} \sin^2 \frac{\beta_0}{2} f_+ - e^{i\pi/2} \cos^2 \frac{\beta_0}{2} f_- \right)
\end{pmatrix}.
\]

When \( F = 0 \), this represents a half-quantum vortex with \( \hat{d} = -\cos \beta_0 \cos(\varphi/2) \hat{x} - \sin(\varphi/2) \hat{y} + \sin \beta_0 \cos(\varphi/2) \hat{z} \). The \( F = 1 \) limit is the vortex-free FM phase with \( \langle \hat{F} \rangle = \sin \beta_0 \hat{x} + \cos \beta_0 \hat{z} \). By allowing \( F(\rho) \) to increase monotonically with the radial distance from \( F = 1 \) and \( F = 0 \), the circulation, \( \nu = h(1 - F)/2m \) from Eq. (F.3), smoothly interpolates between the inner, non-circulating FM phase and the outer polar half-quantum vortex. This is the core structure of the half-quantum vortex studied numerically in Appendix E.

Inspection of Eq. (3.13), representing a singular FM vortex, shows that \( \zeta_0 \) is nonsingular everywhere. It can therefore fill the vortex core. Such a state would have \( F(\rho \to 0) = 0, \beta(\rho \to 0) = \pi/2 \). We now generalise this solution to a spinor that interpolates between an outer singular FM vortex and the inner polar phase. We choose \( \alpha = \varphi \) and \( \phi = 0 \).
with arbitrary $\gamma = \gamma_0$, yielding

$$
\vec{\zeta} = \frac{1}{2} \begin{pmatrix}
\sqrt{2}e^{-i\varphi} \left( e^{i\gamma_0} \sin^2 \frac{\beta(\rho)}{2} f_- - e^{-i\gamma_0} \cos^2 \frac{\beta(\rho)}{2} f_+ \right) \\
- \sin \beta(\rho) \left( e^{i\gamma_0} f_+ + e^{-i\gamma_0} f_- \right) \\
\sqrt{2}e^{i\varphi} \left( e^{i\gamma_0} \cos^2 \frac{\beta(\rho)}{2} f_- - e^{-i\gamma_0} \sin^2 \frac{\beta(\rho)}{2} f_+ \right)
\end{pmatrix}.
$$

(F.5)

In the $F = 0$ limit, the corresponding circulation $\nu = -\hbar F \cos \beta(\rho)/m$ vanishes, and the spinor represents a non-circulating polar condensate with $\hat{d} = \cos \beta(\rho) \hat{\rho} - \sin \beta(\rho) \hat{z}$ when $\gamma_0 = 0$. Note that this corresponds to the nematic coreless vortex (3.32) when $\beta(\rho)$ increases monotonically from $\pi/2$ at $\rho = 0$ so that $\hat{d}$ forms the fountain-like texture. In the $F = 1$ limit, Eq. (F.5) corresponds to the singular FM vortex with $\langle \hat{F} \rangle = \sin \beta(\rho) \hat{\rho} + \cos \beta(\rho) \hat{z}$ forming a radial disgyration when $\sin \beta(\rho) \neq 0$. The inner polar nematic vortex and the outer singular FM vortex are connected by requiring $F(\rho \to 0) = 0$ and $F = 1$ for large $\rho$. When the polar core forms the nematic coreless vortex, the $\beta(\rho)$ required to form the fountain texture in $\hat{d}$ causes $\langle \hat{F} \rangle$ to interpolate between a spin vortex at $\cos \beta(\rho) \to 0$ and a vortex carrying one quantum of mass circulation at $\cos \beta(\rho) \to 1$. Hence as $\beta(\rho)$ and $F(\rho)$ both increase with $\rho$, the wavefunction interpolates between the non-circulating nematic coreless vortex and the outer, circulation-carrying FM vortex. This spinor therefore describes the core-deformed singular vortex of Sec. 5.1.

F.2 Composite Topological Defects

Having constructed vortex states with non-circulating, filled cores, we now apply the same method to construct composite topological defects, which exhibit different small- and large-distance topology. We begin by constructing counter-intuitive defect structures based upon the familiar filled-core structures of Sec. F.1

**Singular polar vortex with vortex-free FM phase:** Notice that the construction of Eq. (F.1) does not depend on the assumption that the FM phase fills the core of the polar vortex. It therefore follows from Eq. (F.1) that it is also possible to construct a counter-intuitive vortex state where a singular polar vortex exists in an otherwise vortex-free FM condensate. The resulting singularity of the polar order parameter at $\rho = 0$ can be accommodated either by requiring the atom density to vanish there, or by forming an inner FM core. Thus the outer non-circulating polar phase exhibits a composite topological defect with a hierarchical core structure. An outer vortex core of the polar phase encloses an inner core of vortex-free FM phase.

**Polar half-quantum vortex with vortex-free FM phase:** Correspondingly, it is also possible to construct the nontrivial state where a polar half-quantum vortex exists inside a vortex-free FM condensate, forming a composite topological defect. Such a vortex would again exhibit an inner core of noncirculating FM phase enclosed by an outer core exhibiting
Appendix F Construction of Defect Structures From Generalised Spinor

the polar half-quantum vortex. Far from the vortex, the noncirculating FM phase is then restored.

**Singular FM vortex with nonsingular polar texture (nematic coreless vortex):** Just as it is possible to construct a spinor describing an outer, vortex-free FM phase exhibiting a composite topological defect, so we may also construct such a spinor with outer, non-circulating polar phase from Eq. \((F.5)\). If the spin \(F(\rho) \to 0\) far from the vortex line, the outer bulk consists of the non-circulating polar phase. Since a \(\hat{d}\) texture does not induce circulation, the polar bulk is not necessarily uniform, as was the case for the FM bulk. This non-circulating polar phase encloses a vortex with a composite core structure. The outer core exhibits the FM phase and the inner core again fills with the non-circulating polar phase.

**Singly-quantised polar vortex with FM coreless vortex:** Similarly to the nematic coreless vortex appearing as the core of a singular FM vortex, the coreless vortex \((3.17)\) may form the FM core of a singly-quantised polar vortex with a \(2\pi\) winding of \(\hat{d}\), represented by Eq. \((3.29)\) with \(b = 1\). We are then led to choose \(\phi = \alpha = \varphi, \gamma = \pi\) to produce

\[
\zeta = \frac{1}{2} \begin{pmatrix}
\sqrt{2} \left( \cos^2 \frac{\beta(\rho)}{2} f_+ - \sin^2 \frac{\beta(\rho)}{2} f_- \right) \\
e^{i\varphi} \sin \beta(\rho) \left( f_+ + f_- \right) \\
\sqrt{2} e^{i2\varphi} \left( \sin^2 \frac{\beta(\rho)}{2} f_+ - \cos^2 \frac{\beta(\rho)}{2} f_- \right)
\end{pmatrix}.
\]

\[(F.6)\]

In the limit \(F = 1\), this represents the coreless vortex when \(\beta(\rho)\) increases monotonically from zero at \(\rho = 0\). In the \(F = 0\) limit, Eq. \((F.6)\) represents a singly-quantised polar vortex with \(\hat{d} = -\cos \beta(\rho) \hat{\rho} + \sin \beta(\rho) \hat{z}\), displaying a radial disgyration for \(\cos \beta(\rho) \neq 0\). The composite vortex is formed as \(F(\rho)\) decreases monotonically from \(F(\rho \to 0) = 1\) to \(F = 0\) at large \(\rho\). Then also the circulation \(\nu = h \left(1 - F \cos \beta(\rho)\right)/m\) interpolates smoothly between the non-quantised circulation in the inner coreless vortex to the single quantum of circulation in the outer polar vortex. By again allowing the spin to increase in the outer bulk, such that the FM coreless vortex is restored at large \(\rho\), a composite topological defect may once more be constructed, with the large-distance topology of the FM coreless vortex and the small-distance topology of a singly-quantised polar vortex.

**Half-quantum vortex with FM coreless vortex:** Given that the FM coreless vortex \((3.17)\) can form inside the core of a singly-quantised polar vortex, we ask whether it can also form the core of a polar half-quantum vortex. Indeed, such a state can be described by \(\phi = -\gamma = \varphi/2\) and \(\alpha = \varphi\), yielding

\[
\zeta = \frac{e^{i\frac{\varphi}{2}}}{2} \begin{pmatrix}
\sqrt{2} \left( e^{-i\frac{\varphi}{2}} \sin^2 \frac{\beta(\rho)}{2} f_- - e^{-i\frac{\varphi}{2}} \cos^2 \frac{\beta(\rho)}{2} f_+ \right) \\
- \sin \beta(\rho) \left( e^{-i\frac{\varphi}{2}} f_- + e^{i\frac{\varphi}{2}} f_+ \right) \\
\sqrt{2} \left( e^{i\frac{\varphi}{2}} \cos^2 \frac{\beta(\rho)}{2} f_- - e^{i\frac{\varphi}{2}} \sin^2 \frac{\beta(\rho)}{2} f_+ \right)
\end{pmatrix}.
\]

\[(F.7)\]
The $F = 1$ limit corresponds to the coreless vortex (3.17). The fountain-like spin texture is formed by $\beta(\rho)$ increasing monotonically from $\beta(\rho = 0) = 0$. In the $F = 0$ limit, Eq. (F.7) represents a half-quantum vortex, as the condensate phase winds by $\pi$ as the vortex line is encircled. However, compared with Eq. (3.25), the corresponding winding of $\hat{d}$ to keep the wavefunction single-valued now acquires a nontrivial dependence on $\beta$:

$$
\hat{d} = \left( \cos \varphi \cos \beta(\rho) \cos \frac{\varphi}{2} + \sin \varphi \sin \frac{\varphi}{2} \right) \hat{x} \\
+ \left( \sin \varphi \cos \beta(\rho) \cos \frac{\varphi}{2} - \cos \varphi \sin \frac{\varphi}{2} \right) \hat{y} \\
- \sin \beta(\rho) \cos \frac{\varphi}{2} \hat{z}.
$$

Equation (F.8)

At $\beta = 0$, $\hat{d}$ stays in the $x$-$y$ plane, and the windings of $\alpha$ and $\gamma$ combine into a $\pi$ winding of $\hat{d}$ around the vortex line. On the other hand, when $\beta = \pi$, the change of sign in the first terms of $d_x$ and $d_y$ means that $\alpha$ and $\gamma$ instead combine into a $3\pi$ winding of $\hat{d}$. Since in the polar phase the winding of $\hat{d}$ does not affect the circulation, these two limits represent topologically equivalent vortices, and $\beta(\rho)$ provides a continuous parametrisation between them.

Since the $F = 0$ limit of Eq. (F.7) thus always represents a half-quantum vortex, the composite vortex formed by $F$ decreasing monotonically from $F(\rho = 0) = 1$, and $\beta$ simultaneously increasing monotonically from $\beta(\rho = 0) = 0$, smoothly connects the inner coreless vortex with an outer polar half-quantum vortex. The circulation $\nu = h \left[ 1 + F - 2F \cos \beta(\rho) \right] / 2m$ correspondingly interpolates from the non-quantised circulation of the coreless vortex to the half quantum of circulation of the large-distance polar vortex.

**FM coreless vortex with nonsingular nematic texture:** In addition to a nonsingular texture forming a composite topological defect with a singular vortex from the opposite phase, it is also possible to form a composite nonsingular vortex, with the FM coreless vortex (3.17) enclosed by a non-circulating outer polar region. The fountain texture of the coreless vortex then again gives rise to a nontrivial texture in $\hat{d}$. The state can be constructed using $\alpha = -\gamma = \varphi$ and $\phi = 0$, yielding

$$
\zeta = \frac{1}{2} \left( \begin{array}{c}
\sqrt{2} \left( e^{-i2\varphi} \sin^2 \frac{\beta(\rho)}{2} f_- - \cos^2 \frac{\beta(\rho)}{2} f_+ \right) \\
- \sin \beta(\rho) \left( e^{-i\varphi} f_- + e^{i\varphi} f_+ \right) \\
\sqrt{2} \left( \cos^2 \frac{\beta(\rho)}{2} f_- - e^{i2\varphi} \sin^2 \frac{2\beta(\rho)}{2} f_+ \right)
\end{array} \right).
$$

Equation (F.9)

In the $F = 1$ limit, this corresponds to the coreless vortex. The $F = 0$ limit exhibits a $\hat{d}$ texture,

$$
\hat{d} = \left( \cos \beta(\rho) \cos^2 \varphi + \sin^2 \varphi \right) \hat{x} \\
+ \left( \cos \beta(\rho) - 1 \right) \sin \varphi \cos \varphi \hat{y} \\
- \sin \beta(\rho) \cos \varphi \hat{z},
$$

Equation (F.10)
that is nonsingular if $\beta(\rho \to 0) = 0$. Similar to Eq. (F.8), the windings of $\alpha$ and $\gamma$ combine nontrivially depending on $\beta$. At $\beta = 0$ the texture is uniform $\mathbf{d} = \hat{x}$, while at $\beta = \pi$, $\mathbf{d} = -\cos(2\varphi)\hat{x} - \sin(2\varphi)\hat{y}$, corresponding to a $4\pi$ winding on a loop around the vortex line. The two textures are topologically equivalent, and $\beta$ thus provides a parametrisation between them in terms of purely local spin rotations.

Since both textures are nonsingular for $\beta(\rho = 0) = 0$, we thus describe this as a composite texture, rather than a composite topological defect. Letting $F(\rho)$ smoothly decrease from $F(\rho \to 0) = 1$ to $F(\rho) = 0$, a FM coreless vortex may be constructed by having $\beta(\rho)$ increase monotonically from 0 at $\rho = 0$. The circulation $\nu = hF(1 - \cos(\beta(\rho))) / m$ then vanishes at the centre of the trap, increasing in the region with $F > 0$ due to the bending of $\beta(\rho)$. The circulation then drops back to zero in the outer polar region. This should be contrasted with the coreless vortex inside the core of a singular polar vortex, in which the outer, polar region carries a nonzero circulation. The difference comes from having a winding of $\gamma$ rather than $\phi$: In the FM phase, only the combined Euler angle $\phi' = \phi - \gamma$ plays a role and so the negative winding in $\gamma$ has the same effect as a winding in $\phi$. However, in the polar phase, $\phi$ and $\gamma$ are distinct and only a winding in $\phi$ gives rise to a circulation.

By changing the profile of $F(\rho)$ such that $F(\rho \to 0) = 0$ and $F(\rho) = 1$ for large $\rho$, a non-circulating inner region of polar phase may then be enclosed by an outer FM coreless vortex. The circulation then again vanishes in the inner, polar region, interpolating to the non-quantised circulation of the outer FM coreless vortex.

**Singular FM vortex with singly-quantised polar vortex:** It is also possible to construct composite topological defects where both the inner and outer vortices are singular (leaving open the question of the core structure of the inner singular vortex). The simplest example to construct is that of a singular FM vortex [Eq. (3.12)], forming the core of the singly-quantised polar vortex [Eq. (3.30)], or vice versa. We construct the corresponding spinor by setting $\phi = \varphi$ and $\alpha = 0$. For any constant $\gamma = \gamma_0$ and $\beta = \beta_0$, we then have

\[
\zeta = \frac{e^{i\varphi}}{2} \begin{pmatrix}
\sqrt{2} \left( e^{i\gamma_0} \sin^2 \frac{\beta_0}{2} f_- - e^{-i\gamma_0} \cos^2 \frac{\beta_0}{2} f_+ \right) \\
- \sin \beta_0 \left( e^{i\gamma_0} f_- + e^{-i\gamma_0} f_+ \right) \\
\sqrt{2} \left( e^{i\gamma_0} \cos^2 \frac{\beta_0}{2} f_- - e^{-i\gamma_0} \sin^2 \frac{\beta_0}{2} f_+ \right)
\end{pmatrix},
\]

with circulation $\nu = h/m$. This vortex is singular for all values of $F$ and $\beta$, such that the singularity cannot be avoided by judicious choice of parameters. In the $F = 1$ limit then, Eq. (F.11) describes a singular FM vortex, with uniform spin texture $\langle \hat{F} \rangle = \sin \beta_0 \hat{x} + \cos \beta_0 \hat{z}$. The $F = 0$ limit similarly corresponds to a singular polar vortex with uniform $\mathbf{d} = \cos \beta_0 \cos \gamma_0 \hat{x} + \sin \gamma_0 \hat{y} - \sin \beta_0 \cos \gamma_0 \hat{z}$. A wavefunction that continuously interpolates between the two singular vortices is then constructed by taking $F(\rho)$ to vary monotonically between $F = 0$ and $F = 1$. The boundary condition on $F(\rho)$ away from the vortex line determines the large-distance topology.
Appendix F Construction of Defect Structures From Generalised Spinor

Singular FM vortex with polar half-quantum vortex: Just as the singly-quantised polar vortex may form inside the core of a singular FM vortex (or vice-versa), a polar half-quantum vortex may form inside the singular FM vortex core (and vice versa). Here we construct an explicit spinor for this composite vortex state by requiring \( \phi = -\gamma = \varphi/2 \) and \( \alpha = 0 \). Taking constant \( \beta = \beta_0 \), Eq. (6.13) then becomes

\[
\zeta = \frac{e^{i\varphi}}{2} \begin{pmatrix}
\sqrt{2} \left( e^{-i\varphi} \sin^2 \frac{\beta_0}{2} f_+ - e^{i\varphi} \cos^2 \frac{\beta_0}{2} f_- \right) \\
- \sin \beta_0 \left( e^{-i\varphi} f_- + e^{i\varphi} f_+ \right) \\
\sqrt{2} \left( e^{-i\varphi} \cos^2 \frac{\beta_0}{2} f_- + e^{i\varphi} \sin^2 \frac{\beta_0}{2} f_+ \right)
\end{pmatrix}.
\]  

(F.12)

In the \( F = 1 \) limit we recover the singular FM vortex (3.12) with uniform spin profile \( \langle \mathbf{F} \rangle = \sin \beta_0 \mathbf{x} + \cos \beta_0 \mathbf{z} \). The \( F = 0 \) limit, on the other hand, is a half-quantum vortex with \( \hat{\mathbf{d}} = \cos \beta_0 \cos(\varphi/2)\hat{\mathbf{x}} - \sin(\varphi/2)\hat{\mathbf{y}} - \sin \beta_0 \cos(\varphi/2)\hat{\mathbf{z}} \) exhibiting the characteristic \( \pi \) winding as the vortex line is encircled. Hence, the half-quantum vortex forms the core of the FM singular vortex when \( F(\rho) \) increases from \( F = 0 \) to \( F = 1 \) with the radial distance. Correspondingly, the circulation \( \nu = h(1+F)/2m \) interpolates smoothly between the inner half-quantum of circulation and the outer singly-quantised FM vortex.

The FM order parameter also allows the formation of a singular vortex on the form of Eq. (3.13), which is topologically equivalent to Eq. (3.12), and the one may be deformed into the other by local spin rotations. We should therefore expect also the core of Eq. (3.13) to be able to host a polar half-quantum vortex. We find an expression for this composite vortex state by taking \( \phi = \gamma = \varphi/2, \alpha = \varphi \). Then

\[
\zeta = \frac{e^{i\varphi}}{2} \begin{pmatrix}
\sqrt{2} \left( e^{-i\varphi} \sin^2 \frac{\beta(\rho)}{2} f_+ - e^{i\varphi} \cos^2 \frac{\beta(\rho)}{2} f_- \right) \\
- \sin \beta(\rho) \left( e^{i\varphi} f_- + e^{-i\varphi} f_+ \right) \\
\sqrt{2} \left( e^{i\varphi} \cos^2 \frac{\beta(\rho)}{2} f_- + e^{-i\varphi} \sin^2 \frac{\beta(\rho)}{2} f_+ \right)
\end{pmatrix},
\]  

(F.13)

The \( F = 1 \) limit represents the FM singular vortex (3.13), exhibiting the radial spin disgyration \( \langle \mathbf{F} \rangle = \sin \beta(\rho)\hat{\mathbf{r}} + \cos \beta(\rho)\hat{\mathbf{z}} \), by construction. The angle \( \beta(\rho) \) increases from \( \pi/2 \) to \( \pi \) as a function of radius. In the \( F = 0 \) limit, this spinor does indeed represent a half-quantum vortex with \( \phi \) winding by \( \pi \). As in Eqs. (F.8) & (F.10), the winding of \( \hat{\mathbf{d}} \) depends on \( \beta \), resulting in a nematic axis profile of \( \hat{\mathbf{d}} = (\cos \varphi \cos \varphi/2 \cos \beta(\rho) - \sin \varphi \sin \varphi/2)\hat{\mathbf{x}} + (\sin \varphi \cos \varphi/2 \cos \beta(\rho) + \cos \varphi \sin \varphi/2)\hat{\mathbf{y}} - \cos \varphi/2 \sin \beta(\rho)\hat{\mathbf{z}} \). Again the composite defect is formed as \( F(\rho) \) is allowed to vary such that \( F(\rho \to 0) = 0 \) and \( F(\rho) = 1 \) at large \( \rho \), and the circulation \( \nu = h(1 - F - 2F \cos \beta(\rho))/2m \) interpolates from the inner half-quantum vortex of the polar phase to the non-quantised circulation of the outer radial spin disgyration.
Appendix G

Glossary

Coreless vortex - a vortex with no singular vortex core.

Disgyration - planar profile of a vector $\mathbf{v}$ such that $\mathbf{v}$ rotates by $2\pi$ in the plane. For example the radial disgyration, where $\mathbf{v}$ everywhere points towards (or away from) a singular point, similar to the electric field generated by a charged particle.

Energetic stability - a state which represents a local minimum of the energy functional is energetically stable as energy must be added to the system in order for the state to decay or dissipate.

Ground-state manifold - the group of physically distinguishable states which minimise the energy functional.

Homeomorphic - two manifolds are homeomorphic if there is a continuous mapping between them with a continuous inverse.

Homotopic - two shapes are homotopic if they can be continuously deformed into one another.

Homotopy group - the $n^{th}$ homotopy group of the manifold $M$ classifies how many distinct classes of $n$-dimensional surfaces may be constructed on $M$, where all surfaces within a single class are homotopic to one another.

Nematic axis - a unit vector, $\hat{d}$, which identifies $\hat{d} \leftrightarrow -\hat{d}$ and is hence unoriented.

Order parameter - a mapping from real space to the ground-state manifold.

Order-parameter space - another name for the ground-state manifold.
Skyrmion - a specific texture which maps from $S^3$ in real space to $S^3$ in the ground-state manifold.

Texture - a nonsingular, nonuniform profile of the order parameter, where the order parameter takes the same value at all points on the boundary of the medium under study, such that the edge of the medium may be treated as a point.

Topological defect - a point, line, surface or hypersurface on which the order parameter is singular.
References


REFERENCES


