Chapter 6
p-Wave Superconductivity and d-Vector Representation

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Abstract Since the mid-80s, new classes of superconductors have been discovered in which the origin of superconductivity cannot be attributed to the electron–ion interactions at the heart of conventional superconductivity. Most of these unconventional superconductors are strongly correlated electron systems, and identifying (or even more difficult, predicting) the precise superconducting state has been, and sometimes remains, an actual challenge. However, in most cases, it has been demonstrated that in these materials the spin state of the Cooper pairs is a singlet state, often associated with a 'd-wave' or '$s+/-$' orbital state. For a few systems, a spin-triplet state is strongly suspected, like in superfluid ^{3}He; this leads to a much more complex superconducting order parameter. This was long supposed to be the case for the d-electron system Sr_2RuO_4, and is very likely realized in some uranium-based (f-electron) 'heavy fermions' like UPt_3 (with multiple superconducting phases) or UGe_2 (with coexisting ferromagnetic order). Beyond the interest for these materials, p-wave superconductivity is presently quite fashionable for its topological properties and the prediction that it could host Majorana-like low energy excitations, seen as a route towards robust (topologically protected) qubits. The aim of these notes is to make students and experimentalists more familiar with the **d**-vector representation used to describe p-wave (spin triplet) superconductivity. The interest of this formalism will be illustrated on some systems where p-wave superconductivity is the prime suspect.

6.1 Introduction

The purpose of these notes is only to cover some aspects of spin-triplet superconductors, not so commonly covered in the excellent textbooks available on superconductivity, in general, and unconventional superconductors, in particular. Among

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those, let us choose to quote only two: the seminal Reviews of Modern Physics paper "A theoretical description of the new phases of liquid ^{3}He" by A. J. Leggett [1], which gives both very advanced and detailed insights on the theory of the p-wave order parameter of superfluid ^{3}He, and pedagogical and enlightening treatment of the microscopic Bardeen–Cooper–Schrieffer (BCS) theory of anisotropic superconductors and the other, which covers the very important symmetry aspects of unconventional superconductors in crystalline materials, is the book 'Introduction to unconventional superconductivity' by V. P. Mineev and K. V. Samokhin [2].

In the following, we concentrate on some basic aspects of the description of spin-triplet superconductors, which are often bewildering, at least to experimentalists.

6.2 Odd-Parity Pairing: BCS Wave Function and Order Parameter

Most known superconductors are 'spin-singlet' superconductors, meaning that the relative wave function of the Cooper pairs $|\Psi(\mathbf{r_1}-\mathbf{r_2})\rangle$, in the real or in the reciprocal space, can be written as a product of an orbital wave function and a spin (singlet) wave function

$$\begin{aligned} |\Psi(\mathbf{r_1}-\mathbf{r_2})\rangle &= \phi(\mathbf{r_1}-\mathbf{r_2})|\uparrow\downarrow-\downarrow\uparrow\rangle\,, \\ |\Psi(\mathbf{k})\rangle &= \varphi(\mathbf{k})|\uparrow\downarrow-\downarrow\uparrow\rangle\,. \end{aligned} \tag{6.1}$$

Antisymmetrization of the total pair wave function imposes, for such a singlet state, that the orbital wave function verifies $\phi(\mathbf{r_1}-\mathbf{r_2})=\phi(\mathbf{r_2}-\mathbf{r_1})$ or $\varphi(\mathbf{k})=\varphi(-\mathbf{k})$ (even-parity state). However, it is also possible to build Cooper pairs in a triplet spin state (see Fig. 6.1). If all electronic interactions including the pairing interactions conserve spin, one could pair separately up- and down-spins, and the total superconducting wave function with a triplet spin state would be the (antisymmetrized) product of both. However, if any non-spin conserving term exists, like the spin–orbit interaction, this is no longer possible. One can just say that Cooper pairs will be formed with a wave function of the form

$$|\Psi\rangle=\phi_{11}(\mathbf{r_1}-\mathbf{r_2})|\uparrow\uparrow\rangle+\phi_{22}(\mathbf{r_1}-\mathbf{r_2})|\downarrow\downarrow\rangle+\phi_{12}(\mathbf{r_1}-\mathbf{r_2})|\uparrow\downarrow+\downarrow\uparrow\rangle\,, \tag{6.2}$$

or in the reciprocal space

$$|\Psi\rangle=\varphi_{11}(\mathbf{k})|\uparrow\uparrow\rangle+\varphi_{22}(\mathbf{k})|\downarrow\downarrow\rangle+\varphi_{12}(\mathbf{k})|\uparrow\downarrow+\downarrow\uparrow\rangle\,. \tag{6.3}$$

Antisymmetrization of the total pair wave function imposes this time that the orbital wave function $\phi(\mathbf{r_1}-\mathbf{r_2})=-\phi(\mathbf{r_2}-\mathbf{r_1})$ or $\varphi(\mathbf{k})=-\varphi(-\mathbf{k})$ (odd-parity state). Note that microscopically, one would write the ground state superconducting wave function for the whole Fermi sea as

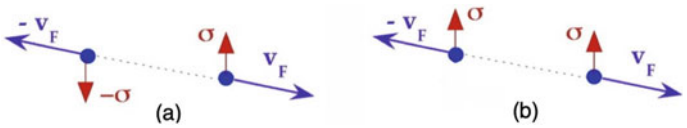

Fig. 6.1 Singlet **a** versus triplet **b** Cooper pairs: they are built with quasiparticles of opposite wave vectors in both cases, but differ by their spin state

$$|\Psi\rangle = \prod_{all\ \mathbf{k}} (u_{\mathbf{k}\uparrow\uparrow} + v_{\mathbf{k}\uparrow\uparrow} c^{+}_{\mathbf{k}\uparrow} c^{+}_{-\mathbf{k}\uparrow})(u_{\mathbf{k}\downarrow\downarrow} + v_{\mathbf{k}\downarrow\downarrow} c^{+}_{\mathbf{k}\downarrow} c^{+}_{-\mathbf{k}\downarrow})(u_{\mathbf{k}\uparrow\downarrow} + v_{\mathbf{k}\uparrow\downarrow} c^{+}_{\mathbf{k}\uparrow} c^{+}_{-\mathbf{k}\downarrow})|0>$$
$$= \prod_{all\ \mathbf{k},\alpha,\beta} (u_{\mathbf{k},\alpha\beta} + v_{\mathbf{k},\alpha\beta} c^{+}_{\mathbf{k}\alpha} c^{+}_{-\mathbf{k}\beta})|0> \tag{6.4}$$

with $u_{\mathbf{k},\alpha\beta} = u_{-\mathbf{k},\alpha\beta}$; $v_{\mathbf{k},\alpha\beta} = -v_{-\mathbf{k},\alpha\beta}$,

and $\varphi_{\alpha\beta}(\mathbf{k}) = \langle c_{-\mathbf{k}\beta} c_{\mathbf{k}\alpha} \rangle = u^{*}_{\mathbf{k}\alpha\beta} v_{\mathbf{k}\alpha\beta} = -\varphi_{\alpha\beta}(-k)$ the order parameter [1] .

The last condition on the parity of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ for the same spin indices ensures that the orbital part is odd (for the exchange of $\mathbf{k}$ and $-\mathbf{k}$), selecting only triplet spin components. Coming back to the order parameter, in the reciprocal space, it should be given by three complex odd functions of $\mathbf{k}$: φ_{11}, φ_{22} and $\varphi_{12} = \varphi_{21}$. The most natural would be to view the order parameter as a 2×2 symmetrical matrix $\varphi_{\alpha\beta}$, where α and β are spin indices ($1 = \uparrow$, $2 = \downarrow$). This is possible, and is used in many calculations. However, it is not very convenient if one needs to change the quantization axis or if (as it commonly happens) the quantization axis changes over the Fermi surface. There are only three independent complex functions of $\mathbf{k}$, so it would be nice to represent the order parameter by a vector.

6.3 Vectors and Cayley–Klein Representation

6.3.1 Position of the Problem

However, this would be meaningful only if this vector transforms properly under rotation of the spin quantization axis. And one would also expect its magnitude to be proportional to the density of condensed Cooper pairs, and its direction to have a meaning relative to the spin orientation. This last point is clearly not so direct, as the vector will necessarily be complex. In order to understand more clearly what is necessary, let us first explore what doesn't work. We could build simply such a vector representation through:

$$\mathbf{V} = \varphi_{11}\mathbf{e_x} + \varphi_{22}\mathbf{e_y} + \varphi_{12}\mathbf{e_z} \ . \tag{6.5}$$

But it would not do the job: the module would be fine, but the direction of $\mathbf{V}$ and so its transformation under rotations of the axis would be meaningless, for example, for the same quantization axis a pure $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ state would lead to perpendicular vectors. Or equivalently, taking an opposite direction of the quantization axis would yield perpendicular vector representations. This is clearly not what is expected from a vector behaviour. The problem stems from the fact that one needs to make a link between the spin state [SU(2)] and three-dimensional vectors. The good news is that this problem has been solved long ago in classical mechanics, with the Cayley–Klein representation, which aimed at simplifying the calculation of rotation effects; in real space, a matrix rotation is a 3×3 matrix; however, it is fully characterized by only three angles (the Euler angles for example); so, in principle, a 2×2 matrix, with four parameters, should be more than enough. The Cayley–Klein representation associates a three-dimensional vector ($\mathbf{a}$) to a 2×2 matrix through … Pauli matrices

$$
\begin{aligned}
&\mathbf{a} \rightarrow \mathbf{a}\cdot\boldsymbol{\sigma} \ , \\
&\boldsymbol{\sigma} = \sigma_1 \mathbf{e_x} + \sigma_2 \mathbf{e_y} + \sigma_3 \mathbf{e_z} \ , \\
&\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ , \\
&\sigma_i = \begin{pmatrix} \delta_{3i} & \delta_{1i} - \mathrm{i}\delta_{2i} \\ \delta_{1i} + \mathrm{i}\delta_{2i} & -\delta_{3i} \end{pmatrix} \quad \mathbf{a}\cdot\boldsymbol{\sigma} = a_i \sigma_i = \begin{pmatrix} a_3 & a_1 - \mathrm{i}a_2 \\ a_1 + \mathrm{i}a_2 & -a_3 \end{pmatrix} \ ,
\end{aligned}
\tag{6.6}
$$

where δ_{ij} is the Kronecker symbol.

6.3.2 *Useful Formula for Pauli Matrices*

As a reminder, for these (Hermitian) Pauli matrices

$$
\begin{aligned}
\sigma_i^2 = \mathbb{1} \quad ; \quad [\sigma_i, \sigma_j] = 2\mathrm{i}\,\epsilon^{ijk}\sigma_k \quad ; \quad \{\sigma_i, \sigma_j\} = 2\,\delta_{ij}\mathbb{1} \ , \\
\sigma_i \sigma_j = \mathrm{i}\epsilon^{ijk}\sigma_k + \delta_{ij}\mathbb{1} \ , \\
\mathrm{tr}(\sigma_i) = 0; \quad \det(\sigma_i) = -1; \quad \text{eigenvalues} = \pm 1 \ ,
\end{aligned}
\tag{6.7}
$$

where ϵ^{ijk} is the Levi-Civita symbol.

From that, a little algebra leads to very useful formulae ($\mathbf{a}$ and $\mathbf{b}$ are real or complex 3D vectors)

$$
(\mathbf{a}\cdot\boldsymbol{\sigma})\sigma_k = (a_i\sigma_i)\sigma_k = a_i\epsilon^{ikj}\mathrm{i}\sigma_j + a_i\delta_{ik}\mathbb{1} = -\mathrm{i}\epsilon^{kij}a_i\sigma_j + a_k\mathbb{1} \ .
$$

So

$$\boxed{\begin{array}{l}(\mathbf{a}\cdot\boldsymbol{\sigma})\boldsymbol{\sigma} = \mathbf{a}\mathbb{1} - \mathrm{i}\mathbf{a}\wedge\boldsymbol{\sigma} \quad ; \quad \boldsymbol{\sigma}(\mathbf{a}\cdot\boldsymbol{\sigma}) = \mathbf{a}\mathbb{1} + \mathrm{i}\mathbf{a}\wedge\boldsymbol{\sigma}\ ; \\ tr((\mathbf{a}\cdot\boldsymbol{\sigma})\boldsymbol{\sigma}) = 2\,\mathbf{a}\ ; \\ (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = (\mathbf{a}\cdot\mathbf{b})\mathbb{1} + \mathrm{i}(\mathbf{a}\wedge\mathbf{b})\cdot\boldsymbol{\sigma}\ .\end{array}} \tag{6.8}$$

Finally, if $\mathbf{a}$ is real, or if at least one can write $\mathbf{a} = a\cdot\hat{\mathbf{a}}$, with a, a complex number, and $\hat{\mathbf{a}}$, a real unit vector, then additional useful relations exist

- the eigenvalues of $\mathbf{a}\cdot\boldsymbol{\sigma}$ are $\pm a$;
- the projectors on each eigenspace can be written as $\frac{1}{2}\left(\mathbb{1}\pm\hat{\mathbf{a}}\cdot\boldsymbol{\sigma}\right)$;
- for any analytic function $f\,(\mathbf{a}\cdot\boldsymbol{\sigma}) = \frac{f(a)}{2}\left(\mathbb{1}+\hat{\mathbf{a}}\cdot\boldsymbol{\sigma}\right) + \frac{f(-a)}{2}\left(\mathbb{1}-\hat{\mathbf{a}}\cdot\boldsymbol{\sigma}\right)$ and
- in particular, if $\boldsymbol{\Omega}$ is a real vector, also written as $\boldsymbol{\Omega} = \Omega\,\hat{\boldsymbol{\Omega}}$, Ω, a real number, and $\hat{\boldsymbol{\Omega}}$, a real unit vector

$$\begin{array}{l}\exp(\mathrm{i}\boldsymbol{\Omega}\cdot\boldsymbol{\sigma}) = \dfrac{\exp(\mathrm{i}\Omega)+\exp(-\mathrm{i}\Omega)}{2}\mathbb{1} + \mathrm{i}\dfrac{\exp(\mathrm{i}\Omega)-\exp(-\mathrm{i}\Omega)}{2\mathrm{i}}\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}\ , \\ \boxed{\exp(\mathrm{i}\boldsymbol{\Omega}\cdot\boldsymbol{\sigma}) = \cos\Omega\,\mathbb{1} + \mathrm{i}\sin\Omega\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}}\ .\end{array} \tag{6.9}$$

6.3.3 Rotation of a 3D Vector: Cayley–Klein Relation

From these relations, it is straightforward to see (proof at the end of the chapter) that if $\mathcal{R}$ is a 3D rotation characterized by an angle Ω around the axis $\hat{\boldsymbol{\Omega}}$, for any vector $\mathbf{a}$

$$\begin{array}{l}\mathcal{R}(\mathbf{a})\cdot\boldsymbol{\sigma} = \exp(-\mathrm{i}/2\boldsymbol{\Omega}\cdot\boldsymbol{\sigma})\,(\mathbf{a}\cdot\boldsymbol{\sigma})\exp(\mathrm{i}/2\boldsymbol{\Omega}\cdot\boldsymbol{\sigma})\ , \\ \boxed{\mathcal{R}(\mathbf{a})\cdot\boldsymbol{\sigma} = \mathcal{R}_{\boldsymbol{\Omega}}\,(\mathbf{a}\cdot\boldsymbol{\sigma})\,\mathcal{R}_{-\boldsymbol{\Omega}}}\ ,\end{array} \tag{6.10}$$

where $\mathcal{R}_{\boldsymbol{\Omega}} = \exp\left(\frac{-\mathrm{i}}{2}\boldsymbol{\Omega}\cdot\boldsymbol{\sigma}\right)$ is the rotation matrix around $\boldsymbol{\Omega}$ for a spin 1/2. So one can work with 2D (complex) matrices to calculate the effect of a 3D rotation $\mathcal{R}$ on a real vector $\mathbf{a}$.

In fact, this is more general in the sense that it is also true when applied on complex vectors (rotating around a real vector $\boldsymbol{\Omega}$). Indeed, the effect of a 3D rotation of angle Ω around the axis $\hat{\boldsymbol{\Omega}}$ on a real vector $\mathbf{a}$ can be easily expressed through the relations (see Fig. 6.2)

$$\begin{array}{l}\mathbf{a} = (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}} + \mathbf{a} - (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\ , \\ \boxed{\mathcal{R}(\mathbf{a}) = (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}} + \cos\Omega\left(\mathbf{a} - (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\right) + \sin\Omega\,(\hat{\boldsymbol{\Omega}}\wedge\mathbf{a})}\ .\end{array} \tag{6.11}$$

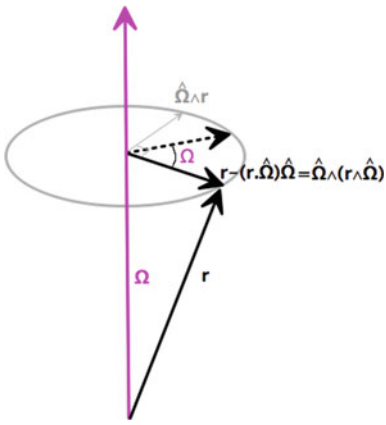

Fig. 6.2 Decomposition of a vector for the calculation of its rotation by an angle Ω around $\hat{\mathbf{\Omega}}$

And (6.11) can be used to define what is the rotation of a complex vector around a real vector $\hat{\mathbf{\Omega}}$. With such a definition, the Cayley–Klein relation (6.10) also works when **a** is a complex 3D vector (see 'proof' in Sect. 6.11).

Exercise 6.1 Show that with the definition of the rotation (6.11) of a complex vector (around a 'real vector $\mathbf{\Omega}$'), the scalar product and the cross product are conserved under rotation:

$$\begin{aligned} \mathcal{R}(\mathbf{d}) \cdot \mathcal{R}(\mathbf{u}) &= \mathbf{d} \cdot \mathbf{u} \ , \\ \mathcal{R}(\mathbf{u}) \wedge \mathcal{R}(\mathbf{d}) &= \mathcal{R}(\mathbf{u} \wedge \mathbf{d}) \ . \end{aligned} \tag{6.12}$$

Solution in Sect. 6.11.

6.4 d-Vector Representation

Coming back to the problem of finding a vector representation of the order parameter, if we could cast the 2×2 matrix order parameter (φ) in the form $(\mathbf{a} \cdot \boldsymbol{\sigma})$, there are good chances that the vector $(\mathbf{a})$ would do the job. Working in the reciprocal space $(\mathbf{k} = k_F \hat{\mathbf{n}})$, where k_F is the radius of the Fermi surface, we start from

$$\begin{aligned} |\Psi(\hat{\mathbf{n}})\rangle &= \sum_{\alpha,\beta} \varphi_{\alpha\beta}(\hat{\mathbf{n}}) |\alpha\beta\rangle \\ &= \Delta^{\uparrow}(\hat{\mathbf{n}}) |\uparrow\uparrow\rangle + \Delta^{\downarrow}(\hat{\mathbf{n}}) |\downarrow\downarrow\rangle + \Delta^{0}(\hat{\mathbf{n}})(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \ , \end{aligned} \tag{6.13}$$

$$(\varphi) = \begin{pmatrix} \varphi_{\alpha\alpha} & \varphi_{\beta\alpha} \\ \varphi_{\alpha\beta} & \varphi_{\beta\beta} \end{pmatrix} \quad \text{with} \quad \varphi_{\alpha\beta} = \varphi_{\beta\alpha} \quad \text{or} \quad (\varphi) = \begin{pmatrix} \Delta^{\uparrow} & \Delta^{0} \\ \Delta^{0} & \Delta^{\downarrow} \end{pmatrix} \ . \tag{6.14}$$

Comparison with expression (6.6) for $\mathbf{a}\cdot\boldsymbol{\sigma}$ doesn't fit, notably as regards the non-diagonal symmetric terms. This is due to the σ_2 component of $\mathbf{a}\cdot\boldsymbol{\sigma}$. It can be eliminated if one calculates

$$\mathrm{i}(\mathbf{a}\cdot\boldsymbol{\sigma})\cdot\sigma_2 = \mathrm{i}\begin{pmatrix} a_3 & a_1-\mathrm{i}a_2 \\ a_1+\mathrm{i}a_2 & -a_3 \end{pmatrix}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} . \tag{6.15}$$

This allows for a straightforward identification of a vector representation of the order parameter, noted as $\mathbf{d}$, of components

$$\varphi_{\alpha\beta} = \quad (\mathrm{i}(\mathbf{d}\cdot\boldsymbol{\sigma})\cdot\sigma_2)_{\alpha\beta} \quad \Longleftrightarrow \quad (\varphi) = \mathrm{i}(\mathbf{d}\cdot\boldsymbol{\sigma})\cdot\sigma_2 . \tag{6.16}$$

Note that, traditionally, $\mathbf{d}$ is normalized to 1 (in a sense to be precised later), like a wave function, whereas the order parameter amplitude reflects the 'superfluid density' and is proportional to the gap in the simplest cases. The equations above do not reflect this subtlety that will be precised later on (see Sect. 6.6.1). Therefore, to be 'in line' with the convention of most papers on the subject, we will introduce a ($\mathbf{k}$-independent) proportionality factor ψ

$$\left.\begin{array}{r} \varphi_{11}=\Delta^{\uparrow}=\psi(-\mathrm{d}_x+\mathrm{i}\mathrm{d}_y) \\ \varphi_{22}=\Delta^{\downarrow}=\psi(\mathrm{d}_x+\mathrm{i}\mathrm{d}_y) \\ \varphi_{12}=\varphi_{21}=\Delta^{0}=\psi(\mathrm{d}_z) \end{array}\right\} \Leftrightarrow \left\{\begin{array}{lll} \psi\mathrm{d}_x= & \frac{1}{2}(-\Delta^{\uparrow}+\Delta^{\downarrow})= & \frac{1}{2}(-\varphi_{11}+\varphi_{22}) \\ \psi\mathrm{d}_y= & -\frac{\mathrm{i}}{2}(\ \Delta^{\uparrow}+\Delta^{\downarrow})= & -\frac{\mathrm{i}}{2}(\ \varphi_{11}+\varphi_{22}) \\ \psi\mathrm{d}_z= & \Delta^{0} \quad = & \frac{1}{2}(\ \varphi_{12}+\varphi_{21}) \end{array}\right. . \tag{6.17}$$

And convenient expressions for calculations deduced from (6.16) and (6.8) read:

$$|\Psi\rangle = \sum_{\alpha,\beta}\varphi_{\alpha\beta}|\alpha\beta\rangle = \mathrm{i}\psi\sum_{\alpha\beta,i=1}^{3}\mathrm{d}_i(\sigma_i\sigma_2)_{\alpha\beta}|\alpha\beta\rangle ,$$

$$\boxed{|\Psi\rangle = \mathrm{i}\psi\sum_{\alpha\beta}\langle\beta|(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle|\alpha\beta\rangle} , \tag{6.18}$$

$$\psi(\mathbf{d}\cdot\boldsymbol{\sigma}) = -\mathrm{i}(\varphi).\sigma_2 \quad \Longrightarrow \quad \boxed{\mathbf{d} = \frac{-\mathrm{i}}{2\psi}tr\,((\varphi)(\sigma_2\boldsymbol{\sigma}))} = -\frac{\mathrm{i}}{2\psi}\sum_{\alpha\beta}(\sigma_2\boldsymbol{\sigma})_{\alpha,\beta}\,\varphi_{\alpha,\beta} ,$$

$$\boxed{\mathbf{d} = \frac{1}{2\psi}[-\Delta^{\uparrow}(\hat{\mathbf{n}})(\hat{\mathbf{k}}_\mathbf{x}+\mathrm{i}\hat{\mathbf{k}}_\mathbf{y})+\Delta^{\downarrow}(\hat{\mathbf{n}})(\hat{\mathbf{k}}_\mathbf{x}-\mathrm{i}\hat{\mathbf{k}}_\mathbf{y})+2\Delta^{0}\hat{\mathbf{k}}_\mathbf{z}]} . \tag{6.19}$$

6.5 Behaviour under Rotations

6.5.1 Rotation in Spin Space

For **d** to be a true vector, it should behave appropriately under rotation. **d** is representing an order parameter which has both orbital and spin degrees of freedom, but the specificity of odd-parity pairing, leading to the necessity of such a vector representation, is coming from the spin degree of freedom. With the relationship to the Cayley–Klein representation, one should expect that this choice leads to a relationship between rotation in spin space and rotation of **d**. In fact, the effect of rotations can be calculated both directly and with the generator of rotations. Let's do both methods.

For the direct evaluation, the important point is that the rotation acts simultaneously on both spins. Starting from the expression (6.18) to evaluate the effect of the rotation on the spin part of the order parameter, we get

$$\begin{aligned}\mathcal{R}_{\mathbf{\Omega}}|\Psi\rangle &= \mathrm{i}\psi \sum_{\alpha\beta}\langle\beta|(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\mathcal{R}_{1,\mathbf{\Omega}}\otimes\mathcal{R}_{2,\mathbf{\Omega}}|\alpha\beta\rangle \\ &= \mathrm{i}\psi \sum_{\alpha\beta\gamma\delta}\langle\delta|\mathcal{R}_{\mathbf{\Omega}}|\beta\rangle\langle\beta|(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\langle\gamma|\mathcal{R}_{\mathbf{\Omega}}|\alpha\rangle|\gamma\delta\rangle \\ &= \mathrm{i}\psi \sum_{\alpha\gamma\delta}\langle\delta|\mathcal{R}_{\mathbf{\Omega}}(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\langle\gamma|\sigma_2^2\cdot\mathcal{R}_{\mathbf{\Omega}}|\alpha\rangle|\gamma\delta\rangle\ .\end{aligned}$$

We have

$$\begin{aligned}\langle\gamma|\sigma_2^2\cdot\mathcal{R}_{\mathbf{\Omega}}|\alpha\rangle &= \sum_{\eta}\langle\gamma|\sigma_2|\eta\rangle\langle\eta|\cos(\Omega/2)\sigma_2 - \mathrm{i}\sin(\Omega/2)\sigma_2\hat{\mathbf{\Omega}}.\sigma|\alpha\rangle \\ &= \sum_{\eta}(-\langle\eta|\sigma_2|\gamma\rangle)\langle\alpha| - \cos(\Omega/2)\sigma_2 - \mathrm{i}\sin(\Omega/2)\sigma_2\hat{\mathbf{\Omega}}.\sigma|\eta\rangle \\ &= \langle\alpha|\sigma_2\mathcal{R}_{-\mathbf{\Omega}}\sigma_2|\gamma\rangle\ ,\end{aligned}$$

as σ_2 is antisymmetric and $\sigma_2(\hat{\mathbf{\Omega}}.\sigma)$ is symmetric. So

$$\begin{aligned}\mathcal{R}_{\mathbf{\Omega}}|\Psi\rangle &= \mathrm{i}\psi \sum_{\alpha\gamma\delta}\langle\delta|\mathcal{R}_{\mathbf{\Omega}}(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\langle\alpha|\sigma_2\mathcal{R}_{-\mathbf{\Omega}}\sigma_2|\gamma\rangle|\gamma\delta\rangle \\ &= \mathrm{i}\psi \sum_{\gamma\delta}\langle\delta|\mathcal{R}_{\mathbf{\Omega}}(\mathbf{d}\cdot\boldsymbol{\sigma})\mathcal{R}_{-\mathbf{\Omega}}\sigma_2|\gamma\rangle|\gamma\delta\rangle \\ &= \mathrm{i}\psi \sum_{\gamma\delta}\langle\delta|\,(\mathcal{R}(\mathbf{d})\cdot\boldsymbol{\sigma})\,\sigma_2|\gamma\rangle|\gamma\delta\rangle\ .\end{aligned}$$

Using (6.10)

$$\mathcal{R}_{\boldsymbol{\Omega}}|\Psi\rangle = |\Psi\left(\mathcal{R}(\mathbf{d})\right)\rangle \ .$$

So indeed, the effect of a change of the spin quantization axis on the order parameter can be evaluated directly by the corresponding rotation of the (complex) **d**-vector in 3D. And the calculation above makes a direct connection between the Cayley–Klein transformation and the rather involved definition of the **d**-vector.

It is also useful (and simple) to evaluate the effect of a rotation using the generator of rotations in spin space: this generator is simply $-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}\cdot\mathbf{S}$, where the total spin $\mathbf{S} = \mathbf{S_1} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbf{S_2}$.

The effect of any operator $\mathbf{O} = O_1 \otimes \mathbb{1} + \mathbb{1} \otimes O_2$ acting in the spin space can be calculated as (remembering that $(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2$ is a symmetric matrix and σ_2 an antisymmetric matrix)

$$\begin{aligned}
\mathbf{O}|\Psi\rangle &= i\psi \sum_{\alpha\beta} \langle\beta|(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle \mathbf{O}|\alpha\beta\rangle \\
&= i\psi \sum_{\alpha\beta\gamma} \langle\beta|(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle \left(\langle\gamma|O|\alpha\rangle|\gamma\beta\rangle + \langle\gamma|O|\beta\rangle|\alpha\gamma\rangle\right) \\
&= i\psi \sum_{\alpha\beta} \langle\beta|O(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle \left(|\alpha\beta\rangle + |\beta\alpha\rangle\right) \quad \text{or} \\
&= i\psi \sum_{\alpha\beta} \left(\langle\beta|O(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle + \langle\alpha|O(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\beta\rangle\right)|\alpha\beta\rangle \ .
\end{aligned} \tag{6.20}$$

Applying (6.20) to the action of generator of rotations in spin space, namely, $-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}\cdot\mathbf{S}$, we get

$$\begin{aligned}
-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}.\mathbf{S}|\Psi\rangle &= \psi\frac{1}{2}\sum_{\alpha\beta}\langle\beta|(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\left(|\alpha\beta\rangle + |\beta\alpha\rangle\right) \\
&= \psi\frac{1}{2}\sum_{\alpha\beta}\langle\beta|(\cancel{\hat{\mathbf{n}}.\mathbf{d}})\cancel{\sigma_2} + i(\hat{\mathbf{n}}\wedge\mathbf{d})\cdot\boldsymbol{\sigma}\sigma_2|\alpha\rangle\left(|\alpha\beta\rangle + |\beta\alpha\rangle\right) \ .
\end{aligned}$$

So

$$-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}.S|\Psi\rangle = |\Psi(\hat{\mathbf{n}}\wedge d)\rangle \ . \tag{6.21}$$

So that applying a rotation in spin space amounts to the same rotation of the **d**-vector [see (6.11)] for an elemental rotation of **d**: $\mathcal{R}_{\boldsymbol{\Omega},\mathbf{S}}|\Psi\rangle = |\Psi\left(\mathcal{R}_{\boldsymbol{\Omega}}(\mathbf{d})\right)\rangle$ (see [3]).

6.5.2 Rotation in Real Space

For rotations in real space (on the orbital degrees of freedom), we should calculate the effect of $-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}.L$, with $L = \mathbf{r}\wedge\left(\frac{\hbar}{\mathrm{i}}\nabla_{\mathbf{r}}\right)$. Writing $D(\mathbf{k}) = [\mathbf{d}(\mathbf{k})\cdot\boldsymbol{\sigma}]\sigma_2$, we get

$$
\begin{aligned}
-\frac{\mathrm{i}}{\hbar}\mathbf{L}|\Psi\rangle &= -(\mathbf{r}\wedge\nabla_{\mathbf{r}})\int \mathrm{d}\mathbf{k}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\psi\sum_{\alpha\beta}\langle\beta|D(\mathbf{k})|\alpha\rangle|\alpha\beta\rangle \\
&= \psi\sum_{\alpha\beta}\int \mathrm{d}\mathbf{k}\,\mathrm{i}(\mathbf{r}\wedge\mathbf{k})\mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}}\langle\beta|D(\mathbf{k})|\alpha\rangle|\alpha\beta\rangle \\
&= \psi\sum_{\alpha\beta}\int \mathrm{d}\mathbf{k}\,\langle\beta|D(\mathbf{k})|\alpha\rangle(\mathbf{k}\wedge\nabla_{\mathbf{k}})\mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}}|\alpha\beta\rangle \\
&= -\psi\sum_{\alpha\beta,i}\int \mathrm{d}\mathbf{k}\,\frac{\partial}{\partial k_i}\left(\langle\beta|D(\mathbf{k})|\alpha\rangle\mathbf{k}\right)\wedge\hat{\mathbf{k}}_i\,\mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}}|\alpha\beta\rangle \\
&= -\psi\sum_{\alpha\beta}\int \mathrm{d}\mathbf{k}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}}\langle\beta|(\mathbf{k}\wedge\nabla)D(\mathbf{k})|\alpha\rangle|\alpha\beta\rangle\ ,
\end{aligned}
$$

so

$$
-\frac{\mathrm{i}}{\hbar}\hat{\mathbf{n}}.L|\Psi\rangle = |\Psi(-\mathrm{i}\hat{\mathbf{n}}\cdot\mathbf{L}_{\mathbf{k}}\mathbf{d}(\mathbf{k}))\rangle,\ \text{with}\ \ \mathbf{L}_{\mathbf{k}} = \mathbf{k}\wedge\frac{1}{\mathrm{i}}\nabla_{\mathbf{k}}\ . \tag{6.22}
$$

This last expression shows that a rotation in real space acts, as it should, on the order parameter according to its orbital state: p-wave, f-wave, … for a triplet superconductor, transposed as usual in the reciprocal space.

6.5.3 *Change of Quantization Axis: Application to ESP States*

In order to get more familiar with rotations of the **d**-vector, let us start with an exercise:

Exercise 1 Consider the very first example of Sect. 6.3.1 to observe the fate of the **d**-vector under a change of orientation of the quantization axis on a simple $|\uparrow\uparrow\rangle$ state. Solution in Sect. 6.11.

Beyond this 'trivial' example, understanding the behaviour under rotation of the **d**-vector is particularly useful to get a more precise idea about some specific spin states. For example, we can easily understand that any state $|\Psi\rangle = \Delta_0|\uparrow\downarrow + \downarrow\uparrow\rangle$ can be considered as an 'equal spin pairing' (ESP) state, with equal weight on $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ spin components. Indeed, its **d**-vector is simply

$$
\mathbf{d} = \frac{1}{\psi}\begin{pmatrix}0\\0\\\Delta_0\end{pmatrix}\ .
$$

Let us rotate the quantization axis by $-\pi/2$ around an axis $\hat{\Omega}$ in the x-y-plane with an angle φ from the x-axis. To get the coordinates of **d** in the new frame, we should rotate it by $\pi/2$ around $\hat{\Omega}$ [remember (6.11)]

$$\hat{\mathbf{\Omega}} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix} ,$$

$$\mathcal{R}_{\mathbf{\Omega}}(\mathbf{d}) = \sin(\pi/2)\,\hat{\mathbf{\Omega}} \wedge d = \frac{1}{\psi} \begin{pmatrix} \sin\varphi\Delta_0 \\ -\cos\varphi\Delta_0 \\ 0 \end{pmatrix} ,$$

$$\Delta_\uparrow = \psi(-\mathrm{d}_x + \mathrm{i}\mathrm{d}_y) = -\mathrm{i}e^{\mathrm{i}\varphi}\Delta_0 \quad ; \quad \Delta_\downarrow = \psi(\mathrm{d}_x + \mathrm{i}\mathrm{d}_y) = -\mathrm{i}e^{-\mathrm{i}\varphi}\Delta_0 ,$$

which is indeed an ESP state with only $\uparrow\uparrow$ and $\downarrow\downarrow$ spin components. It is a good exercise to check that, reciprocally, any ESP state with equal weight for the up- and down-spin components can also be written as a pure $S_z = 0$ state for some choice of the quantization axis.

Exercise 6.2 Show that any ESP state with equal weight for the up- and down-spin component can also be written as a pure $|S_z = 0\rangle$ state. Solution in Sect. 6.11.

6.6 Some Uses of the d-Vector Representation

6.6.1 Amplitude of the d-Vector

As promised, let us say a few words on the question of normalization of the **d**-vector. For s-wave superconductors, in the simplest cases, we know that the order parameter can be taken as proportional to the gap. Of course, this is wrong in the general case, e.g. gapless superconductivity exists (induced by a critical amount of magnetic impurities for example). But the idea is that $|\psi|^2$ somehow represents the superfluid density. For a spin-triplet superconductor, we can define this quantity as

$$\begin{aligned} \langle\Psi|\Psi\rangle &= \oint \frac{\mathrm{d}\Omega}{4\pi} \sum_{\alpha,\beta} \varphi^*_{\beta\alpha}\varphi_{\alpha\beta} = \oint \frac{\mathrm{d}\Omega}{4\pi} tr(\varphi^*(\hat{\mathbf{n}})\varphi(\hat{\mathbf{n}})) \\ &= |\psi|^2 \oint \frac{\mathrm{d}\Omega}{4\pi} tr(\sigma_2(\mathbf{d}^* \cdot \boldsymbol{\sigma})(\mathbf{d} \cdot \boldsymbol{\sigma})\sigma_2) = 2|\psi|^2 \oint \frac{\mathrm{d}\Omega}{4\pi} |\mathbf{d}(\hat{\mathbf{n}})|^2 . \end{aligned}$$

Note that the definition above is coherent with the fact that from the very beginning, we did not normalize (by $\frac{1}{\sqrt{2}}$) the $|\uparrow\uparrow + \downarrow\downarrow\rangle$ component of $|\psi\rangle$ in (6.3). $|\mathbf{d}(\hat{\mathbf{n}})|^2$ can be interpreted as the angular-dependent superconducting (or superfluid) density, and by convention, one takes

$$\oint \frac{\mathrm{d}\Omega}{4\pi} |\mathbf{d}(\hat{\mathbf{n}})|^2 = 1 . \tag{6.23}$$

So on calculating averaged quantities $\langle\Psi|O|\Psi\rangle/\langle\Psi|\Psi\rangle$, one should remember that $\langle\Psi|\Psi\rangle = 2|\psi|^2$.

6.6.2 Spin Direction

Up to now, we discussed the properties of the **d**-vector under rotation but we did not unveil the signification of its direction. As announced, it cannot be straightforward, as in the general case, **d** is a complex vector. But it should be related to the spin. So let us calculate $\mathbf{S}|\psi\rangle$, in the same way we performed the calculation of the effects of rotations in spin space, using the generator [Sect. 6.5.1, (6.21)]

$$\begin{aligned}\mathbf{S}|\Psi\rangle &= \frac{\mathrm{i}\hbar}{2}\sum_{\alpha\beta}\psi\langle\beta|\boldsymbol{\sigma}(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_2|\alpha\rangle\left(|\alpha\beta\rangle+|\beta\alpha\rangle\right)\\ &= \frac{\hbar}{2}\sum_{\alpha\beta}\psi\langle\beta|(\cancel{\mathrm{i}\mathbf{d}\sigma_2}-(\mathbf{d}\wedge\boldsymbol{\sigma})\sigma_2|\alpha\rangle)\left(|\alpha\beta\rangle+|\beta\alpha\rangle\right)\ ,\end{aligned}$$

from which we deduce immediately that

$$\mathbf{d}\cdot\mathbf{S}|\Psi\rangle = 0\ . \tag{6.24}$$

This means that if **d** is real (up to a phase factor), it is perpendicular to the direction of the Cooper pairs spin (quantization axis). More explicitly the average spin at a given wave vector **k** of the Fermi surface can be calculated as

$$\begin{aligned}\frac{\langle\Psi|\mathbf{S}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \quad & \frac{\mathrm{i}\hbar}{2}\sum_{\gamma,\delta}\sum_{\alpha,\beta}\langle\gamma|\sigma_2(\mathbf{d}^*\cdot\boldsymbol{\sigma})|\delta\rangle\langle\beta|(\mathbf{d}\wedge\boldsymbol{\sigma})\sigma_2|\alpha\rangle\langle\gamma\delta|\left(|\alpha\beta\rangle+|\beta\alpha\rangle\right)\\ &= \frac{\mathrm{i}\hbar}{2}\,tr\left((\mathbf{d}^*\cdot\boldsymbol{\sigma})(\mathbf{d}\wedge\boldsymbol{\sigma})\right) = \frac{\mathrm{i}\hbar}{2}\,tr\left((\mathbf{d}\wedge(\mathbf{d}^*\cdot\boldsymbol{\sigma})\boldsymbol{\sigma})\right)\\ &= \frac{\mathrm{i}\hbar}{2}\left(tr\left((\mathbf{d}\wedge\mathbf{d}^*)\mathbb{1}\right)-\mathrm{i}\,tr\left(\mathbf{d}\wedge(\mathbf{d}^*\wedge\boldsymbol{\sigma})\right)\right)\\ &= \mathrm{i}\hbar(\mathbf{d}\wedge\mathbf{d}^*)-\frac{\hbar}{2}\cancel{tr\left((\mathbf{d}.\boldsymbol{\sigma})\mathbf{d}^*-\mathbf{d}(\mathbf{d}^*\cdot\boldsymbol{\sigma})\right)}\\ &\qquad\boxed{\langle\mathbf{S}(\mathbf{k})\rangle = \mathrm{i}\hbar\mathbf{d}(\mathbf{k})\wedge\mathbf{d}^*(\mathbf{k})}\ .\end{aligned} \tag{6.25}$$

6.6.3 Non-unitary States

The above equation is important. Indeed, if $\mathbf{d}(\mathbf{k})\wedge\mathbf{d}^*(\mathbf{k})$ is non-zero, the state is called a 'non-unitary state' and it has some more involved properties. Moreover, in general, the fact that $\mathbf{d}(\mathbf{k})\wedge\mathbf{d}^*(\mathbf{k})$ is non-zero means that locally, on the Fermi surface, the Cooper pairs spin is non-zero. But it does not mean that globally, the superconductor is spin-polarized. Conversely, if the superconductor is globally spin-

polarized, it is necessarily in a non-unitary state, where $\mathbf{d}^*$ is not proportional to $\mathbf{d}$, see Sect. 6.9 on ferromagnetic superconductors.

This notion of 'non-unitary' state is usually bewildering, and it is useful to make some simple calculations in order to get more used to it. For example, we can check what are the conditions under which an ESP state can also be non-unitary. An ESP state has only $\Delta_\uparrow$ and $\Delta_\downarrow$ components, so that its $\mathbf{d}$-vector will be of the form

$$\mathbf{d} = \psi \begin{pmatrix} \frac{1}{2}(-\Delta^\uparrow + \Delta^\downarrow) \\ -\frac{i}{2}(\ \ \Delta^\uparrow + \Delta^\downarrow) \\ 0 \end{pmatrix} . \tag{6.26}$$

Then

$$\begin{aligned} \mathbf{d} \wedge \mathbf{d}^* &= (\mathrm{d}_x \mathrm{d}_y^* - \mathrm{d}_y \mathrm{d}_x^*)\mathbf{e}_z \\ &= \frac{\mathrm{i}|\psi|^2}{4}[(-\Delta^\uparrow + \Delta^\downarrow)(\Delta^{\uparrow *} + \Delta^{\downarrow *}) + (\Delta^\uparrow + \Delta^\downarrow)(-\Delta^{\uparrow *} + \Delta^{\downarrow *})]\mathbf{e}_z \\ &= \frac{-\mathrm{i}|\psi|^2}{2}[|\Delta^\uparrow|^2 - |\Delta^\downarrow|^2]\mathbf{e}_z . \end{aligned}$$

From (6.23), we get that $\frac{|\psi|^2}{2}(|\Delta^\uparrow|^2 + |\Delta^\downarrow|^2) = 1$. So

$$\mathrm{i}\hbar \mathbf{d} \wedge \mathbf{d}^* = \hbar \frac{[|\Delta^\uparrow|^2 - |\Delta^\downarrow|^2]}{|\Delta^\uparrow|^2 + |\Delta^\downarrow|^2} \mathbf{e}_z . \tag{6.27}$$

The conclusion is simple: an ESP state is non-unitary only if the amplitude of the $\Delta_\uparrow$ and $\Delta_\downarrow$ components is different on some part of the Fermi surface.

6.6.4 Orbital Moment

In the same way, from (6.22), we calculate that the average orbital moment per Cooper pair is [1]

$$\begin{aligned} \frac{\langle \Psi | \mathbf{L} | \Psi \rangle}{\langle \Psi | \Psi \rangle} &= \oint \frac{\mathrm{d}\Omega}{4\pi} \frac{\hbar}{2\mathrm{i}} \sum_{\alpha,\beta,\gamma,\delta} \langle \gamma | \sigma_2 (\mathbf{d}^* \cdot \boldsymbol{\sigma}) | \delta \rangle \ \langle \beta | (\mathbf{k} \wedge \nabla_\mathbf{k})(\mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}) \sigma_2 | \alpha \rangle \langle \gamma \delta | \alpha \beta \rangle \\ &= \oint \frac{\mathrm{d}\Omega}{4\pi} \frac{\hbar}{2\mathrm{i}} \, tr \left((\mathbf{d}^* \cdot \boldsymbol{\sigma})(\mathbf{k} \wedge \nabla_\mathbf{k})(\mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}) \right) , \end{aligned}$$

$$\boxed{\langle \mathbf{L}(\mathbf{k}) \rangle = \frac{\hbar}{\mathrm{i}} \oint \frac{\mathrm{d}\Omega}{4\pi} \sum_i \mathrm{d}_i^* (\mathbf{k} \wedge \nabla_\mathbf{k}) \mathrm{d}_i(k)} . \tag{6.28}$$

Note that if $\mathbf{d}$ is real, $\langle \mathbf{L} \rangle$ is zero (if not, it would be imaginary!). This appears in (6.28) from

$$\oint \frac{\mathrm{d}\Omega}{4\pi} \sum_i \mathrm{d}_i^*(\mathbf{k} \wedge \nabla_{\mathbf{k}})\mathrm{d}_i(k) = \oint \frac{\mathrm{d}\Omega}{8\pi} \sum_{i,j} (\mathbf{k} \wedge \mathbf{e}_j) \frac{\partial}{\partial k_j} \mathrm{d}_i^2(k)$$
$$= -\oint \frac{\mathrm{d}\Omega}{8\pi} \sum_{i,j} (\mathbf{e}_j \wedge \mathbf{e}_j)\mathrm{d}_i^2(k) = 0 \,.$$

A last remark on this point: superconductors for which $\langle \mathbf{L} \rangle$ is non-zero are nowadays called 'chiral superconductors' and quite looked-after for their potential topological properties [4]. Note, however, that if only triplet superconductors can have a non-zero $\langle \mathbf{S} \rangle$, this is not the case for $\langle \mathbf{L} \rangle$: both spin-singlet and spin-triplet can be chiral. Naturally, in case of spin-singlet, the superconductor needs to be unconventional (not s-wave), and intrinsically complex, so that $\langle \mathbf{L} \rangle$ can be non-zero. This is the case, for example, of d-wave superconductors of type "$d + \mathrm{i}d$" or $(k_x \pm \mathrm{i}k_y)k_z \ldots$

6.6.5 *Excitation Energy of Quasiparticles*

We will not derive the energy spectrum from microscopic theory, just report the results (see [2] for example): for triplet superconductors in a unitary state, the expression of the energy of elementary excitations is very similar to that of singlet anisotropic superconductors, with the $\mathbf{k}$ dependence of the energy gap controlled by the amplitude of $\mathbf{d}(\mathbf{k})$

$$E_k = \sqrt{\xi_k^2 + \Delta^2 \left(|\mathbf{d}(\mathbf{k})|^2\right)} \,. \tag{6.29}$$

However, for non-unitary states, two branches appear in the spectrum, depending on the spin orientation of the excitations with respect to $\langle \mathbf{S} \rangle$: it is as if they are 'Zeeman split' by $\langle \mathbf{S} \rangle$. So the energy gap is expressed in such a case as

$$E_k = \sqrt{\xi_k^2 + \Delta^2 \left(|\mathbf{d}(\mathbf{k})|^2 \pm |\mathbf{d}(\mathbf{k}) \wedge \mathbf{d}^*(\mathbf{k})|\right)} \,. \tag{6.30}$$

Hence, this is another true difference with respect to singlet superconductors.

We can also see how both (6.29) and (6.30) read when using not the $\mathbf{d}$-vector notation, but expression like (6.17) for the order parameter. In the unitary case, the gap $\Delta(\mathbf{k})$ would be expressed as

$$\Delta(\mathbf{k}) = \sqrt{\frac{1}{2}\left(|\Delta^{\uparrow}(\mathbf{k})|^2 + |\Delta^{\downarrow}(\mathbf{k})|^2\right) + |\Delta^0(\mathbf{k})|^2} \,.$$

And in the case of non-unitary states, if we take the 'simple' example of ESP states, using expression (6.27) for $\mathbf{d} \wedge \mathbf{d}^*$ we derive easily that

$$\begin{aligned}\Delta(\mathbf{k}) &= \sqrt{\Delta^2\left(|\mathbf{d}(\mathbf{k})|^2 \pm |\mathbf{d}(\mathbf{k}) \wedge \mathbf{d}^*(\mathbf{k})|\right)} \\ &= |\Delta^{\uparrow}(\mathbf{k})| \quad \text{or} \quad |\Delta^{\downarrow}(\mathbf{k})| \,.\end{aligned} \tag{6.31}$$

This last expression shows concretely why 'non-unitary states' are a distinctive feature of spin-triplet superconductors. It can be also anticipated that this expression will be particularly useful for ferromagnetic superconductors, where band polarization can lead to a large difference between $|\Delta^{\uparrow}(\mathbf{k})|$ and $|\Delta^{\downarrow}(\mathbf{k})|$ (see Sect. 6.9). Expression (6.30) gives a general formula for the two gap values of a non-unitary state, even if it is not an ESP state: as will be seen later, UPt_3 in its B-phase could produce such a case (see Sect. 6.8.2.3).

6.7 The Spin–Orbit Issue

Before discussing some emblematic examples of p-wave superconductors, let us say a few words concerning the question of spin–orbit coupling. Indeed, when discussed for real materials (except for superfluid ^{3}He), it covers two different aspects which should be distinguished to avoid confusion. The first is the usual spin–orbit coupling at the atomic scale, discussed already in the normal phase as it prevents the spin $\mathbf{S}$ to be a good quantum number. In a solid, symmetries can help to overcome this problem:

- If the system has an inversion centre and time-reversal symmetry, quasiparticles with a given wave vector $\mathbf{k}$ are necessarily degenerate. This allows to define a 'pseudo-spin 1/2' and to build Cooper pairs with this pseudo-spin state: replacing 'spin' by 'pseudo-spin' is all that is required to keep everything else unchanged.
- If the system has an inversion centre, but not necessarily time-reversal symmetry, then, at least, one can distinguish between odd-parity and even-parity states.
- If there is no inversion centre, but time-reversal symmetry, one can still build Cooper pairs; however, there is no such distinction any more between even- or odd-parity states. Abusively, one can say that singlet and triplet pairings are mixed together. Experimentally, large upper critical fields outpassing the paramagnetic limit are commonly found for such systems.

6.7.1 Spin–Orbit and the Superconducting Order Parameter

However, there is also another issue for 'triplet' superconductors with spin–orbit interaction: we are now speaking of spin–orbit coupling between the spin and orbital parts of the Cooper pairs, as done in the case of superfluid ^{3}He: the problem is that the 'atomic-scale' spin–orbit coupling can be very large (see, for example, what happens in the ^{3}He nuclei!), whereas the coupling between the total orbital moment

of the Cooper pair (an object of a coherence length scale) and the total spin of the Cooper pairs can be much weaker. And in real solid, it is very difficult to either calculate (predict) or to measure this spin–orbit interaction. This question is very important because it determines the symmetry group which has to be considered for the classification of the different superconducting states. If spin–orbit is weak, the relative orientation of spin and orbit should be decoupled: so, for example, one can imagine that the spin could reorient 'freely' under the action of an external field. If spin–orbit is strong, the orbital state (the gap nodes for example) expected to be pinned on the crystal lattice will prevent such a reorientation of the spin state. Therefore

- If the spin–orbit interaction is weak, the symmetry group considered for the classification of the possible superconducting states will be $G \otimes U(1) \otimes \mathcal{T} \otimes \mathcal{R}_{\mathcal{S}}$, where $\mathcal{R}_{\mathcal{S}}$ are the (3D) rotations in spin space, G is the crystal point group, $U(1)$ the gauge symmetry (always broken in the superconducting state) and $\mathcal{T}$ the time-reversal symmetry. Due to $\mathcal{R}_{\mathcal{S}}$, $\mathbf{d}$ should reorient under field to minimize the Zeeman energy.
- If the spin–orbit interaction is strong, the symmetry group considered for the classification of the possible superconducting states will be $G \otimes U(1) \otimes \mathcal{T}$, meaning that the $\mathbf{d}$-vector is expected to be 'pinned' on the lattice. In such a case, additional spin anisotropy may appear in the superconducting state, possibly detected, for example, by an anisotropy of the Knight-shift reduction below T_{SC}, or by an anisotropic paramagnetic limitation.

For most of the candidate p-wave superconductors, determining what is the best of the two limits for the description of the system remains an open issue (see, for example, the discussion on UPt_3 in Sects. 6.8.2.2 and 6.8.2.3).

6.7.2 Anisotropy of the Susceptibility for the Strong Spin–Orbit Case

Experimentally, an important question when analysing the behaviour of a potential triplet superconductor is the Pauli depairing effect and its anisotropy on the upper critical field, or equivalently, the anisotropy of the change of the Knight shift below T_{SC}, both of which depending on the Cooper pairs spin susceptibility. Supposing that we are in the strong spin–orbit limit, the question is to derive from the possible order parameters, in which directions there will be no change of the electronic spin susceptibility between normal and superconducting phases, and in which directions, if any, there will be at least a partial suppression of this spin susceptibility.

As a matter of fact, it is important to realize that even spin-triplet superconductors, whatever the spin–orbit regime, can present a reduction of the susceptibility for all orientations of the magnetic field. We will see below (Sect. 6.8.1) that superfluid ^{3}He realize, in its B-phase, an A_{1u} state for which $\mathbf{d} \propto \mathbf{k}$. This means that, on each point of the Fermi surface, the order parameter is described by a pure $|S_z = 0\rangle$ state if the

quantization z-axis is taken along $\mathbf{k}$. Such a $|S_z = 0\rangle$ state is equivalent to the spin-singlet case as regards susceptibility, leading to a vanishing susceptibility. In fact, it can be shown that for such an A_{1u} state, on average, the susceptibility is reduced to two-third of the normal state susceptibility at $T = 0$, as if for a given field direction, one-third of the spins were in the $|S_z = 0\rangle$ state [1].

At the opposite, for an ESP state, where Cooper pairs are formed only with spins of the same direction, we expect no change of the susceptibility for fields along the quantization axis. However, this does not tell us what to expect in the perpendicular directions.

Maybe the easiest way to understand if the spin susceptibility is reduced or not for a given field direction, and whatever the order parameter, is to rewrite the **d**-vector with the new quantization axis in this field direction, and check in this representation, whether or not the z-component of the **d**-vector (corresponding to the amplitude of the $|S_z = 0\rangle$ state for that direction) is zero. Changing the quantization axis, and rewriting the **d**-vector for this new quantization axis, amounts to rotate the reference frame, or rotate in the opposite direction the **d**-vector in spin space (see Sect. 6.5.1). It is easy to see [see (6.11) for the rotation of the **d**-vector] that the z-component of the **d**-vector, when changing the quantization axis for the x- or y-axis, is, respectively, $-\mathrm{d}_x$ or d_y. What it means is that, in the case of strong spin–orbit coupling, where the **d**-vector cannot reorient depending on the field (**H**) direction:

- The $|S_z = 0\rangle$ component of the order parameter, where z is the field direction, is proportional to the **d**-vector projection along the field direction [which generalizes (6.24), which had a physical meaning only for real **d**-vectors]: if $(\mathbf{d}\cdot\mathbf{H})$ is non-zero, there will be at least a partial suppression of the spin susceptibility and so, Pauli depairing for the upper critical field, for fields applied in this direction.
- Whatever the **d**-vector, there is always at least one direction, where there will be Pauli depairing (otherwise, **d** should be the null vector).

Coming back to the question of ESP states, if the phase between the $\Delta^{\uparrow}$ and $\Delta^{\downarrow}$ is constant on the Fermi surface and it is a unitary state, on top of the quantization axis, there is another direction (hence a whole plane) for which there is no change of the spin susceptibility (and no Pauli depairing) and a perpendicular direction for which the spin susceptibility is completely suppressed (see Sect. 6.11.5). For example, if **d** is of the form (6.26)

$$\mathbf{d} = \psi \begin{pmatrix} \frac{1}{2}(-\Delta^{\uparrow} + \Delta^{\downarrow}) \\ -\frac{i}{2}(\ \Delta^{\uparrow} + \Delta^{\downarrow}) \\ 0 \end{pmatrix},$$

with $\Delta^{\uparrow} = \Delta^{\downarrow}$, then there is no Pauli depairing for fields in the x-z-plane and full Pauli depairing (as in the singlet case) for field along the y-axis. If the ESP state is non-unitary ($|\Delta^{\uparrow}| \neq |\Delta^{\downarrow}|$ on some part of the Fermi surface), then for sure, there is at least partial Pauli depairing in the two directions perpendicular to the quantization axis and still no Pauli depairing for fields along the quantization axis.

6.8 d-vector Representation of Some Known (or Suspected) *p*-Wave Superconductors

6.8.1 Phases of Superfluid ^{3}He

^{3}He has been the very first case for *p*-wave superconductivity (superfluidity, to be precise!), and it is, beyond contest, a true paradigm for this state of matter. The reasons are that, despite its very low superfluid transition temperature ($\approx$ 1 mK on the melting curve), the spin state and most of the superfluid properties could be identified and studied with tremendous precision thanks to nuclear magnetic resonance (NMR): in superfluid ^{3}He, the Cooper pairs spin is the nuclear spin of the ^{3}He atoms, which are directly probed by NMR. Moreover, the system is rotationally invariant, so with the simplest (spherical) possible Fermi surface, and with spherical harmonics as basis for the irreducible representations of the superconducting order parameter. In **k**-space, for a *p*-wave state, they read

$$Y_{11}(\hat{\mathbf{k}}) = -\sqrt{\frac{3}{2}}(\hat{\mathbf{k}}_x + \mathrm{i}\hat{\mathbf{k}}_y)\ ;\ Y_{1-1}(\hat{\mathbf{k}}) = \sqrt{\frac{3}{2}}(\hat{\mathbf{k}}_x - \mathrm{i}\hat{\mathbf{k}}_y)\ ;\ Y_{10}(\hat{\mathbf{k}}) = -\sqrt{3}\hat{\mathbf{k}}_z\ . \tag{6.32}$$

It can be explicitly checked that [see (6.22)]

$$\hat{\mathbf{k}}_z \cdot L_k\, Y_{1m} = \hat{\mathbf{k}}_z \cdot (k \wedge \frac{1}{\mathrm{i}}\boldsymbol{\nabla}_{\mathbf{k}}\, Y_{1m}) = m\, Y_{1m}\ . \tag{6.33}$$

Another reason for which superfluid ^{3}He is a paradigm of *p*-wave superconductors is that it presents a rich phase diagram (shown in Fig. 6.3[1]), with three well-identified phases: two (called *A* and *B*) in the temperature–pressure plane, and an additional (A_1) phase under magnetic fields, which are key references. A main topic these days is that of the topological properties of some superconductors, which has been addressed in great detail some tens of years ago for superfluid ^{3}He [5]. Let us examine them quickly.

6.8.1.1 *B*-Phase

The *B*-phase of superfluid ^{3}He is simply characterized by

$$\begin{aligned} &\mathbf{d}(\mathbf{k}) = \hat{\mathbf{k}}\ ;\ \text{or explicitely} \\ &|\Psi(\hat{\mathbf{k}})\rangle = \psi\left((-\hat{k}_x + \mathrm{i}\hat{k}_y)|\uparrow\uparrow\rangle + (\hat{k}_x + \mathrm{i}\hat{k}_y)|\downarrow\downarrow\rangle + \hat{k}_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\right)\ . \end{aligned} \tag{6.34}$$

[1] Adapted from 'Heliums egenskaper vid låga temperaturer', P. Berglund, Kosmos 1988, s. 63 (Courtesy of the Swedish Physical Society).

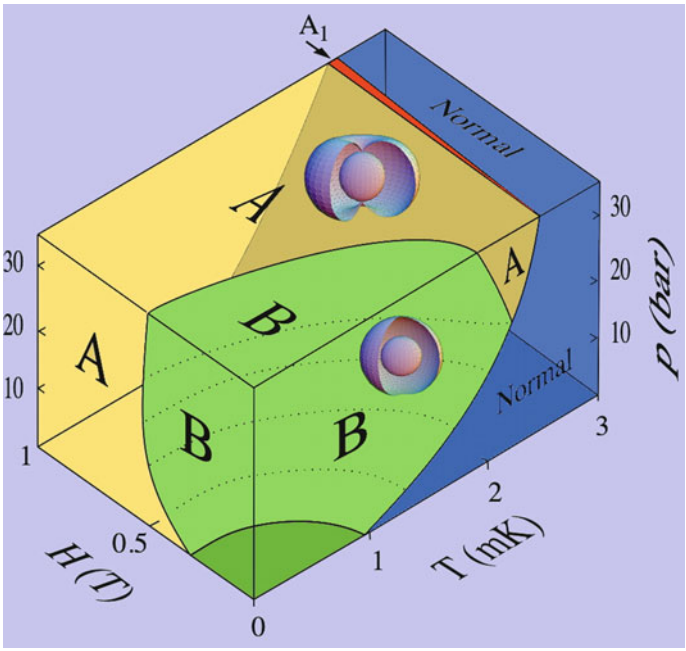

Fig. 6.3 Phase diagram, in the temperature–pressure–magnetic field space, of the superfluid phases of ^{3}He. Three different phases, called B, A and A_1, corresponding to different symmetries and **d**-vectors have been identified. The gap structure is also shown, represented by the distance between the inner sphere (the Fermi surface) and the exploded view of the outer surface. There is a uniform gap in the B-phase, and a nodal gap (with two nodes at the poles) in the A-phase. The A_1 phase, which appears only under magnetic field, is non-unitary and the gap is like that of the A-phase on the majority spin Fermi sheet, and zero on the other (only half the Fermi surface is paired)

As $\mathbf{d}^*(\mathbf{k}) = \mathbf{d}(\mathbf{k})$, this state is unitary and has both $\langle \mathbf{S} \rangle = 0$ and $\langle \mathbf{L} \rangle = 0$. Moreover, $|\mathbf{d}(\mathbf{k})| = 1$, so that the gap is uniform on the Fermi surface, even though the average of $\mathbf{d}(\mathbf{k})$ is zero.

In the simplest models, this B-phase should be the state of lowest free energy, notably due to the fact that the gap is fully open over the whole Fermi surface. However, this state has a reduced spin susceptibility deep in the superfluid state (see the discussion in Sect. 6.7.2). As the pairing mechanism involves spin fluctuations, this may be unfavourable compared to other states, notably ESP states, where such a reduction of the susceptibility is absent (this is the so-called 'feedback' mechanism). Therefore, as seen in Fig. 6.3, another phase, the A-phase, is stable notably along the melting line and becomes the dominant phase under field. As will be seen below, this A-phase is indeed an ESP state and it has a nodal gap structure.

6.8.1.2 *A*-Phase

The *A*-phase of superfluid ^{3}He is simply characterized by

$$\begin{aligned} \mathbf{d}(\mathbf{k}) &= \sqrt{\frac{3}{2}}(\hat{k}_y + \mathrm{i}\hat{k}_z, 0, 0) \ , \\ |\Psi(\hat{\mathbf{k}})\rangle &= -\psi\sqrt{\frac{3}{2}}(\hat{k}_y + \mathrm{i}\hat{k}_z)(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \ . \end{aligned} \tag{6.35}$$

So, in the *A*-phase, the excitation gap vanishes for $k_y = k_z = 0$; as shown in Fig. 6.3, it has two nodes on the poles of the Fermi surface. Moreover, this ESP state is unitary, as $\langle \mathbf{S} \rangle = \mathbf{0}$ (since $\mathbf{d^*(k)} \wedge \mathbf{d(k)} = \mathbf{0}$). But $\langle \mathbf{L} \rangle$ is non-zero. In fact, the orbital state is selected (by dipolar coupling), so that $\mathbf{d}$ and $\langle \mathbf{L} \rangle$ are either parallel or antiparallel. Following (6.28)

$$\begin{aligned} \langle \mathbf{L} \rangle &= \frac{\hbar}{\mathrm{i}} \oint \frac{d\Omega}{4\pi}(\hat{k}_y - \mathrm{i}\hat{k}_z)(\hat{\mathbf{k}} \wedge (\mathbf{e_y} + \mathrm{i}\mathbf{e_z}))/\oint \frac{d\Omega}{4\pi}(k_y^2 + k_z^2) \ , \\ \langle \mathbf{L} \rangle &\sim \frac{\hbar}{\mathrm{i}} \oint \frac{d\Omega}{4\pi}(\hat{k}_y - \mathrm{i}\hat{k}_z)\left(\mathrm{i}(\hat{k}_y + \mathrm{i}\hat{k}_z)\mathbf{e_x} + \hat{k}_x(\mathbf{e_z} - \mathrm{i}\mathbf{e_y})\right) \ , \\ \langle \mathbf{L} \rangle &\sim \hbar \oint \frac{d\Omega}{4\pi}\left((\hat{k}_y^2 + \hat{k}_z^2)\mathbf{e_x} + \cancel{(\hat{k}_y - \mathrm{i}\hat{k}_z)\hat{k}_x}(\mathbf{e_z} - \mathrm{i}\mathbf{e_y})\right) \ , \\ \langle \mathbf{L} \rangle &= \hbar\, \mathbf{e_x} \ . \end{aligned} \tag{6.36}$$

The physics of this phase is very rich, notably when considering the weak coupling between the orbital and spin moments due to spin–orbit interaction, the existence of spin currents, the chirality of the excitations close to the nodes… Again, the review by A. J. Leggett [1] is a seminal paper.

6.8.1.3 A_1 Phase

The A_1 phase appears under field with only one spin direction paired: it has the same orbital moment but in addition also a finite average spin. If we keep the same convention for the normalization of $|\Psi(\hat{\mathbf{k}})\rangle$ and $\mathbf{d(k)}$, despite the fact that only half the Fermi surface is paired, we get

$$\begin{aligned} |\Psi(\hat{\mathbf{k}})\rangle &= -\psi\sqrt{3}(\hat{k}_y + \mathrm{i}\hat{k}_z)|\uparrow\uparrow\rangle \ , \\ \mathbf{d(k)} &= \frac{\sqrt{3}}{2}((\hat{k}_y + \mathrm{i}\hat{k}_z), -\mathrm{i}(\hat{k}_y + \mathrm{i}\hat{k}_z), 0) \ . \end{aligned} \tag{6.37}$$

For this A_1 phase

$$\begin{aligned}\langle \mathbf{S}\rangle &= \mathrm{i}\hbar \oint \frac{\mathrm{d}\Omega}{4\pi}(\mathrm{d}_x \mathrm{d}_y^* - \mathrm{d}_y \mathrm{d}_x^*)\mathbf{e_z} \\ &= 2\,\hbar \oint \frac{\mathrm{d}\Omega}{4\pi}|k_y + i\ k_z|^2 \mathbf{e_z}/2 \oint \frac{\mathrm{d}\Omega}{4\pi}(k_y^2 + k_z^2) \\ &= \hbar\,\mathbf{e_z}\ , \\ \langle \mathbf{L}\rangle &= \hbar\,\mathbf{e_z}\ .\end{aligned} \tag{6.38}$$

Its stability arises from the fact that when the Fermi surface is polarized, the density of states increases with k_F, and from the fact that, in ^{3}He, the spin–orbit interaction is very weak. So, the up-spin and down-spin Fermi surfaces are almost completely decoupled and the largest Fermi surface may have a larger transition temperature than the other. Hence, the stability range of this A_1 phase grows under field (see Fig. 6.3).

As we shall see, the situation should be completely different in uranium-based ferromagnetic superconductors, where such a phase is very unlikely due to the coupling between the different Fermi sheets induced by spin–orbit interaction: like for most multigap superconductors, in such a case, there is a unique transition temperature, even if the different gaps may have different sizes. A possible very singular exception will be discussed in Sect. 6.10. Coming back to ^{3}He, the A_1 phase is the paradigm of a non-unitary state, with a finite value of $\langle \mathbf{S}\rangle$, a vanishing gap on one Fermi surface, and a nodal gap (axial gap) identical to that of the A-phase on the other Fermi surface.

6.8.1.4 Planar and Polar Phases

Some other states may also be favoured in ^{3}He, due to peculiar constraints [lower dimensions, aerogel (disordered) background, …]. These are in any case useful reference states for the more complicated cases of superconductors in crystal lattices. Notably, there is the planar phase and the polar phase, which are derived from the B-phase. The planar phase is defined by

$$\begin{aligned}\mathbf{d}(\mathbf{k}) &= \sqrt{\frac{3}{2}}(\hat{k}_x, \hat{k}_y, 0)\ , \\ |\Psi(\hat{\mathbf{k}})\rangle &= \psi\sqrt{\frac{3}{2}}\left((-\hat{k}_x + \mathrm{i}\hat{k}_y)|\uparrow\uparrow\rangle + (\hat{k}_x + \mathrm{i}\hat{k}_y)|\downarrow\downarrow\rangle\right)\ .\end{aligned} \tag{6.39}$$

Conversely, the polar phase is defined by

$$\begin{aligned}\mathbf{d}(\mathbf{k}) &= \sqrt{3}(0, 0, \hat{k}_z)\ , \\ |\Psi(\hat{\mathbf{k}})\rangle &= \psi\sqrt{3}\hat{k}_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\ .\end{aligned} \tag{6.40}$$

These two states have also $\langle \mathbf{S} \rangle = 0$ and $\langle \mathbf{L} \rangle = 0$; however, the planar state has point nodes along the z-axis whereas the polar state has a line of nodes on the equator. Both are also unitary, ESP states (see Sect. 6.5.3).

6.8.2 *UPt_3 and Sr_2RuO_4*

UPt_3 is a 'heavy fermion' metal, meaning that it is an inter-metallic system with very strong electronic correlation effects, leading to a strong renormalization of the effective mass of the electronic quasiparticles. It has been the first heavy fermion where these effective masses have been directly measured (up to 160 times the free electron mass) on the different Fermi sheets, by quantum oscillations, and it has also been the first superconducting system (after superfluid ^{3}He) where phase transitions between different superconducting phases have been observed (see [6] for a review and Fig. 6.4).

6.8.2.1 Phases of UPt_3

The reasons leading to these phase transitions and the nature of the various superconducting phases have been the subject of many different proposals. There is a global consensus that superconductivity in UPt_3 should be triplet (odd parity). Nevertheless, many questions remain without a definite answer. A first (still open) question, for example, is whether or not the spin component is free to rotate in the hexagonal crystal lattice of UPt_3. This will determine the response of UPt_3 under the application of an external field when it is superconducting. The orbital part (the **k**-dependence) of the superconducting order parameter is constrained by the broken symmetries in the superconducting state inducing, for example, nodes of the order parameter and so of the gap in some particular directions: if spin–orbit coupling is strong enough, then the **d**-vector is expected to be pinned in some crystal direction; if spin–orbit coupling is weak, as in superfluid ^{3}He, the **d**-vector should be free to rotate and the response to a magnetic field should have the same anisotropy as in the normal phase. Because pairing is mainly driven by the $5f$ electrons, spin–orbit coupling is expected to be strong also for the Cooper pair wave function, and pinning of the **d**-vector is likely. However, this hypothesis has no definite experimental support (see Sect. 6.8.2.3).

6.8.2.2 E_{2u} Representation

Among the models assuming such a strong spin–orbit coupling pinning the **d**-vector in a fixed crystallographic direction, the so-called E_{2u} representation has been strongly developed. It is an 'f-wave' order parameter, which can have various symmetries (six basis functions are necessary to describe the most general order parameter). Among these, the most successful [7] proposes a **d**-vector with some

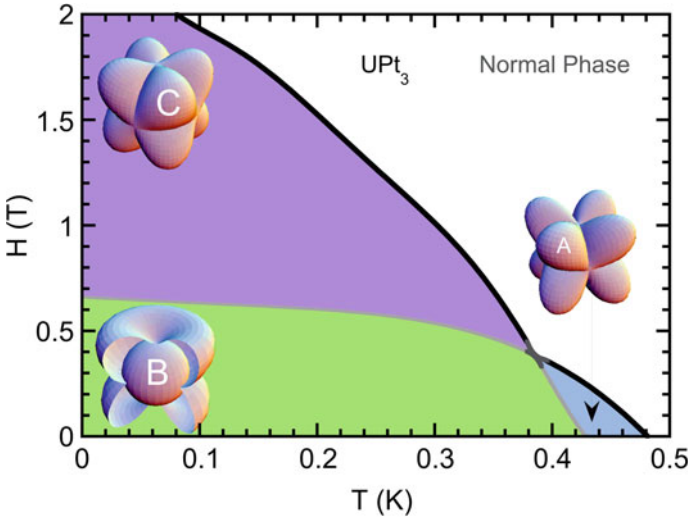

Fig. 6.4 Phase diagram, in the temperature–magnetic field space, of the superconducting phases of UPt_3. Three different phases called A, B and C corresponding to different symmetries and **d**-vectors have been identified. The gap structure is also shown for the different phases, like for superfluid ^{3}He in Fig. 6.3, as proposed for the 'E_{2u} model'. This E_{2u} model is coherent with results from thermal transport and upper critical field measurements, but not with NMR measurements of the Knight shift (see Sect. 6.8.2.3)

accidental restrictions (like the fact that the **d**-vector would only have components along the hexagonal c-axis); with these restrictions, it matches numerous experimental probes.

$$\mathbf{d}(\mathbf{k}) = \left(\varphi_A(T) 2k_x k_y k_z + \varphi_C(T) k_z (k_x^2 - k_y^2)\right) \mathbf{e}_z \ . \tag{6.41}$$

In the A-phase, $\varphi_C(T) = 0$, in the C-phase, $\varphi_A(T) = 0$, and in the B-phase, at low temperature and low field, $\varphi_A(T) = \pm i\ \varphi_C(T)$: $\mathbf{d}(\mathbf{k}) = \varphi(T) k_z (k_x \pm \mathrm{i} k_y)^2 \mathbf{e}_z$. For this model, all phases are unitary, but the B-phase is chiral, with a non-zero $\langle \mathbf{L} \rangle$. Muon experiments or recently polar Kerr effect [8] could have detected such a chiral component.

With its pinned **d**-vector, in the A- and C-phases, the spin component is zero along the c-axis ($\mathbf{d} \parallel \mathbf{e}_z$), and for any field direction in the basal plane, the order parameter behaves as an ESP state (see Sect. 6.5.3). So the Pauli spin susceptibility should be suppressed (like for a singlet superconductor), whereas it will be unchanged in the basal plane. This feature, which guided the choice of this E_{2u} representation, can explain the famous 'crossing' of the upper critical fields (H_{c2}) of UPt_3 [9] along the basal plane (no Pauli limitation of H_{c2}) and the c-axis (Pauli limitation of H_{c2}).

6.8.2.3 E_{1u} Representation

However, NMR experiments seem to be in contradiction with this interpretation of the crossing of the upper critical fields of UPt_3. Indeed Knight-shift measurements, which are the closest to a measure of the spin susceptibility in the superconducting state, found no change in the superconducting state for fields applied along the **a** or **b** directions in the C-phase, but also no change for field along the c-axis except at very low field deep inside the B-phase [11]. Therefore, other models have been proposed for UPt_3, which are much closer to the situation of superfluid ^{3}He, with a weak spin–orbit coupling allowing for a field reorientation of the **d**-vector as long as the field is 'strong enough'. Knight-shift measurements can tell nothing on the gap nodes, but combining angle-dependent thermal conductivity measurements [10] with the NMR result, a E_{1u} scenario has been proposed, predicting a non-chiral state [$\mathbf{d}(\mathbf{k}) \propto (5\hat{k}_c^2 - 1)(\hat{k}_a \mathbf{e}_b + \hat{k}_b \mathbf{e}_c)$ in the B-phase]. This scenario can also more easily give account of some other features of the phase diagram (like the existence of a tetracritical point in all field directions): see Fig. 6.5. For the different phases, in this model, the **d**-vector would be as shown in Table 6.1.

So, as can be seen from Table 6.1, at low fields the **d**-vector does not depend on the field orientation [check the A-phase and B-phase-(low H) lines of the table]. In the B-phase, for $\mathbf{H} \parallel \mathbf{c}$, there is a field-induced reorientation of the **d**-vector: at low field, with $\mathbf{d} \propto (\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$, the **d**-vector is not perpendicular to the c-axis (except on the line $\hat{k}_b = 0$) so there is a finite $|S_z = 0\rangle$ component of the spin along the field. This would be imposed by the orbital part of the wave function and spin–orbit interaction or coupling to the small antiferromagnetic moments acting as a symmetry breaking field. But for fields above 0.22 T, with $\mathbf{d} \propto (\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_a)$, the **d**-vector is real and always perpendicular to the c-axis, so we know that it is equivalent to an ESP state in that direction. Hence, the field-induced rotation of the **d**-vector. In the high-field C-phase, where the Pauli limitation could be at play, we note that in Table 6.1 the **d**-vector is always perpendicular to the field direction, so that again, it is an ESP state explaining the observed absence of change of the Knight shift (but in contradiction with the H_{c2} anisotropy). Note also that all these features are preserved if in the B-phase, the **d**-vector is a complex combination of $\mathbf{e}_b$ and $\mathbf{e}_c$, or $\mathbf{e}_b$ and $\mathbf{e}_a$: $(\hat{k}_a\, \mathbf{e}_b \pm \mathrm{i}\hat{k}_b\, \mathbf{e}_c)$; $(\hat{k}_a\, \mathbf{e}_b \pm \mathrm{i}\hat{k}_b\, \mathbf{e}_a)$.

Then, the B-phase would be chiral (as in the E_{2u} model), but also non-unitary ($\mathbf{d}(\mathbf{k}) \wedge \mathbf{d}^*(\mathbf{k}) \neq 0$, see Sect. 6.6.3). So was the original proposal in [11]. It is an interesting example of a non-unitary state with no global spin polarization, e.g. with $\mathbf{d} \propto (5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \mathrm{i}\hat{k}_b\, \mathbf{e}_a)$, we derive from (6.25) and (6.31) that $\langle \mathbf{S}(\mathbf{k}) \rangle \propto (5\hat{k}_c^2 - 1)^2 \hat{k}_a \hat{k}_b \mathbf{e}_c$ and $\Delta^{\uparrow}(\mathbf{k}) \propto |(5\hat{k}_c^2 - 1)(\hat{k}_a + \hat{k}_b)|$, $\Delta^{\downarrow}(\mathbf{k}) \propto |(5\hat{k}_c^2 - 1)(\hat{k}_a - \hat{k}_b)|$. So indeed, averaging over the Fermi surface leads to no net spin and equal averaged gap amplitudes for up-spins and down-spins, even though they are different for most **k** of the Fermi surface.

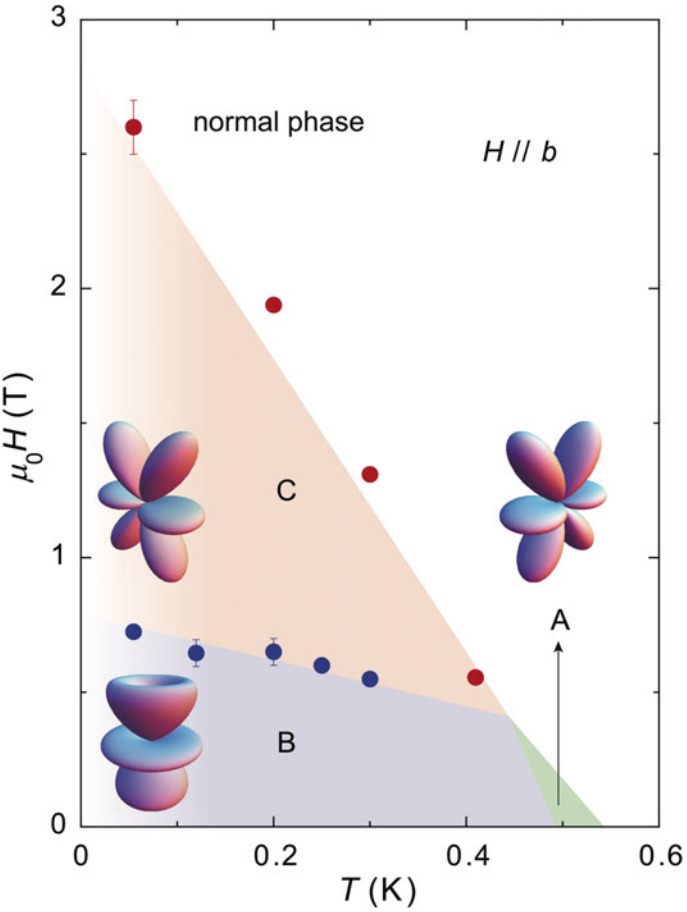

Fig. 6.5 Phase diagram in the temperature–magnetic field space of the superconducting phases of UPt_3 : the same phases as in Fig. 6.4 are represented, but different gap structures are proposed, according to the E_{1u} symmetry (the Fermi surface is reduced to a point in this representation). The magnetic field H is parallel to the lattice vector **b**. Reproduced from [10] with permission (Copyright 2012, American Physical Society)

6.8.2.4 p-Wave Superconductivity in Sr_2RuO_4

This system has also early been proposed as a candidate for p-wave superconductivity. In fact, due to the accessible range for the studies (T_{SC} is slightly larger than 1K), and the absence of radioactive elements, as well as the popularity of oxides, it is certainly the most studied 'p-wave' superconductor ever (for a review, see [12]). The most 'fashionable' order parameter is very similar to the superfluid ^{3}He A-phase

$$\mathbf{d}(\mathbf{k}) \propto (k_x \pm i\, k_y)\mathbf{e}_z \,. \tag{6.42}$$

Table 6.1 The **d**-vector for the various phases and magnetic field orientations in the E_{1u} model of UPt_3, as proposed in [10, 11]. The distinction 'low field' or 'high field' is meaningful only in the B-phase for $\mathbf{H} \parallel \mathbf{c}$, and is suggested by NMR measurements which show a decrease of the Knight shift in the whole B- and A-phases for $\mathbf{H} \parallel \mathbf{b}$, and for $\mathbf{H} \parallel \mathbf{c}$ in the B-phase only, and for fields lower than 0.22 T. Above this value, the **d**-vector would rotate and the change of the Knight shift disappears (see [11])

Phase	$\mathbf{H} \parallel \mathbf{a}$	$\mathbf{H} \parallel \mathbf{b}$	$\mathbf{H} \parallel \mathbf{c}$
A	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b)$
C	$(5\hat{k}_c^2 - 1)(\hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_b\, \mathbf{e}_a)$
B (low H)	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$
B (high H)	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_c)$	$(5\hat{k}_c^2 - 1)(\hat{k}_a\, \mathbf{e}_b + \hat{k}_b\, \mathbf{e}_a)$

It is a unitary chiral state with $\langle \mathbf{L} \rangle = \pm\hbar\, \mathbf{e_z}$ and point nodes along the c-axis. However, due to its quasi-2D Fermi surface, there is no $\mathbf{k}$ vector on the Fermi surface at the node position. There are many contradictory experiments on this system and several have claimed to have detected or refuted the time-reversal symmetry breaking in this compound (this is also true for the B-phase of UPt_3). So today, there is still no firm conclusion on whether or not (6.42) is the correct gap symmetry for Sr_2RuO_4, and even on whether or not it is really a p-wave superconductor. Indeed, the most recent NMR studies corrected previous results and demonstrate now that the Knight shift does decrease in the superconducting phase when the field is applied in the basal plane, ruling out one of the strongest support for an order parameter of the above form [13, 14].

6.9 Ferromagnetic Superconductors

Since 2000, three systems with a true homogeneous coexistence of ferromagnetic order and superconductivity have been discovered; all of them are uranium based. The first, UGe_2 [15], is only superconducting under pressure, the other two, URhGe [16] and UCoGe [17], are superconducting at ambient pressure. In the three cases, the same $5f$ electrons from the uranium ions are responsible for the ferromagnetic and the superconducting orders, and the Curie temperature (T_{Curie}) is always larger than the superconducting transition temperature (T_{SC}). Intuitively, these two orders seem antagonistic, as it is known that superconductivity is suppressed by large fields. However, it is important to be more precise in order to understand why and how ferromagnetism and superconductivity might coexist.

The first point to have in mind is the two kinds of magnetic fields associated with ferromagnetic order: there is an internal magnetic field B_{int} also called the 'dipolar field', arising from the spontaneous magnetization in the sample ($\mathbf{B} \approx \mathbf{M}$,

Table 6.2 Orders of magnitude of some important parameters, including an estimate of the internal (dipolar) magnetic field B_{int} (coming from the spontaneous magnetization) and the effective exchange field B_{exc}, in the three known uranium-based ferromagnetic superconductors. For UGe_2, which is superconducting only under pressure, we have indicated the Curie temperature and the ordered moment μ_{ord} at the pressure of 1.2 GPa, where T_{SC} is maximum. For B_{exc} we only give a lower bound deduced from the value of the Curie temperature

	UGe_2 (1.2 GPa)	URhGe	UCoGe
T_{Curie}	35 K	9.5 K	2.5 K
T_{SC}	0.8 K	0.25 K	0.5 K
μ_{ord}	$\approx 1\ \mu_{\text{B}}$	$0.4\ \mu_{\text{B}}$	$0.05\ \mu_{\text{B}}$
$B_{int} \approx M$	0.2 T	0.09 T	0.1 T
$B_{exc} > \frac{k_{\text{B}}}{\mu_{\text{B}}} T_{\text{Curie}}$	50 T	13 T	4.5 T

if one neglects demagnetization effects) and there is the exchange field B_{exc} which is a very short range effective magnetic field, acting only on the electron spins, and arising from the Coulomb interaction and the exclusion principle. This exchange field appears in a mean-field treatment of the spin–spin exchange interaction term. These two fields have very different orders of magnitude. The first is rather small in these systems, owing to the weak ordered moment (see Table 6.2); indeed, the three compounds, when they are not in the itinerant limit, remain close to it, so that this internal field is in any case much smaller than the (large) orbital upper critical field. However, the exchange field, whose scale is fixed by $k_{\text{B}} T_{\text{Curie}}/\mu_{\text{B}}$, is much larger than the Pauli paramagnetic limit (of the order of $2k_{\text{B}} T_{SC}/\mu_{\text{B}}$). Table 6.2 reports the values of these fields for the different compounds; a recent review has been published in [18].

6.9.1 ESP States

In these uranium-based ferromagnetic superconductors, superconductivity sets in below T_{Curie}, so that Cooper pairs are formed from a spin-polarized Fermi surface. Intuitively, one can guess that if the polarization is large enough (typically, if the difference in the Fermi wave vectors is larger than the inverse coherence length), this leaves little choice but to form Cooper pairs 'independently' on the Fermi sheets with different spin orientations (see Fig. 6.6). In other words, the strong exchange field present in the uranium-based ferromagnetic superconductors seems only consistent with an odd-parity (triplet) superconducting order parameter. Moreover, in case of large polarization of the bands (compared to Δ), one expects only ESP states to be favoured. Choosing the quantization axis along the easy axis

$$|\Psi\rangle = \Delta^{\uparrow} |\uparrow\uparrow\rangle + \Delta^{\downarrow} |\downarrow\downarrow\rangle \,. \tag{6.43}$$

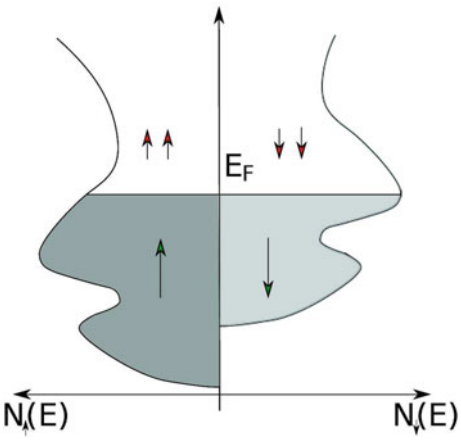

Fig. 6.6 Scheme of the spin-dependent density of states in a ferromagnetic metal. If superconductivity develops on spin-polarized Fermi surfaces, due to the difference of wave vectors at the Fermi level, mainly up-up and down-down Cooper pairs can be formed (short arrows). This leads to an ESP state with different weights for the majority and minority spins, so to a non-unitary ESP state

In such a case, the **d**-vector would have the general form:

$$\begin{cases} d_x = \dfrac{1}{2\psi}(-\Delta^{\uparrow} + \Delta^{\downarrow}) \\ d_y = \dfrac{-i}{2\psi}(\Delta^{\uparrow} + \Delta^{\downarrow}) \\ d_z = 0 \end{cases} . \tag{6.44}$$

Then $\langle \mathbf{S} \rangle$ at a given $\mathbf{k}$ is

$$\begin{aligned} \langle \mathbf{S} \rangle &= i\,\hbar(\mathbf{d} \wedge \mathbf{d}^*) \\ &= -\frac{\hbar}{4\psi}\left((-\Delta^{\uparrow} + \Delta^{\downarrow})(\Delta^{\uparrow *} + \Delta^{\downarrow *}) + \Delta^{\uparrow} + \Delta^{\downarrow})(-\Delta^{\uparrow *} + \Delta^{\downarrow *})\right)\mathbf{e}_z \\ &= \hbar\frac{\left(|\Delta^{\uparrow}|^2 - |\Delta^{\downarrow}|^2\right)}{\left(|\Delta^{\uparrow}|^2 + |\Delta^{\downarrow}|^2\right)}\mathbf{e}_z \,. \end{aligned} \tag{6.45}$$

This has been already seen when discussing ESP states [see (6.27)]. It is a very natural result; for an ESP state, there is a finite spin (and non-unitary state) if and only if the weights of the $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ components are unbalanced. Conversely, for a ferromagnetic superconductor with at least partial band polarization, one does expect to have such a non-unitary state, which should be an ESP for a 'strong enough' exchange field. It could also be chiral, but it should be at least non-unitary. Before that, let us see what are the possible order parameter from group theory considerations for orthorhombic systems [19].

6.9.2 Symmetries

Only two one-dimensional representations are left, called A and B, due to the low orthorhombic symmetry. In the paramagnetic state, the first one (A) looks very much like the B-phase of superfluid ^{3}He

$$\mathbf{d}_A(\mathbf{k}) \propto u_x \hat{k}_x \mathbf{e}_x + u_y \hat{k}_y \mathbf{e}_y + u_z \hat{k}_z \mathbf{e}_z \ , \tag{6.46}$$

where u_x, u_y, u_z are real functions of $\mathbf{k}$ with full orthorhombic symmetry. So in the paramagnetic state, we start from

$$\begin{cases} \Delta_A^{\uparrow} = -u_x \hat{k}_x + \mathrm{i} u_y \hat{k}_y \\ \Delta_A^{\downarrow} = +u_x \hat{k}_x + \mathrm{i} u_y \hat{k}_y \\ \Delta_A^{0} = u_z \hat{k}_z \end{cases} . \tag{6.47}$$

In the ferromagnetic state, the amplitude (and possibly the phase) of the $\Delta_A^{\uparrow}$ and $\Delta_A^{\downarrow}$ components can differ. So the order parameter should read

$$\begin{cases} \Delta_A^{\uparrow} = \eta^{\uparrow}(-u_x \hat{k}_x + \mathrm{i} u_y \hat{k}_y) = -\eta_x^{\uparrow} \hat{k}_x + \mathrm{i} \eta_y^{\uparrow} \hat{k}_y \\ \Delta_A^{\downarrow} = \eta^{\downarrow}(+u_x \hat{k}_x + \mathrm{i} u_y \hat{k}_y) = \eta_x^{\downarrow} \hat{k}_x + \mathrm{i} \eta_y^{\downarrow} \hat{k}_y \\ \Delta_A^{0} = \eta^{0} u_z \hat{k}_z = \eta_z^{0} \hat{k}_z \end{cases} \tag{6.48}$$

with no phase difference between the complex amplitudes $\eta^{\uparrow}$, $\eta^{\downarrow}$, η^0. In terms of $\mathbf{d}$-vectors

$$\begin{aligned} \mathbf{d} &= \frac{1}{2\psi}[-\Delta^{\uparrow}(\hat{\mathbf{n}})(\mathbf{e}_x + \mathrm{i}\mathbf{e}_y) + \Delta^{\downarrow}(\hat{\mathbf{n}})(\mathbf{e}_x - \mathrm{i}\mathbf{e}_y)] + \Delta^0 \mathbf{e}_z \\ &= \frac{1}{2\psi}[(\eta_x^{\uparrow} \hat{k}_x - \mathrm{i}\eta_y^{\uparrow} \hat{k}_y)(\mathbf{e}_x + \mathrm{i}\mathbf{e}_y) + (\eta_x^{\downarrow} \hat{k}_x + \mathrm{i}\eta_y^{\downarrow} \hat{k}_y)(\mathbf{e}_x - \mathrm{i}\mathbf{e}_y)] + \eta_z^0 \hat{k}_z \mathbf{e}_z \\ &= \frac{1}{2\psi} \left\{ \left[\left(\eta_x^{\uparrow} + \eta_x^{\downarrow}\right) \hat{k}_x - \mathrm{i} \left(\eta_y^{\uparrow} - \eta_y^{\downarrow}\right) \hat{k}_y \right] \mathbf{e}_x \right. \\ &\quad \left. + \left[\left(\eta_y^{\uparrow} + \eta_y^{\downarrow}\right) \hat{k}_y + \mathrm{i} \left(\eta_x^{\uparrow} - \eta_x^{\downarrow}\right) \hat{k}_x \right] \mathbf{e}_y + 2\eta_z^0 \hat{k}_z \mathbf{e}_z \right\} . \end{aligned} \tag{6.49}$$

Similarly for the B-phase, the order parameter reads

$$\begin{cases} \Delta_B^{\uparrow} = \zeta_z^{\uparrow} \hat{k}_z \\ \Delta_B^{\downarrow} = \zeta_z^{\downarrow} \hat{k}_z \\ \Delta_B^{0} = \zeta_x^{0} \hat{k}_x + \mathrm{i} \zeta_y^{0} \hat{k}_y \end{cases} \tag{6.50}$$

$$\begin{aligned}\mathbf{d} &= \frac{1}{2\psi}[-\Delta^{\uparrow}(\hat{\mathbf{n}})(\mathbf{e}_x + \mathrm{i}\mathbf{e}_y) + \Delta^{\downarrow}(\hat{\mathbf{n}})(\mathbf{e}_x - \mathrm{i}\mathbf{e}_y)] + \Delta^0\mathbf{e}_z \\ &= \frac{1}{2\psi}[(-\zeta_z^{\uparrow}\hat{k}_z)(\mathbf{e}_x + \mathrm{i}\mathbf{e}_y) + (\zeta_z^{\downarrow}\hat{k}_z)(\mathbf{e}_x - \mathrm{i}\mathbf{e}_y)] + (\zeta_x^0\hat{k}_x + \mathrm{i}\zeta_y^0\hat{k}_y)\mathbf{e}_z \\ &= \frac{1}{2\psi}\left\{\left(\zeta_z^{\downarrow} - \zeta_z^{\uparrow}\right)\hat{k}_z\mathbf{e}_x - \mathrm{i}\left(\zeta_z^{\uparrow} + \zeta_z^{\downarrow}\right)\hat{k}_z\mathbf{e}_y + 2\left(\zeta_x^0\hat{k}_x + \mathrm{i}\zeta_y^0\hat{k}_y\right)\mathbf{e}_z\right\}.\end{aligned} \tag{6.51}$$

In the general case, neither the A- nor the B-phase have symmetry-enforced nodes. However, if an ESP state is enforced by strong band splitting, meaning that the Δ^0 component vanishes in (6.48) and (6.50), then

- the order parameter of the A-phase vanishes for $k_x = k_y = 0$: the A-phase has poles on the z-axis and
- the order parameter of the B-phase vanishes for $k_z = 0$: the B-phase has a line of nodes on the equator.

This is correct, but maybe more important insights on these ferromagnetic superconductors can be learned, notably on the relationship between up and down components, from a more general microscopic model [19]. The equations look unfriendly at first sight, but at the end, a nice physical picture emerges.

6.9.3 Microscopic Model

For these ferromagnetic superconductors, all models start from the same pairing interaction, supposed to arise from the magnetic interactions: this was already proposed in the de Gennes book on superconductivity ([20] page 104)! So they start from a Hamiltonian

$$H_{int} = -\frac{1}{2}\mu_B^2 I^2 \int \mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{r}' S_i(\mathbf{r})\chi_{ij}(\mathbf{r}-\mathbf{r}')S_j(\mathbf{r}') \,, \tag{6.52}$$

where I is an exchange constant and χ_{ij} the medium magnetic susceptibility (matrix). The models differ notably on the expression for this susceptibility. However, starting from such an Hamiltonian, the derived gap equations necessarily couple the different components of the order parameter. In the case of ferromagnetic superconductors, a peculiarity found in all systems is that the susceptibility has a marked uniaxial anisotropy (Ising type), so that if z is the easy magnetization axis, χ_{zz} will be a dominant term in the susceptibility matrix.

In the following, we will just present and comment the linearized gap equations (in the weak-coupling limit) to show where the approximations come into play and what are the physical consequences. To understand the derivation of these equations, please refer to [19]. The gap equations (at T_{SC}) read

$$\begin{cases} \Delta^{\uparrow}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{\uparrow\uparrow}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') \\ \qquad\qquad + V^{\uparrow\downarrow}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}') + V^{\uparrow 0}(G^{\downarrow}G^{\uparrow} + G^{\uparrow}G^{\downarrow})\Delta^{0}(\mathbf{k}')] \\ \Delta^{\downarrow}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{\downarrow\uparrow}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') \\ \qquad\qquad + V^{\downarrow\downarrow}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}') + V^{\downarrow 0}(G^{\downarrow}G^{\uparrow} + G^{\uparrow}G^{\downarrow})\Delta^{0}(\mathbf{k}')] \\ \Delta^{0}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{0\uparrow}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') \\ \qquad\qquad + V^{0\downarrow}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}') + V^{00}(G^{\downarrow}G^{\uparrow} + G^{\uparrow}G^{\downarrow})\Delta^{0}(\mathbf{k}')] \end{cases}, \tag{6.53}$$

where the different interaction terms $V^{\alpha\beta}$ are expressed from the susceptibility by

$$\begin{cases} V^{\uparrow\uparrow} = -\mu_{\mathrm{B}}^2 I^2 \chi^u_{zz} & ;\ V^{\downarrow\downarrow} = -\mu_{\mathrm{B}}^2 I^2 \chi^u_{zz} \\ V^{\uparrow\downarrow} = -\mu_{\mathrm{B}}^2 I^2 (\chi^u_{xx} - \chi^u_{yy} - 2\mathrm{i}\chi^u_{xy}) & ;\ V^{\downarrow\uparrow} = -\mu_{\mathrm{B}}^2 I^2 (\chi^u_{xx} - \chi^u_{yy} + 2\mathrm{i}\chi^u_{xy}) \\ V^{\uparrow 0} = -\mu_{\mathrm{B}}^2 I^2 (\chi^u_{xz} - \mathrm{i}\chi^u_{yz} + 2\mathrm{i}\chi^u_{xy}) & ;\ V^{\downarrow 0} = -\mu_{\mathrm{B}}^2 I^2 (-\chi^u_{xz} - \mathrm{i}\chi^u_{yz} + 2\mathrm{i}\chi^u_{xy}) \\ V^{00} = -\mu_{\mathrm{B}}^2 I^2 \dfrac{\chi^u_{xx} + \chi^u_{yy} - \chi^u_{zz}}{2} & \end{cases}. \tag{6.54}$$

In the above equations,

$$V^{\alpha\beta} = V^{\alpha\beta}(\mathbf{k}, \mathbf{k}') \text{ and } \chi^u_{ij} = \chi^u_{ij}(\mathbf{k}, \mathbf{k}') = \tfrac{1}{2}\left(\chi_{ij}(\mathbf{k} - \mathbf{k}') - \chi_{ij}(\mathbf{k} + \mathbf{k}')\right).$$

Strong band polarization (like that due to an 'exchange field') much larger than T_{SC} means that we can cancel all terms with Green functions arising from bands of opposite spins ($G^{\downarrow}G^{\uparrow}$-type terms). However, (6.53) shows that this is not enough to ensure an ESP state with $\Delta^0(\mathbf{k}) = 0$. Indeed, the different components are all coupled together as a multigap system and a non-zero $\Delta^0(\mathbf{k})$ can be induced by the $\Delta^{\uparrow}$, $\Delta^{\downarrow}$ components

$$\begin{cases} \Delta^{\uparrow}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{\uparrow\uparrow}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') + V^{\uparrow\downarrow}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}')] \\ \Delta^{\downarrow}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{\downarrow\uparrow}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') + V^{\downarrow\downarrow}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}')] \\ \Delta^{0}(\mathbf{k}) = -T\sum\limits_{n}\sum\limits_{\mathbf{k}'}[V^{\uparrow 0}G^{\uparrow}G^{\uparrow}\Delta^{\uparrow}(\mathbf{k}') + V^{\downarrow 0}G^{\downarrow}G^{\downarrow}\Delta^{\downarrow}(\mathbf{k}')] \end{cases}. \tag{6.55}$$

To go further, we need to make approximations based on the characteristics of the susceptibility. All non-diagonal terms of χ_{ij} are zero at $k = 0$, but, in principle, can be finite at finite $\mathbf{k}$. In a Landau framework, they would arise from gradient terms of the form $\frac{\partial M_i}{\partial x_j}$, so from spin–orbit coupling. If the spin–orbit coupling is weak enough, we can further neglect these terms, then $V^{\uparrow 0}$ and $V^{\downarrow 0}$ are suppressed and we do get an ESP state: $\Delta^0(\mathbf{k}) = 0$. However, in uranium-based systems, spin–orbit

coupling is usually considered as 'strong' and most models suppose that the **d**-vector has a fixed direction, imposed by the orbital part of the order parameter and … spin–orbit coupling. Therefore, considering these systems as pure ESP states is probably only an approximation: spin–orbit coupling most likely induces a (small?) Δ^0 finite component, even with strong band polarization! But this is not the only surprise which emerges from these microscopic equations. Even if we suppose that $\Delta^0 = 0$, another counter-intuitive result emerges. The equations in the 'ESP approximation' are written as

$$\begin{cases} \Delta^{\uparrow}(\mathbf{k}) = -T \sum\limits_{n} \sum\limits_{\mathbf{k}'} [V^{\uparrow\uparrow} G^{\uparrow} G^{\uparrow} \Delta^{\uparrow}(\mathbf{k}') \; + V^{\uparrow\downarrow} G^{\downarrow} G^{\downarrow} \Delta^{\downarrow}(\mathbf{k}')] \\ \Delta^{\downarrow}(\mathbf{k}) = -T \sum\limits_{n} \sum\limits_{\mathbf{k}'} [V^{\downarrow\uparrow} G^{\uparrow} G^{\uparrow} \Delta^{\uparrow}(\mathbf{k}') \; + V^{\downarrow\downarrow} G^{\downarrow} G^{\downarrow} \Delta^{\downarrow}(\mathbf{k}')] \end{cases} \tag{6.56}$$

with

$$\begin{cases} V^{\uparrow\uparrow} = \quad V^{\downarrow\downarrow} = -\mu_{\mathrm{B}}^2 I^2 \chi_{zz}^{u} \\ V^{\uparrow\downarrow} = \quad V^{\downarrow\uparrow} = -\mu_{\mathrm{B}}^2 I^2 (\chi_{xx}^{u} - \chi_{yy}^{u}) \end{cases} . \tag{6.57}$$

It corresponds to the equations of a two-band superconductor, with intra-band coupling controlled by the longitudinal susceptibility χ_{zz}^{u} and inter-band coupling controlled by transverse susceptibilities.

For such ESP states, the possible order parameters of ferromagnetic superconductors are the above-mentioned A or B states, with **d**-vector

$$\begin{aligned} \mathbf{d}_A = \frac{1}{2\psi} \Big\{ \Big[\left(\eta_x^{\uparrow} + \eta_x^{\downarrow}\right) \hat{k}_x - \mathrm{i} \left(\eta_y^{\uparrow} - \eta_y^{\downarrow}\right) \hat{k}_y \Big] \mathbf{e}_x \\ + \Big[\left(\eta_y^{\uparrow} + \eta_y^{\downarrow}\right) \hat{k}_y + \mathrm{i} \left(\eta_x^{\uparrow} - \eta_x^{\downarrow}\right) \hat{k}_x \Big] \mathbf{e}_y \Big\} \; , \\ \mathbf{d}_B = \frac{1}{2\psi} \Big\{ \left(\eta_z^{\downarrow} - \eta_z^{\uparrow}\right) \hat{k}_z \mathbf{e}_x \; - \mathrm{i} \left(\eta_z^{\uparrow} + \eta_z^{\downarrow}\right) \hat{k}_z \mathbf{e}_y \Big\} \; . \end{aligned} \tag{6.58}$$

At the same level of approximation, equations for η_x, η_y are decoupled. So, for both the A and B states, the equation for the largest T_{SC} is that of a two-band superconductor (where ϵ is a characteristic energy)

$$\begin{aligned} T_{SC} &= \epsilon \exp\left(-\frac{1}{g}\right) \; , \\ g &= \frac{g_1^{\uparrow} + g_1^{\downarrow}}{2} + \sqrt{\frac{\left(g_1^{\uparrow} - g_1^{\downarrow}\right)^2}{4} + g_2^{\uparrow} g_2^{\downarrow}} \; . \end{aligned} \tag{6.59}$$

Here, $g_1^{\uparrow,\downarrow} \propto V^{\uparrow\uparrow,\downarrow\downarrow} \propto \chi_{zz}$, $g_2^{\uparrow,\downarrow} \propto V^{\uparrow\downarrow,\downarrow\uparrow} \propto (\chi_{xx} - \chi_{yy})$. Equation (6.59) shows that, as for any two-band superconductor, T_{SC} should increase if the inter-band coupling is increased. In this case, T_{SC} should increase if the difference between the transverse susceptibilities increases. This is surprising for two reasons.

The first is that it was believed, since the pioneering work of D. Fay and J. Appel [21], that Ising anisotropy was most favourable for ferromagnetic superconductors because transverse fluctuations would be pair-breaking as they would force scattering from one Fermi sheet to the opposite polarization Fermi sheet. However, this paper was written before the discovery of superconducting MgB_2 and the following boost of work on multigap superconductivity: we understand now that these transverse fluctuations do also induce exchange of Cooper pairs from one Fermi sheet to the other, which is favourable to superconductivity. And so the prediction is that 2D anisotropy (rather than uniaxial anisotropy) is the most favourable for ferromagnetic superconductors (maximizing both χ_{zz} and $\chi_{xx} - \chi_{yy}$).

The second reason is that, experimentally, all the systems where ferromagnetic superconductivity has been discovered did show a strong uniaxial anisotropy, confirming the prediction from [21]. But making statistics on few elements is always dangerous. We also found that reducing this uniaxial anisotropy in URhGe, using stress along the b-axis which increases the χ_{bb} susceptibility without changing χ_{cc} (for stress below 0.6 GPa), does increase T_{SC} in URhGe: a factor 2 between 0 and 1 GPa [22]. Ising anisotropy is probably not the most favourable, and larger T_{SC} ferromagnetic superconductors might be awaiting to be discovered.

Coming back to the consequences of (6.58) in terms of order parameter, with decoupling of the equations for η_x and η_y, the order parameter should have a line of node, (k_x or k_y or $k_z = 0$), a finite $\langle \mathbf{S} \rangle$ of order (at given $\mathbf{k}$)

$$\begin{aligned} \langle \mathbf{S}(\mathbf{k}) \rangle &= \hbar \left(\frac{\delta}{\eta} \right) \left(\frac{k_i^2}{\langle k_i^2 \rangle} \right) \mathbf{e}_z \ , \\ \delta = \frac{\eta_i^{\uparrow} - \eta_i^{\downarrow}}{2} \ ; &\qquad \eta = \frac{\eta_i^{\uparrow} + \eta_i^{\downarrow}}{2} \ . \end{aligned} \tag{6.60}$$

But it is not chiral ($\langle \mathbf{L} \rangle = 0$). The A state could be chiral if η_x and η_y remain coupled (in this model, if $\chi_{xy} \neq 0$), with

$$\langle \mathbf{L} \rangle = \hbar \frac{(\delta_y \eta_x + \delta_x \eta_y) \langle k_x^2 + k_y^2 \rangle}{(\eta_x^2 + \delta_x^2) \langle k_x^2 \rangle + (\eta_y^2 + \delta_y^2) \langle k_y^2 \rangle} \mathbf{e}_z \ . \tag{6.61}$$

Note that in principle too, if such is the case, $\mathbf{d}$ is probably not an ESP state any more, meaning that the Δ_0 component should be non-negligible and all expressions should be much more complex.

6.10 UTe_2

The last discovered p-wave superconductor is again an uranium-based system, also orthorhombic, and again close to a ferromagnetic instability but not ferromagnetic: UTe_2. This time, the T_{SC} is even more accessible: between 1.4 and 1.6 K from bulk measurements depending on the samples [23, 24]! Moreover, it presents similar astonishing field-reinforced superconductivity [23, 25, 26], with an absolute record (for such a low-T_{SC} system) of an upper critical field higher than 60 T [26]! An interesting point concerning the possible **d**-vector for such a paramagnetic system is the observation, on all samples, of a finite residual term of about half the normal state value of the specific heat C/T. The origin of this term is still unsettled, but an interesting proposal was that it would arise from a state similar to the A_1 state of superfluid ^{3}He (see Sect. 6.8.1.3).

Naturally, this can only happen if spin–orbit coupling is weak enough (otherwise, it would not be possible to form Cooper pairs on one Fermi surface and not on the other), and in this case, indeed, group theory classification leads to the possibility of such states (see Table 1 in [27])

$$\mathbf{d}(\mathbf{k}) = (1, i, 0)\varphi(\mathbf{k}) \ . \tag{6.62}$$

Moreover, because this is for a weak spin–orbit case, any rotation of the **d**-vector is a possible order parameter. According to (6.17), this means that the order parameter would be simply $\Delta(\mathbf{k}) = \Delta^{\uparrow}\varphi(\mathbf{k})$, with no other component. In the case of UTe_2, the largest susceptibility axis is the a-axis, so the quantization axis should be along **a**. In such a case, the Fermi surface with down-spin would remain unpaired, explaining the residual specific heat term.

Another consequence of such an order parameter is that it is non-unitary, with a finite spin for the Cooper pairs (along the a-axis). For the total system, this spin of the Cooper pairs would be compensated by that of the unpaired electrons (from the down-spin Fermi surface). This might lead to a total null magnetization. Nevertheless, in such a case, there is no reason that the state with such a **d**-vector would be stabilized, as half the condensation energy is lost compared to any other state, where pairing occurs on Fermi sheets of each spin direction. For such a state to be favoured, one needs some advantage of having this spin polarization in the superconducting state, so, for example, a form of coupling between the spin Cooper pairs and the normal state magnetization [27]. Then, this would also induce, like for superfluid ^{3}He in the A_1 state [28], a finite magnetization when entering the superconducting phase; globally, it is as if the system would become ferromagnetic on entering the superconducting state, with a (weak?) magnetization increasing linearly with temperature below T_{SC} [27]. Up to now, this has not been detected, and it remains to be settled if this (rather improbable) hypothesis is valid or not.

In any case, this last system beautifully confirms that p-wave superconductors are an incredible playground, where almost every new system brings its own share of surprise and stimulating challenges.

6.11 Proofs and Exercise Solutions

6.11.1 Proof of the Cayley–Klein Relation

Proof

$$
\begin{aligned}
&\mathcal{R}_{\boldsymbol{\Omega}}(\mathbf{a}\cdot\boldsymbol{\sigma})\mathcal{R}_{-\boldsymbol{\Omega}} \\
&\quad= \left(\cos\Omega/2\,\mathbb{1} - \mathrm{i}\,\sin\Omega/2\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}\right)(\mathbf{a}\cdot\boldsymbol{\sigma})\left(\cos\Omega/2\,\mathbb{1} + \mathrm{i}\,\sin\Omega/2\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}\right) \\
&\quad= \left(\cos\Omega/2\,\mathbb{1} - \mathrm{i}\,\sin\Omega/2\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}\right)\Big[\cos\Omega/2\,(\mathbf{a}\cdot\boldsymbol{\sigma}) \\
&\qquad+\mathrm{i}\,\sin\Omega/2\,\left((\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\mathbb{1} + \mathrm{i}(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\cdot\boldsymbol{\sigma}\right)\Big] \\
&\quad= \cos^2\Omega/2\,(\mathbf{a}\cdot\boldsymbol{\sigma}) + \mathrm{i}\,\cos\Omega/2\,\sin\Omega/2\,(\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\mathbb{1} \\
&\qquad- \cos\Omega/2\,\sin\Omega/2\,(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\cdot\boldsymbol{\sigma} \\
&\qquad- \mathrm{i}\,\cos\Omega/2\,\sin\Omega/2\,\left(\mathbf{a}\cdot\hat{\boldsymbol{\Omega}}\mathbb{1} - \mathrm{i}(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\cdot\boldsymbol{\sigma}\right) \\
&\qquad+ \sin^2\Omega/2\,\left((\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})(\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}) + \mathrm{i}^2\,\left(\hat{\boldsymbol{\Omega}}\wedge(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\right)\cdot\boldsymbol{\sigma}\right) \\
&\quad= (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})(\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}) + \cos^2\Omega/2\left(\mathbf{a} - (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\right)\cdot\boldsymbol{\sigma} + \sin\Omega\,(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\cdot\boldsymbol{\sigma} \\
&\qquad- \sin^2\Omega/2\,\left(\hat{\boldsymbol{\Omega}}\wedge(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\right)\cdot\boldsymbol{\sigma} \\
&\quad= (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})(\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\sigma}) + \cos\Omega\left(\mathbf{a} - (\mathbf{a}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\right)\cdot\boldsymbol{\sigma} + \sin\Omega\,(\mathbf{a}\wedge\hat{\boldsymbol{\Omega}})\cdot\boldsymbol{\sigma} \\
&\quad= \mathcal{R}_{\boldsymbol{\Omega}}(\mathbf{a})\cdot\boldsymbol{\sigma}\,.
\end{aligned}
$$

6.11.2 Conservation of the Scalar Product under Rotation with the Definition (6.11)

Solution 6.1 Let us note that we can write, for any (complex) vectors $\mathbf{u}$, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$, …

$$
\begin{aligned}
u &= (\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\boldsymbol{\Omega} + \left(\mathbf{u} - (\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\boldsymbol{\Omega}\right) = \mathbf{u}\mathbf{d}_{\parallel} + \mathbf{u}\mathbf{d}_{\perp} \\
\mathcal{R}(\mathbf{u}) &= \mathbf{u}\mathbf{d}_{\parallel} + \mathcal{R}(\mathbf{u}\mathbf{d}_{\perp}) = \mathbf{u}\mathbf{d}_{\parallel} + \cos\Omega\,\mathbf{u}\mathbf{d}_{\perp} + \sin\Omega\,(\hat{\boldsymbol{\Omega}}\wedge\mathbf{u}) \\
\mathbf{a}\wedge(\mathbf{b}\wedge\mathbf{c}) &= \epsilon^{ijk}\epsilon^{klm}a_j b_l c_m = (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c} \\
(\mathbf{a}\wedge\mathbf{b})\wedge\mathbf{c} &= (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{c}\cdot\mathbf{b})\mathbf{a}\,.
\end{aligned}
$$

$$
\mathcal{R}(\mathbf{d})\cdot\mathcal{R}(\mathbf{u}) = \mathbf{d}_{\parallel}\cdot\mathbf{u}\mathbf{d}_{\parallel} + \mathcal{R}(\mathbf{d}_{\perp})\cdot\mathcal{R}(\mathbf{u}_{\perp}) \quad \text{so}
$$

$$
\begin{aligned}
&\mathcal{R}(\mathbf{d})\cdot\mathcal{R}(\mathbf{u})\\
&\quad=(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\\
&\qquad+\cos^2\Omega\left[\mathbf{d}\cdot\mathbf{u}-(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})-\cancel{(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})}+\cancel{(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})}\right]\\
&\qquad+\sin^2\Omega\left[\hat{\boldsymbol{\Omega}}\cdot(\mathbf{d}\wedge(\hat{\boldsymbol{\Omega}}\wedge u))\right]\\
&\qquad+\sin\Omega\cos\Omega\left[\cancel{\mathbf{d}\cdot(\hat{\boldsymbol{\Omega}}\wedge\mathbf{u})}+\cancel{\mathbf{u}\cdot(\hat{\boldsymbol{\Omega}}\wedge\mathbf{d})}\right]\\
&\quad=(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\\
&\qquad+\cos^2\Omega\left[\mathbf{d}\cdot\mathbf{u}-(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\right]\\
&\qquad+\sin^2\Omega\left[\mathbf{d}\cdot\mathbf{u}-(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}}(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\right]\\
&\mathcal{R}(\mathbf{d})\cdot\mathcal{R}(\mathbf{u})=\mathbf{d}\cdot\mathbf{u}.
\end{aligned}
$$

6.11.3 *Conservation of the Cross Product under Rotation with the Definition (6.11)*

We want to check if $\mathcal{R}(\mathbf{u}\wedge\mathbf{d})=\mathcal{R}(\mathbf{u})\wedge\mathcal{R}(\mathbf{d})$. To evaluate $\mathcal{R}(\mathbf{u}\wedge\mathbf{d})$, let us decompose $\mathbf{u}\wedge\mathbf{d}$ in parallel and perpendicular parts to $\boldsymbol{\Omega}$ (called $(\mathbf{ud})_\parallel$ and $(\mathbf{ud})_\perp$)

$$
\begin{aligned}
\mathbf{u}\wedge\mathbf{d}&=\underbrace{\cancel{(\mathbf{ud})_\parallel\wedge\mathbf{d}_\parallel}+(\mathbf{ud})_\perp\wedge\mathbf{d}_\perp)}_{(\mathbf{ud})_\parallel}+\underbrace{(\mathbf{ud})_\parallel\wedge\mathbf{d}_\perp)-(\mathbf{d}_\parallel\wedge(\mathbf{ud})_\perp)}_{(\mathbf{ud})_\perp}\\
&=\underbrace{[(\mathbf{u}\wedge\mathbf{d})\cdot\hat{\boldsymbol{\Omega}}]\hat{\boldsymbol{\Omega}}}_{(\mathbf{ud})_\parallel}+\underbrace{\left[(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathbf{d}_\perp\right]-\left[(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathbf{u}_\perp\right]}_{(\mathbf{ud})_\perp}
\end{aligned}
$$

$$
\mathcal{R}(\mathbf{u}\wedge\mathbf{d})=(\mathbf{ud})_\parallel+\mathcal{R}\left((\mathbf{ud})_\perp\right)
$$

$$
\begin{aligned}
&\mathcal{R}((\mathbf{ud})_\perp)\\
&\quad=\cos\Omega\,(\mathbf{ud})_\perp+\sin\Omega\,\hat{\boldsymbol{\Omega}}\wedge(\mathbf{ud})_\perp\\
&\quad=(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\left[\cos\Omega\,\mathbf{d}+\sin\Omega\,\hat{\boldsymbol{\Omega}}\wedge\mathbf{d}\right]-(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\left[\cos\Omega\,\mathbf{u}+\sin\Omega\,\hat{\boldsymbol{\Omega}}\wedge\mathbf{u}\right]\\
&\quad=(\mathbf{u}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathcal{R}(\mathbf{d})-(\mathbf{d}\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathcal{R}(\mathbf{u})\\
&\quad=(\mathcal{R}(\mathbf{u})\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathcal{R}(\mathbf{d})-(\mathcal{R}(\mathbf{d})\cdot\hat{\boldsymbol{\Omega}})\hat{\boldsymbol{\Omega}}\wedge\mathcal{R}(\mathbf{u})\\
&\quad=\hat{\boldsymbol{\Omega}}\wedge\left[\hat{\boldsymbol{\Omega}}\wedge(\mathcal{R}(\mathbf{d})\wedge\mathcal{R}(\mathbf{u}))\right]
\end{aligned}
$$

$$
\mathcal{R}(\mathbf{u}\wedge\mathbf{d})=\mathcal{R}(\mathbf{u})\wedge\mathcal{R}(\mathbf{d})+(\mathbf{ud})_\parallel-(\mathcal{R}(\mathbf{u})\wedge\mathcal{R}(\mathbf{d}))_\parallel
$$

$$
\begin{aligned}
&(\mathcal{R}(\mathbf{u}) \wedge \mathcal{R}(\mathbf{d}))_{\parallel} \\
&\quad = \mathcal{R}(\mathbf{u})_{\perp} \wedge \mathcal{R}(\mathbf{d})_{\perp} \\
&\quad = \Big(\cos\Omega\,\mathbf{u}_{\perp} + \sin\Omega\,(\hat{\mathbf{\Omega}} \wedge \mathbf{u}_{\perp})\Big) \wedge \Big(\cos\Omega\,\mathbf{d}_{\perp} + \sin\Omega\,(\hat{\mathbf{\Omega}} \wedge \mathbf{d}_{\perp})\Big) \\
&\quad = \cos^2\Omega\,(\mathbf{u}_{\perp} \wedge \mathbf{d}_{\perp}) \\
&\qquad + \sin^2\Omega\,(\hat{\mathbf{\Omega}} \wedge \mathbf{u}_{\perp}) \wedge (\hat{\mathbf{\Omega}} \wedge \mathbf{d}_{\perp}) \\
&\qquad + \sin\Omega\cos\Omega\Big(\mathbf{u}_{\perp} \wedge (\hat{\mathbf{\Omega}} \wedge \mathbf{d}_{\perp}) - \mathbf{d}_{\perp} \wedge (\hat{\mathbf{\Omega}} \wedge \mathbf{u}_{\perp})\Big) \\
&\quad = \cos^2\Omega\,(\mathbf{ud})_{\parallel} \\
&\qquad + \sin^2\Omega\,\Big((\hat{\mathbf{\Omega}} \wedge \mathbf{u}_{\perp})\cdot\mathbf{d}_{\perp}\Big)\,\hat{\mathbf{\Omega}} \\
&\qquad + \sin\Omega\cos\Omega\Big(\cancel{(\mathbf{u}_{\perp}\cdot\mathbf{d}_{\perp})\,\hat{\mathbf{\Omega}}} - \cancel{(\mathbf{d}_{\perp}\cdot\mathbf{u}_{\perp})\,\hat{\mathbf{\Omega}}}\Big) \\
&\quad = \cos^2\Omega\,(\mathbf{ud})_{\parallel} + \sin^2\Omega\,\Big((\mathbf{u} \wedge \mathbf{d}) \cdot \hat{\mathbf{\Omega}}\Big)\,\hat{\mathbf{\Omega}} = (\mathbf{ud})_{\parallel}
\end{aligned}
$$

So indeed, $\mathcal{R}(\mathbf{u} \wedge \mathbf{d}) = \mathcal{R}(\mathbf{u}) \wedge \mathcal{R}(\mathbf{d})$.

6.11.4 *Rotation of the* d*-Vector of a Simple "Up-Up" State*

Solution 6.2 For such a state, from (6.17), we get that

$$
\mathbf{d} = \frac{1}{\psi}\begin{pmatrix} -\frac{1}{2}\Delta_{\uparrow} \\ -\frac{\mathrm{i}}{2}\Delta_{\uparrow} \\ 0 \end{pmatrix}.
$$

Changing the orientation of the (z) quantization axis amounts to a rotation of 6.17 by π around $\mathbf{e}_x$. From (6.11), we get

$$
\begin{aligned}
\mathcal{R}(\mathbf{d}) &= \mathrm{d}_x\,\mathbf{e}_x - (\mathbf{d} - \mathrm{d}_x\,\mathbf{e}_x) \\
&= -\mathbf{d}\,,
\end{aligned}
$$

which is indeed what we would expect!

6.11.5 *Equivalence of ESP Unitary States and Pure* $|S_z = 0\rangle$ *States*

Solution 6.3 Such an ESP state would have only $\Delta_{\uparrow}$ and $\Delta_{\downarrow}$ components, equal within a phase factor. Let us write $\Delta_{\downarrow} = \mathrm{e}^{-2\mathrm{i}\varphi}\Delta_{\uparrow}$. The $\mathbf{d}$-vector of such a state will be [see (6.17)]

$$\mathbf{d} = \frac{1}{\psi}\begin{pmatrix} \frac{\Delta_\uparrow}{2}\left(\mathrm{e}^{-2\mathrm{i}\varphi}-1\right) \\ -\frac{\mathrm{i}\Delta_\uparrow}{2}\left(1+\mathrm{e}^{-2\mathrm{i}\varphi}\right) \\ 0 \end{pmatrix} = \frac{1}{\psi}\begin{pmatrix} -\mathrm{i}\mathrm{e}^{-\mathrm{i}\varphi}\Delta_\uparrow \sin\varphi \\ -\mathrm{i}\mathrm{e}^{-\mathrm{i}\varphi}\Delta_\uparrow \cos\varphi \\ 0 \end{pmatrix} .$$

If we rotate this state by $\pi/2$ around a vector $\hat{\mathbf{\Omega}} = \begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix}$ in the (x, y)-plane, we obtain from (6.11)

$$\begin{aligned} \mathcal{R}_\Omega(\mathbf{d}) &= (\mathbf{d}\cdot\hat{\mathbf{\Omega}})\hat{\mathbf{\Omega}} + (\hat{\mathbf{\Omega}}\wedge\mathbf{d}) \\ &= \frac{1}{\psi}\begin{pmatrix} \sin(\theta+\varphi)\mathrm{e}^{-\mathrm{i}\varphi}\Delta_\uparrow \cos\theta \\ \sin(\theta+\varphi)\mathrm{e}^{-\mathrm{i}\varphi}\Delta_\uparrow \sin\theta \\ -\mathrm{i}\mathrm{e}^{-\mathrm{i}\varphi}\Delta_\uparrow \cos(\theta+\varphi) \end{pmatrix} . \end{aligned}$$

So indeed, if we choose $\theta = -\varphi$, we recover a pure $|S_z = 0\rangle$ state. Note that it is the phase between the $\Delta_\uparrow$ and $\Delta_\downarrow$ components of the order parameter, which determines the precise direction of the required $\pi/2$ rotation.

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