

The invariant polarisation–tensor field and the Bloch equations for spin-1 particles in storage rings, I: mathematical foundations *

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Abstract

We complement the concept of the invariant spin field in storage rings by defining the invariant polarisation–tensor field for spin-1 particles and we suggest how to calculate it by stroboscopic averaging or directly from the invariant spin field. The invariant polarisation–tensor field and the invariant spin field are used to construct equilibrium spin density–matrix fields, and thereby offer a clean framework for describing equilibrium spin-1 ensembles in storage rings. We also introduce a formalism for describing the effect of noise and damping on the polarisation tensor.

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1 Introduction

This is the first of two papers in which we explore the concept of the invariant polarisation-tensor field for spin-1 particles in storage rings. This paper deals with the mathematical foundations. The second paper will present numerical results for a simple but important model.

Spin motion in electric and magnetic fields is governed by the T-BMT equation [1]. This describes the rate of precession of the rest-frame, pure-state, spin expectation value \vec{S} (“the spin”) of a particle and in general, the independent variable is the time. In circular particle accelerators and storage rings the electric and magnetic guide fields are fixed in space so that it is more convenient to take the distance around the ring as the independent variable [2]. Then, at the position s along the design orbit and the point u in the 6-dimensional phase space, we write the T-BMT equation as $d\vec{S}/ds = \vec{\Omega}(u; s) \times \vec{S}$ where the vector $\vec{\Omega}(u; s)$ describing the precession axis and the rate of precession, depends on the electric and magnetic fields in the laboratory, and on the reference energy of the ring. The motion of a particle is governed by the Lorentz force [1]. Thus both the motion of the particle and the motion of the spin expectation value can be treated classically. Nevertheless, as we shall see, for some aspects of spin motion we still need to look at the quantum mechanics. For this we exploit the spin density matrix.

Earlier works have emphasised the utility of the invariant spin field (ISF) for describing equilibrium spin distributions for beams of spin-1/2 fermions and have shown how the amplitude dependent spin tune (ADST) can be exploited [3, 4, 5, 6, 7]. In this paper we embrace spin-1 particles too by introducing the concept of the invariant field of the Cartesian polarisation tensor, which we call the “invariant tensor field” (ITF). Then we show how to define equilibrium density-matrix fields (EDMF) in terms of the ISF and ITF and explain how they can be diagonalised by rotations of the coordinate system when a certain ansatz for the ITF is valid. We continue our discussion by giving examples of ensembles with and without EDMF’s. Following this, we address the matter of adiabatic invariants and mention other representations for the spin-1 density matrix. The paper is rounded off by extending earlier work on the effect of noise and damping on the evolution of the so-called vector-polarisation density to include their effect on the tensor-polarisation density.

We begin by reviewing the concept of the ISF for spin-1/2 fermions.

2 Equilibrium spin distributions for spin-1/2 fermions

The properties of a mixed spin state for spin-1/2 fermions are completely defined by the 2×2 density matrix ρ [8]. The density matrix is Hermitian and its trace is constrained to a definite value (in fact unity) and it is therefore defined by just three real parameters which can be chosen as the three components of the vector polarisation \vec{P} . Then we write

$$\rho = \frac{1}{2} \{ I + \vec{P} \cdot \vec{\sigma} \}, \quad (2.1)$$

where the $\vec{\sigma}$ is the matrix-valued 3-vector formed from the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (2.2)$$

representing the normalised spin operators \hat{s}_i ($i = 1, 2, 3$) and I is the unit matrix. The labels 1, 2 and 3 are chosen to be consistent with those in [6, 9] and refer to the axes of a right-handed Frenet–Serret coordinate system attached to the design orbit whereby in the arcs of a flat ring, axis 2 is vertical, axis 1 is radial and axis 3 is longitudinal. For spin-1/2 particles we normalise the length of \vec{S} to unity. The polarisation vector is the mixed-state expectation value of the normalised spin operator and it can be written as $\vec{P} = Tr(\rho\vec{\sigma})$. Its components are $P_i = \langle \hat{s}_i \rangle$ where the brackets $\langle \rangle$ signal taking the expectation value. In accelerator physics, we define a density matrix for each point u and s . Then at u and s we write the density matrix in terms of the local vector polarisation $\vec{P}_{loc}(u; s)$ [10, 11, 7] as $\rho = \frac{1}{2}\{I + \vec{P}_{loc}(u; s) \cdot \vec{\sigma}\}$. In general one should describe the system by a combined spin-orbit density matrix and the corresponding Wigner function as in [10] but in Sections 2 and 3, the orbital motion is defined by a Hamiltonian so that the density in phase space is conserved along a trajectory. This allows us to focus our attention on the spin density matrix. The degree of polarisation at a point in phase space, $P_{loc} \equiv |\vec{P}_{loc}|$, is at most unity. Of course, since the density of particles in phase space is finite, the notion of a mixed spin state at each position (u, s) is an idealisation, but this and other idealisations in this paper will not detract from the value of the basic concepts presented. In Section 4 we show how to proceed when the phase space density is not preserved along a trajectory.

2.1 The invariant spin field

Since the T-BMT equation is linear in \vec{S} and since the particles at (u, s) all see the same $\vec{\Omega}(u; s)$, $\vec{P}_{loc}(u(s); s)$ obeys the T-BMT equation along trajectories. Of course, the same result emerges by exploiting the equation of motion for ρ [12, Section 1–8c] [10]. Furthermore, P_{loc} is constant along a trajectory. For a storage ring at fixed energy, $\vec{\Omega}$ is 1-turn periodic in s at a fixed position in phase space u so that $\vec{\Omega}(u; s) = \vec{\Omega}(u; s + C)$ where C is the circumference. This opens the possibility of a configuration for the polarisation that is the same from turn to turn in the sense that $\vec{P}_{loc}(u; s)$ is 1-turn periodic in s for fixed u , i.e., $\vec{P}_{loc}(u; s + C) = \vec{P}_{loc}(u; s)$. For reasons that will become clear we denote such a \vec{P}_{loc} by \vec{P}_{eq} . Since \vec{P}_{eq} also obeys the T-BMT equation we then have

$$\vec{P}_{eq}(M(u; s + C, s); s + C) = \vec{P}_{eq}(M(u; s + C, s); s) = R(u; s + C, s)\vec{P}_{eq}(u; s), \quad (2.3)$$

where $M(u; s + C, s)$ is the new position in phase space after one turn starting at u and s , $R(u; s + C, s)$ is the corresponding 3×3 spin transfer matrix representing the solution to the T-BMT equation for one turn from s to $s + C$ and where here, \vec{P}_{eq} is represented by a column matrix of its components. By writing the T-BMT equation in matrix form we have

$$\frac{d}{ds}R(u(s); s, s_0) = \tilde{\Omega}(u(s); s)R(u(s); s, s_0), \quad (2.4)$$

where

$$\tilde{\Omega} = \begin{pmatrix} 0 & -\vec{\Omega}_3 & \vec{\Omega}_2 \\ \vec{\Omega}_3 & 0 & -\vec{\Omega}_1 \\ -\vec{\Omega}_2 & \vec{\Omega}_1 & 0 \end{pmatrix}. \quad (2.5)$$

The relations (2.3) motivate the introduction of a vector *field* $\hat{n}(u; s)$ of fixed, and in particular, unit length, obeying similar constraints, namely

$$\hat{n}(M(u; s + C, s); s + C) = \hat{n}(M(u; s + C, s); s) = R(u; s + C, s)\hat{n}(u; s). \quad (2.6)$$

where \hat{n} is represented by a column matrix of its components. Where appropriate, a similar convention will be used in the rest of this paper. When it exists, the field \hat{n} is simply a 3–vector function of u and s obeying the T–BMT equation and the periodicity conditions as in (2.6). No reference to real particles and their spin states is required. Since the vector field $\hat{n}(u; s)$ is invariant from turn to turn and independent of the real state of a beam it is called the invariant spin field (ISF). The ISF can be used to define the amplitude dependent spin tune (ADST) and together they provide a most elegant way to systematise spin motion in storage rings and circular accelerators [3, 4, 5, 6, 7]. Note that if all parameters of the system, such as the energy, are fixed, the scalar product $I_{\text{sn}} = \vec{S} \cdot \hat{n}$ is invariant along a trajectory, since both vectors obey the T–BMT equation. Thus the motion of \vec{S} is simply a precession around the local \hat{n} .

On the closed, i.e., periodic, orbit, $u = 0$ and we denote the vector \hat{n} on the closed orbit by $\hat{n}_0(s) \equiv \hat{n}(0; s)$. The vector $\hat{n}_0(s)$ is 1–turn periodic and is given by the real, unit–length eigenvector of $R(0; s + C, s)$.

For the remainder of the paper we assume that the orbital motion is integrable to a good approximation so that u can be parametrised in terms of three pairs of action–angle variables $(J_i, \phi_i, i = 1, 2, 3)$ which we abbreviate by (J, ϕ) . We will use the symbols u and (J, ϕ) interchangeably. The actions J are constants of motion. Thus the orbital phase space is partitioned into disjoint tori, each of which is characterised by a unique set J . We also assume that the orbital motion is nonresonant so that, in time, a trajectory could cover its torus. Then from (2.3) P_{eq} must have the same value at all points ϕ on a torus but can depend on the J . Furthermore we will only consider ISF’s which are continuous in ϕ and we avoid spin–orbit resonances [7]. Then apart from the sign, $\hat{n}(J, \phi; s)$ is a unique function of ϕ and s , 2π –periodic in ϕ [7]. So we may write $\vec{P}_{\text{eq}}(J, \phi; s) = P_{\text{eq}}(J)\hat{n}(J, \phi; s)$, bearing in mind that $|\hat{n}| = 1$. The requirement that \hat{n} be continuous reflects our expectation that the polarisation in a real ring varies continuously in ϕ ¹. If we also require that the particles on a torus are distributed uniformly in ϕ , we find that the polarisation for the torus, defined as the average $P_{\text{eq}}(J)/(2\pi)^3 \int_0^{2\pi} \hat{n}(J, \phi; s)d\phi$, is invariant from turn to turn, i.e., in equilibrium. Examples in which the polarisation is not in equilibrium are presented in [3, 9].

We close this section by listing key aspects of the ISF and the ADST.

1. For a turn–to–turn invariant particle distribution in phase space, a distribution of spins in which each is initially aligned parallel to the ISF at its position in phase space, remains invariant (in equilibrium) from turn to turn, and the ISF gives the direction of the equilibrium polarisation \vec{P}_{eq} at each (u, s) .
2. For integrable orbital motion and away from orbital resonances and spin–orbit resonances [7, 14] the ISF determines both the maximum attainable time averaged po-

¹However, an infinite number of totally discontinuous ISF’s can easily be envisaged through the so–called “filling–up method” [13].

larisation and the maximum equilibrium polarisation $P_{\text{lim}} = |\langle \hat{n}(J, \phi; s) \rangle_\phi|$ on a phase space torus at each s , where the brackets $\langle \rangle_\phi$ denote the average over the orbital phases.

3. As shown in [15], under appropriate conditions I_{sn} is an adiabatic invariant, i.e., it does not change as parameters such as J or the reference energy are slowly varied. It is pointed out there, that this result does *not* rely on defining a spin Hamiltonian for the system but emerges from the T–BMT equation and the properties of \hat{n} . The proof is therefore independent of whether it deals with fermions or bosons. We return to this later.
4. The ISF provides the main axis for orthonormal coordinate systems constructed at each point in phase space for defining the ADST. This, in turn, is used to define the concept of spin–orbit resonance. Away from orbital resonance and spin–orbit resonance, $\hat{n}(u; s)$ is unique up to a sign [7, 14].
5. On the closed orbit, the ADST reduces to the number of precessions of a spin, per turn, around \hat{n}_0 . We denote this spin tune by ν_0 . Its fractional part can be extracted from the complex eigenvalues $e^{\pm 2\pi i \nu_0}$ of $R(\vec{0}; s + C, s)$. For a perfectly aligned flat ring with no solenoids, $\nu_0 = a\gamma_0$ where a is the gyromagnetic anomaly and γ_0 is the Lorentz factor for the beam energy.

These and other matters are explained and illustrated in great detail in the sources cited above. In order to limit this paper to a reasonable length we will assume that the reader is familiar with that material.

The most general, *model-independent* way, to construct the ISF is by so-called stroboscopic averaging [3, 5, 6, 13]. This just requires a spin–orbit tracking code such as SPRINT [6] which delivers 3×3 spin transport matrices along particle orbits. As explained in [3, 5, 6, 13], the ISF, $\hat{n}(u_0; s_0)$, at the starting positions u_0 and $s = s_0$ can be found in terms of multi–turn spin transfer matrices by taking the average

$$\langle \vec{f} \rangle_N(u_0; s_0) \equiv \frac{1}{N+1} \sum_{k=0}^N R(u(s_0 - kC); s_0, s_0 - kC) \hat{n}_0(s_0), \quad (2.7)$$

for very large N and normalising this to unity: $\hat{n}(u_0; s_0) = \langle \vec{f} \rangle_N(u_0; s_0) / |\langle \vec{f} \rangle_N(u_0; s_0)|$. In this expression we have used notation similar to that in eqn. 22 in [3] and chosen \hat{n}_0 as the “seed” spin field, although more general choices could be used [13]. If the orbital motion is integrable and nonresonant, the vector \hat{n} need only be calculated by this means at one position (u_0, s_0) . After that, \hat{n} can be found all over the corresponding torus by propagating this initial \hat{n} along the trajectory. Thus for integrable, nonresonant orbital motion, there is usually *no* need to execute stroboscopic averages on a grid of pre–chosen positions ϕ on a torus since the approach just suggested suffices for obtaining the significant information, namely averages.

Typical plots of P_{lim} , the ADST or the components of the ISF, can be found in [3, 5, 6, 15, 16, 9] and we give examples in Part II. For rational orbital tunes, ISF’s can always be extracted trivially as the normalised real eigenvectors of multi–turn spin maps [9]. But for other cases we know of no analytical proof that the ISF always exists and indeed we know of

examples for irrational tunes, off orbital resonance, where there is no numerical convergence for the stroboscopic averages, implying that the ISF perhaps does not exist in those cases. Nevertheless, in most cases of interest we have found ISF's via stroboscopic averaging. For detailed discussions on convergence of stroboscopic averages, see [13, 3, 5].

2.2 The equilibrium density–matrix field for spin-1/2 particles

The existence of a 1–turn periodic \vec{P}_{eq} and the corresponding ISF implies the existence of an equilibrium density–matrix field (EDMF), ρ^{eq} , obeying the periodicity condition $\rho^{\text{eq}}(u; s + C) = \rho^{\text{eq}}(u; s)$ and which we can write in the form:

$$\rho_{P_{\text{eq}}(J)}^{\text{eq}}(J, \phi; s) = \frac{1}{2} \{ I + P_{\text{eq}}(J) \hat{n}(J, \phi; s) \cdot \vec{\sigma} \}, \quad (2.8)$$

in an obvious notation. Different ensembles of spins at a (u, s) with the same \vec{P}_{eq} cannot be distinguished by measurements from a mixture of spins in eigenstates of the operator $\hat{n} \cdot \vec{\sigma}$ with that \vec{P}_{eq} . The corresponding density matrix at each (u, s) is diagonal in a coordinate system in which the components of \hat{n} are $(0, 1, 0)$.

3 Equilibrium spin distributions for spin-1 particles

Spin–1 particles such as deuterons have three eigenvalues, namely $+1, 0, -1$, for the projection of the normalised spin operator \hat{s} onto a chosen quantisation axis, and a 3×3 density matrix. Since it is Hermitian and its trace is constrained to a definite value, this density matrix can be completely specified in terms of eight real parameters. Three of these can be the components of vector polarisation \vec{P} analogous to those for spin-1/2 fermions and the other five are the so–called tensor polarisations. Various representations of the latter are in use. For us, a particularly useful parametrisation for the density matrix ρ is that given in [8, Section 3.1.12] in terms of a rank–2, 3×3 , real, symmetric, traceless, Cartesian tensor T as:

$$\rho = \frac{1}{3} \left\{ I + \frac{3}{2} \vec{P} \cdot \vec{\mathfrak{J}} + \sqrt{\frac{3}{2}} \sum_{i,j} T_{ij} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) \right\}, \quad (3.1)$$

where the three matrices \mathfrak{J}

$$\mathfrak{J}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \mathfrak{J}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \mathfrak{J}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad (3.2)$$

representing the normalised spin operators \hat{s}_i ($i = 1, 2, 3$), are the analogues for spin-1 of the Pauli matrices and where $\vec{\mathfrak{J}}$ is the corresponding matrix–valued 3–vector. The tensor T has just five independent components and is irreducible in that it contains no non–zero tensors of lower rank [17, 18]. The tracelessness of the tensor and the matrices \mathfrak{J} ensures that $Tr(\rho) = 1$ as required. The matrices \mathfrak{J} are cyclically permuted with respect to the corresponding matrices in [8] because of the labelling of the axes explained in Section 2. See the Appendix for a way to derive (3.1).

The vector polarisation, with its components $P_i = \langle \hat{s}_i \rangle$, is now $\vec{P} = Tr(\rho \vec{\mathfrak{J}})$ and again, $P = |\vec{P}|$ is at most unity. However, the components of T which are also needed for the spin-1 density matrix, depend of quadratic combinations of spin operators. In particular,

$$T_{ij} = \frac{1}{2} \sqrt{\frac{3}{2}} \left\{ \langle \hat{s}_i \hat{s}_j + \hat{s}_j \hat{s}_i \rangle - \frac{4}{3} \delta_{ij} \right\} \quad (3.3)$$

where the Kronecker delta has been used [8]. This can be seen by computing the $\langle \hat{s}_i \hat{s}_j \rangle$ using $Tr(\rho \vec{\mathfrak{J}}_i \vec{\mathfrak{J}}_j)$. The degree of tensor polarisation $\mathfrak{T} \equiv \sqrt{\sum_{i,j} T_{ij}^2} = \sqrt{Tr(TT^T)} = \sqrt{Tr(T^2)}$ is at most unity [8].

In contrast to the case of spin-1/2 particles, for spin-1 particles, there are pure states for which $|\vec{S}|$ is zero. In that case $|\vec{S}|$ cannot be normalised to unity [19]. If $|\vec{S}|$ is zero I_{sn} vanishes and it is automatically adiabatically invariant since $|\vec{S}|$ is invariant under rotations. For the other pure states, $|\vec{S}|$ can be normalised to unity but we have no need to do this. The overall degree of polarisation for spin-1 particles is $\frac{3}{4}P^2 + \mathfrak{T}^2$ [8, eqs. 3.1.55, 3.1.65]. So an ensemble is unpolarised only when *both* P and \mathfrak{T} are zero. In that case $\rho = \frac{1}{3}I$ so that the probabilities for the three substates are equal at 1/3.

3.1 The invariant tensor field

Given the existence of ISF's in most cases of interest, it is natural to ask if invariant tensor fields (ITF) can exist. We now examine this possibility by defining the ITF and then suggesting how to construct it by stroboscopic averaging and in terms of the ISF.

For this we use the analogue for T of solutions of the T-BMT equation for spin. In particular, if an initial spin, \vec{S}^i , is transformed to a final spin, \vec{S}^f , by a spin transfer matrix R according to the relation

$$\vec{S}^f = R \vec{S}^i, \quad (3.4)$$

then the components of T are transformed according to the rule [17]

$$T^f = R T^i R^T. \quad (3.5)$$

Of course, $\vec{P}^f = R \vec{P}^i$. Equation (3.5) conserves the trace and the symmetry of the tensor as well as \mathfrak{T} . Moreover,

$$\frac{dT}{ds} = [\tilde{\Omega}, T] \equiv \tilde{\Omega} T - T \tilde{\Omega} \quad \text{while} \quad \frac{d\vec{P}}{ds} = \tilde{\Omega} \vec{P}. \quad (3.6)$$

We emphasise the fact, obvious from (3.4) and (3.5), that as soon as the matrix R for rotating spins is known, the transformation for T follows trivially.

We now define the ITF T^I , in analogy with the definition for the ISF, by the periodicity condition

$$T^I(M(u; s + C, s); s + C) = T^I(M(u; s + C, s); s) = R(u; s + C, s) T^I(u; s) R^T(u; s + C, s) \quad (3.7)$$

with $\sqrt{\text{Tr}(T^I)^2} = 1$. This normalisation is preserved along a trajectory. Just as with the ISF, when it exists, the ITF is simply a tensor function of u and s obeying (3.5) and the periodicity conditions as in (3.7). No reference to real particles and their spin states is required. Intuition suggests that the ITF is unique up to a sign away from orbital resonances and spin-orbit resonances. We also expect that the ITF can be constructed using stroboscopic averaging in analogy with the ISF:

$$\langle g \rangle_N(u_0; s_0) \equiv \frac{1}{N+1} \sum_{k=0}^N R(u(s_0 - kC); s_0, s_0 - kC) T(s_0) R^T(u(s_0 - kC); s_0, s_0 - kC) \quad (3.8)$$

where N is very large and $T(s_0)$ is a fixed 3×3 symmetric matrix with zero trace. The symmetry and tracelessness ensure that the 3×3 matrix $\langle g \rangle_N(u_0; s_0)$ is traceless and symmetric. The ITF is obtained as $T^I(u_0; s_0) \equiv \langle g \rangle_N / \sqrt{\text{Tr}(\langle g \rangle_N^2)}$.

Just as with $\hat{n}(u_0; s_0)$, once $T^I(u_0; s_0)$ is known, and if the orbital motion is integrable and non-resonant, one simply propagates it forward using (3.5) to obtain T^I all over the corresponding torus.

Given the simplicity of the form (3.5) it is also tempting to try to express the ITF in terms of the ISF, and the form

$$T^I = \pm \sqrt{\frac{3}{2}} \left\{ \hat{n} \hat{n}^T - \frac{1}{3} I \right\}, \quad (3.9)$$

suggests itself. The term with the 3×3 unit matrix ensures that the tensor is traceless and the factor $\sqrt{\frac{3}{2}}$ ensures the chosen normalisation. Since a spin transfer matrix R is orthogonal, it is trivial that this ansatz satisfies (3.5). Note that the required periodicity conditions (3.7) are fulfilled owing to the analogous periodicity of \hat{n} . The ansatz (3.9) clearly satisfies all requirements for T^I . So, if T^I is unique, any other ansatz must give the same result up to a sign. Alternatively, if this ansatz is unique, then T^I is unique up to a sign when \hat{n} is unique.

If the stroboscopic average in (3.8) is calculated for many different, non-zero, traceless, symmetric matrices $T(s_0)$ in the simple, non-trivial but important model of Part II, then, away from orbital resonances and spin-orbit resonances, the same normalised stroboscopic average is obtained (up to a sign) and it is a single valued function of the orbital phases. This suggests, but does not prove, that the ITF is indeed unique up to a sign. One also finds that the normalised stroboscopic average agrees with the ansatz of (3.9).

If T^I is unique, it can be obtained using (3.9) as soon as the ISF is known, without further stroboscopic averaging. Then, for example, in a parameter regime where the so-called single resonance model [9, 20] provides an approximation to the spin dynamics, one not only has an approximate analytical formula for the ISF, but also for the ITF.

Later we shall see that the ansatz (3.9) is supported by another consideration. So we will adopt this form in the remainder of the paper. Moreover it will suffice to choose the + sign. Then, for example, $T_{2,2}^I = \sqrt{\frac{2}{3}} (\frac{3}{2} \cos^2 \theta - \frac{1}{2})$ where $\theta = \cos^{-1}(\hat{n}_2)$.

3.2 The EDMF for spin-1 particles

The kind of argument that leads to the concept of the equilibrium polarisation $\vec{P}_{\text{eq}}(J, \phi; s) = P_{\text{eq}} \hat{n}(J, \phi; s)$ on a torus, also leads to the concept of the equilibrium polarisation tensor $T_{\text{eq}}(J, \phi; s) \equiv \mathfrak{T}_{\text{eq}}(J) T^{\text{I}}(J, \phi; s)$ where $\mathfrak{T}_{\text{eq}}(J)$ is the degree of equilibrium tensor polarisation. If the particles are distributed uniformly in ϕ on the torus J and $T(J, \phi; s) = T_{\text{eq}}(J, \phi; s)$ at some s , the polarisation tensor for the torus, defined as $\mathfrak{T}_{\text{eq}}(J)/(2\pi)^3 \int_0^{2\pi} T^{\text{I}}(J, \phi; s) d\phi$, is invariant from turn to turn.

With the ITF we can now construct an EDMF for spin-1 particles:

$$\rho_{[P_{\text{eq}}, \mathfrak{T}_{\text{eq}}](J)}^{\text{eq}}(J, \phi; s) = \frac{1}{3} \left\{ I + \frac{3}{2} P_{\text{eq}}(J) \hat{n} \cdot \vec{\mathfrak{J}} + \sqrt{\frac{3}{2}} \mathfrak{T}_{\text{eq}}(J) \sum_{i,j} T_{ij}^{\text{I}} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) \right\}. \quad (3.10)$$

So on a torus, the EDMF is defined by two free parameters, $P_{\text{eq}}(J)$ and $\mathfrak{T}_{\text{eq}}(J)$. As required, $\text{Tr}(\rho^{\text{eq}}) = 1$ for any pure or mixed state. However, for a pure state we require that $\text{Tr}(\rho^2) = 1$. Then in a pure state, from (3.10) and (3.9) and after some matrix algebra, we find the constraint

$$1 = \frac{1}{9} \left\{ 3 + \frac{9}{2} P_{\text{eq}}^2 + 6 \mathfrak{T}_{\text{eq}}^2 \right\} \quad \Rightarrow \quad 1 = \frac{3}{4} P_{\text{eq}}^2 + \mathfrak{T}_{\text{eq}}^2. \quad (3.11)$$

which is clearly independent of the precise values of the components of \hat{n} and T^{I} . In this context it should be emphasised that the ISF and the ITF just encode the relative sizes of their components and that to specify actual invariant spin states on tori we need $P_{\text{eq}}(J)$ and $\mathfrak{T}_{\text{eq}}(J)$ too. Relation (3.11) corresponds to the fact that pure states are fully polarised according to the definition in [8, eqs. 3.1.55, 3.1.65].

As we are reminded in [8], although the density matrix for spin-1/2 particles can always be diagonalised by a rotation of the coordinate system (see Section 2), this is not always the case for spin-1 particles. However, it is always possible for the EDMF of spin-1 particles when the ansatz in (3.9) is valid since the ITF, and thus the EDMF, will be diagonal if \hat{n} has components (0, 1, 0) and this can always be achieved at each (u, s) by rotating the coordinate frame to make \hat{n} vertical in that frame. According to the definition in [8], the ISF therefore defines the quantisation axes for the EDMF on a torus for spin-1 particles too. In particular, different ensembles of spins at a (u, s) with the same \vec{P}_{eq} and T_{eq} cannot be distinguished by measurements from a mixture of spins in eigenstates of the operator $\hat{n} \cdot \vec{\mathfrak{J}}$ with those \vec{P}_{eq} and T_{eq} . Of course, since all spin transformations here are rotations according to the matrices R , it is clear that if ρ^{eq} can be diagonalised at one point on a trajectory, it can be diagonalised by a rotation everywhere else along the trajectory.

We now illustrate these concepts with simple examples in which we choose some special configurations of spins and then check to see if they can be described by EDMF's

3.2.1 Example 1

Consider the case where all particles at some arbitrary (J, ϕ_0, s_0) are in the eigenstate of $\hat{n} \cdot \vec{\mathfrak{J}}$ whose eigenvalue is +1 so that $P_{\text{loc}} = 1$. We write this eigenstate as $|n^+\rangle$. The corresponding

3-spinor is

$$e^{i\varphi} \begin{pmatrix} \frac{1+n_2}{2} \\ \frac{n_1+in_3}{\sqrt{2}} \\ \frac{1-n_2}{2} \frac{n_1+in_3}{n_1-in_3} \end{pmatrix} \quad (3.12)$$

where φ is an arbitrary phase. Then, by evaluating the expectation values in (3.3) for $|n^+\rangle$, we find for the local polarisation tensor:

$$T_{\text{loc}} = \frac{1}{2} \sqrt{\frac{3}{2}} \left\{ \hat{n} \hat{n}^T - \frac{1}{3} I \right\}. \quad (3.13)$$

So $T_{\text{loc}}(J, \phi_0; s_0)$ is proportional to the $T^1(J, \phi_0; s_0)$ of (3.9). The proportionality factor is $1/2$ and the same value will be obtained at any other (J, ϕ_0, s_0) . Also, it is preserved as the ensemble moves over the torus. So there is an EDMF. In particular we have $T_{\text{eq}}(J, \phi_0; s_0) = T_{\text{loc}}(J, \phi_0; s_0) = T^1(J, \phi_0; s_0)/2$ and we define $T_{\text{eq}}(J, \phi; s) \equiv \mathfrak{T}_{\text{eq}}(J) T^1(J, \phi; s)$ where $\mathfrak{T}_{\text{eq}}(J) = 1/2$. With $P_{\text{loc}} = P_{\text{eq}} = 1$, this value of $\mathfrak{T}_{\text{eq}}(J)$ satisfies (3.11), as expected for a pure state. We can now write

$$\begin{aligned} \rho^{\text{eq}} &= \left\{ \frac{I}{3} + \frac{1}{2} P_{\text{eq}} \hat{n} \cdot \vec{\mathfrak{J}} + \mathfrak{T}_{\text{eq}} \sum_{i,j} (\hat{n}_i \hat{n}_j - \frac{1}{3} \delta_{ij}) \frac{(\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i)}{2} \right\} \\ &= \left\{ \frac{I}{3} + \frac{1}{2} \hat{n} \cdot \vec{\mathfrak{J}} + \frac{1}{2} \sum_{i,j} (\hat{n}_i \hat{n}_j - \frac{1}{3} \delta_{ij}) \frac{(\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i)}{2} \right\}, \end{aligned} \quad (3.14)$$

where we have suppressed the dependences on J, ϕ and s for convenience. It is now clear that the ansatz (3.9) is natural if (3.10) is to be able to encompass these pure states on a torus. It is easily checked that this density matrix is idempotent as required for pure states.

Note that these states are the so-called coherent states appearing in the discussion of the matter of defining the classicality of spin states in [21]. There, the density operator for the pure state with a spin expectation value \hat{n} of unit magnitude, is given by the projector

$$|\hat{n}\rangle\langle\hat{n}| = \left\{ \frac{I}{3} + \frac{1}{2} \hat{n} \cdot \vec{\mathfrak{J}} + \frac{1}{2} \sum_{i,j} (\hat{n}_i \hat{n}_j - \frac{1}{3} \delta_{ij}) \frac{(\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i)}{2} \right\}, \quad (3.15)$$

With the explicit representation (3.12), the equality of the 3×3 matrices on each side of (3.15) is readily confirmed.

Of course, if all particles are in the eigenstate $|n^-\rangle$ of $\hat{n} \cdot \vec{\mathfrak{J}}$ whose eigenvalue is -1 , $P_{\text{eq}} = -1$. However, \mathfrak{T}_{eq} is again $1/2$.

3.2.2 Example 2

Consider the case where all particles at some (J, ϕ_0, s_0) are in the eigenstate $|n^0\rangle$ of $\hat{n} \cdot \vec{\mathfrak{J}}$ whose eigenvalue is 0 so that $P_{\text{loc}} = 0$. The corresponding 3-spinor is

$$e^{i\varphi} \sqrt{\frac{1-n_2^2}{2}} \begin{pmatrix} 1 \\ -\frac{\sqrt{2}n_2}{n_1-in_3} \\ -\frac{n_1+in_3}{n_1-in_3} \end{pmatrix} \quad (3.16)$$

where φ is an arbitrary phase. Then, by evaluating the expectation values in (3.3) for $|n^0\rangle$, we find for the local polarisation tensor:

$$T_{\text{loc}} = -\sqrt{\frac{3}{2}} \left\{ \hat{n} \hat{n}^T - \frac{1}{3} I \right\} . \quad (3.17)$$

So the ansatz (3.9) for T^I appears again. Thus there is again an EDMF and in this case $\mathfrak{T}_{\text{eq}}(J) = -1$. Since $P_{\text{eq}} = 0$, (3.11) is satisfied as expected for a pure state.

3.2.3 Example 3

Although ensembles in the pure states $|n^+\rangle$ or $|n^-\rangle$ can be described by EDMF's, this is not necessarily true for ensembles in coherent superpositions of these states. For example, consider the case where all particles at some (J, ϕ_0, s_0) are in the pure state $|N^+\rangle \equiv \{|n^+\rangle + |n^-\rangle\}/\sqrt{2}$ or where all particles are in the pure state $|N^-\rangle \equiv \{|n^+\rangle - |n^-\rangle\}/\sqrt{2}$. In both cases $P_{\text{loc}} = 0$ and $\mathfrak{T} = 1$ so that the relation $1 = \frac{3}{4}P^2 + \mathfrak{T}^2$ for pure states is fulfilled. However, neither of the local polarisation tensors, T_{loc}^+ for $|N^+\rangle$ and T_{loc}^- for $|N^-\rangle$, is proportional to the T^I calculated using (3.9). So ensembles in one or the other of these pure states are not described by an EDMF.

Alternatively we may say that the states $|N^\pm\rangle$ cannot be represented by a projector of the form (3.15). This is in contrast to the case of spin-1/2 particles. There, all pure states can be represented in the corresponding form namely, $|\mathbf{n}\rangle\langle\mathbf{n}| = \frac{1}{2}\{I + \hat{\mathbf{n}} \cdot \vec{\sigma}\}$, since every pure state is an eigenstate of $\mathbf{n} \cdot \vec{\sigma}$ for some unit vector \mathbf{n} .

3.2.4 Example 4

We now turn to mixed states. Consider the mixed state at some arbitrary (J, ϕ_0, s_0) comprised of equal proportions of the pure states $|N^+\rangle$ and $|N^-\rangle$. The density matrix is the average of the density matrices for the two pure states. Then $T_{\text{loc}} = \frac{1}{2}T_{\text{loc}}^+ + \frac{1}{2}T_{\text{loc}}^-$ and we find

$$T_{\text{loc}} = \frac{1}{2} \sqrt{\frac{3}{2}} \left\{ \hat{n} \hat{n}^T - \frac{1}{3} I \right\} , \quad (3.18)$$

so that there is an EDMF and $\mathfrak{T}_{\text{eq}}(J) = 1/2$. Since $P_{\text{eq}} = 0$, $\frac{3}{4}P_{\text{eq}}^2 + \mathfrak{T}_{\text{eq}}^2 < 1$ as expected in a mixed state.

This example illustrates nicely how an EDMF can exist for a mixture of states which individually do not have EDMF's. There is an unlimited number of such examples.

3.2.5 Example 5

Consider now the mixed state at some arbitrary (J, ϕ_0, s_0) in which the fraction p_+ is in the state $|n^+\rangle$ and the remainder is in the state $|n^-\rangle$. Then

$$T_{\text{loc}} = \frac{1}{2} \sqrt{\frac{3}{2}} \left\{ \hat{n} \hat{n}^T - \frac{1}{3} I \right\} \quad (3.19)$$

and there is an EDMF with $P_{\text{eq}} = 2p_+ - 1$ and $\mathfrak{T}_{\text{eq}}(J) = 1/2$. With $p_+ = 1/2$, the EDMF is the same as that in Example 4 so that the two ensembles cannot be distinguished by measurements.

3.2.6 Example 6

As a final example, consider the mixed state at some arbitrary (J, ϕ_0, s_0) comprising equal proportions of the pure states $|n^+\rangle$, $|n^-\rangle$ and $|n^0\rangle$. As we have seen, each of these pure states has a $T_{\text{loc}}(J, \phi_0; s_0)$ proportional to the $T^{\text{I}}(J, \phi_0; s_0)$ of (3.9) and thus an EDMF. The $\mathfrak{T}_{\text{eq}}(J)$ is the average of those for the three pure states and is zero. Since $P_{\text{eq}} = 0$ as well, this ensemble is fully unpolarised.

3.3 Adiabatic invariants based on the ISF and ITF

With \hat{n} , we have the adiabatic invariant I_{sn} . Then it is clear from (3.9) that

$$I_{\text{st}} \equiv \sqrt{\frac{3}{2}} \left\{ I_{\text{sn}}^2 - \frac{1}{3} |\vec{S}|^2 \right\} = \vec{S}^{\text{T}} T^{\text{I}} \vec{S} = \text{Tr}(\vec{S} \vec{S}^{\text{T}} T^{\text{I}}) \quad (3.20)$$

is the corresponding adiabatic invariant associated with T^{I} . For a 3×3 tensor T satisfying (3.5), $I_{\text{tt}} \equiv \text{Tr}(T T^{\text{I}})$ is invariant along a trajectory if the parameters of the system are fixed. We comment on the adiabatic invariance of this in Part II.

3.4 Other parametrisations

Once the Cartesian version of the ITF has been established, the five components of the corresponding invariant spherical polarisation–tensor field follow trivially using the relations in [8, eqs. 3.1.66 - 67]. See [22, 23] too. Thus it is simple to find the invariant spherical polarisation–tensor field for the single resonance model. In analogy with the expansion for spin-1/2 particles in (2.1), the density matrix for spin-1 particles can also be expanded in terms of the generators of the group $\text{SU}(3)$ and the so-called coherence (or Bloch) vector [24, 25]. Other matrix bases and the corresponding Bloch vectors can be used too: see [26] and also the Appendix. However, the expansion in terms of the polarisation and the Cartesian tensor seems to be the most convenient for calculating and discussing the EDMF.

Not all Bloch vectors inside their so-called Bloch hyper-spheres lead to admissible density matrices [26]. So perhaps some ITF's constructed by the purely numerical technique of stroboscopic averaging could also lead to inadmissible density matrices. However, that will not be the case for mixed or pure states constructed with the ansatz (3.9).

4 The Bloch equations

In the previous sections, the orbital motion is deterministic and governed just by a Hamiltonian so that the density in phase space is conserved along a trajectory and one can work with spin density matrices instead of spin-orbit density matrices. However, if the particles are subject to noise and damping, the evolution of the density of particles in phase space is

more complicated and spin–orbit density matrices and their Wigner functions come into play [10, 27]. Alternatively, we can work with the classical phase space density and the so–called polarisation density as in [11, 28]. The effect of noise and damping on the polarisation tensor can be studied in an analogous way. So we round off this paper on the polarisation tensor by showing how to do this. In order to avoid undue repetition we assume that the reader is familiar with the concepts in [11, 28]. The final result of this section is perhaps no more than a curiosity but we include this material for completeness.

Charged particles suffering deflection in magnetic fields emit synchrotron radiation and, as is well known, this has important consequences for the properties of electron beams in storage rings. For example, the stochastic nature of photon emission together with damping mechanisms cause the phase space density $W_{\text{orb}}(u; s)$ to reach equilibrium, ie., to become 1–turn periodic: $W_{\text{orb}}(u; s + C) = W_{\text{orb}}(u; s)$ [29]. It often suffices to approximate the effects of the photon emission as a Gaussian white noise process so that if interparticle forces can be ignored, the evolution of W_{orb} can be described in terms of the Fokker–Planck equation [29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39]. For our purposes it is sufficient to write the Fokker–Planck equation somewhat symbolically as in [11] in the form

$$\frac{\partial W_{\text{orb}}}{\partial s} = \mathcal{L}_{\text{FP,orb}} W_{\text{orb}} , \quad (4.1)$$

where the orbital Fokker–Planck operator can be decomposed into the form:

$$\mathcal{L}_{\text{FP,orb}} = \mathcal{L}_{\text{ham}} + \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2 \quad (4.2)$$

whereby \mathcal{L}_0 , \mathcal{L}_1 , \mathcal{L}_2 are terms due to damping and noise containing respectively zeroth, first and second order derivatives w.r.t. the components of u . The term \mathcal{L}_{ham} is the Poisson bracket $\{H_{\text{orb}}, W_{\text{orb}}\}$ of W_{orb} with the orbital Hamiltonian. Detailed forms for the other \mathcal{L} 's can be found in [34, 35, 36] but are not important for the argument that follows. After a few damping times W_{orb} approaches the periodic form. We normalise W_{orb} to unity: $\int d^6 u W_{\text{orb}}(u; s) = 1$.

We have introduced the Fokker–Planck equation by mentioning synchrotron radiation but the Fokker–Planck equation can be applied when the particles are subject to other sources of noise and damping by adopting appropriate forms for \mathcal{L}_0 , \mathcal{L}_1 and \mathcal{L}_2 . Of course, except at very large energies, synchrotron radiation is irrelevant for particles other than electrons or positrons. But as in the case of synchrotron radiation, noise can lead to irreversible loss of vector polarisation [10], and even when W_{orb} has reached periodicity. The chief mechanism is simple: the noise causes random perturbations in the trajectories and thereby causes random perturbations in $\vec{\Omega}$ in the non–uniform fields of the quadrupoles.

Since the local vector polarisation \vec{P}_{loc} is not a density, its evolution cannot be described by a Fokker–Planck equation. However, as explained in [11, 28], if the noise has no *direct* effect on spins, the vector–polarisation density $\vec{\mathcal{P}} \equiv W_{\text{orb}} \vec{P}_{\text{loc}}$ evolves according to the equation

$$\frac{\partial \vec{\mathcal{P}}}{\partial s} = \mathcal{L}_{\text{FP,orb}} \vec{\mathcal{P}} + \vec{\Omega} \times \vec{\mathcal{P}} . \quad (4.3)$$

where the Poisson bracket \mathcal{L}_{ham} is now $\{H_{\text{orb}}, \vec{\mathcal{P}}\}$. Thus, if $\mathcal{L}_{\text{FP,orb}}$ is known, we have an immediate, succinct, classical encapsulation of the way in which \vec{P}_{loc} is modified both by

precession and by the effect of noise and damping on the mixture of spin states at each (u, s) . We call (4.3) the Bloch equation for the vector-polarisation density². Although (4.3) was derived with spin-1/2 fermions in mind, it applies to spin-1 particles too. The vector-polarisation density is proportional to the density in phase space of \vec{S} . To obtain $\vec{P}_{\text{loc}}(u; s)$, (4.1) and (4.3) should be solved in parallel and then $\vec{P}(u; s)/W_{\text{orb}}(u; s)$ should be calculated.

Although (4.3) might appear to lack transparency, it is easy to appreciate it in two limits. For example, if \mathcal{L}_0 , \mathcal{L}_1 and \mathcal{L}_2 vanish leaving just the Poisson bracket \mathcal{L}_{ham} , (4.3) then reduces to the T-BMT equation for \vec{P} along a trajectory, just as expected when we recall that in this case W_{orb} is preserved along the trajectory. On the other hand, if there is no direct spin-orbit coupling in (4.3) ($\vec{\Omega} = \vec{0}$), the components of \vec{P} reach equilibrium forms proportional to the equilibrium form for W_{orb} so that the components of $\vec{P}_{\text{loc}}(u; s)$ become independent of (u, s) . In this case, the spins do not precess but are mixed by the motion of the particles. It is then not too surprising that the polarisation becomes uniform. However, in reality, $\vec{\Omega}$ does not vanish but instead mixes the components of the polarisation directly. This is the route, in this picture, leading to variation of $P_{\text{loc}}(u; s)$ even when W_{orb} has reached equilibrium. Further aspects of this formalism and the connection with the spin-orbit density operator are discussed in [11, 28, 10].

In order to study the evolution of the Cartesian polarisation tensor we introduce the tensor-polarisation density $\mathcal{T} \equiv W_{\text{orb}}T_{\text{loc}}$. Then, from the previous discussion we expect that the Bloch-like equation for \mathcal{T} is

$$\frac{\partial \mathcal{T}}{\partial s} = \mathcal{L}_{\text{FP,orb}} \mathcal{T} + [\tilde{\Omega}, \mathcal{T}], \quad (4.4)$$

where the commutator derives from (3.6) and where the Poisson bracket \mathcal{L}_{ham} is $\{H_{\text{orb}}, \mathcal{T}\}$. To obtain $T_{\text{loc}}(u; s)$, (4.1) and (4.4) should be solved in parallel and then $\mathcal{T}(u; s)/W_{\text{orb}}(u; s)$ should be calculated.

If the spin-orbit coupling terms in (4.4) were to vanish ($\vec{\Omega} = \vec{0}$), the components of \mathcal{T} would each reach equilibrium forms proportional to the equilibrium form for W_{orb} so that the components of $T_{\text{loc}}(u; s)$ would become independent of (u, s) . However $\vec{\Omega}$ does not vanish but instead mixes the components. Since, by definition, \mathcal{T} is symmetric and traceless at all (u, s) , the right-hand side of (4.4) is traceless and symmetric too. Therefore (4.4) preserves the symmetry and tracelessness of T_{loc} . As a next step we must prove that (4.3) ensures that $P_{\text{loc}} \leq 1$, that (4.4) ensures that the local tensor polarisation $\mathfrak{T}_{\text{loc}}$ is at most unity and that $\frac{1}{4}P_{\text{loc}}^2 + T_{\text{loc}}^2 \leq 1$. These matters will be the subjects of a separate work. Other formalisms [10, 34] show that in the absence of a polarising mechanism, P_{loc} tends to fall to zero in beams of spin-1/2 particles subject to noise and damping. This will also happen in this case for spin-1 particles and we suspect that $\mathfrak{T}_{\text{loc}}$ will fall to zero too.

Note that the relationships between (4.1) and (4.3) and between (4.1) and (4.4) survive if $\mathcal{L}_{\text{FP,orb}}$ is replaced by any physically admissible transport operator \mathcal{K}_{orb} — which could even contain derivatives beyond second order.

²This equation has nothing directly to do with the Bloch vectors mentioned earlier.

5 Summary

We have proposed a definition of an invariant rank-2 Cartesian polarisation-tensor field for spin-1 particles, and a procedure for calculating it numerically by stroboscopic averaging or analytically once the ISF is known. The ISF and ITF provide “scaffolding” on which to “hang” equilibrium spin distributions for spin-1 particles on a phase-space torus and the two fields can be combined to construct equilibrium density-matrix fields which depend on just two parameters, the degree of equilibrium vector polarisation $P_{\text{eq}}(J)$ and the degree of equilibrium tensor polarisation $\mathfrak{T}_{\text{eq}}(J)$. We have also pointed out that the EDMF for spin-1 particles can always be diagonalised by a rotation of the coordinate system when the ansatz (3.9) for the ITF is valid and we have shown with examples how that ansatz is entirely natural. Moreover, we have identified adiabatic invariants associated with the ITF.

Finally, we have extended earlier work to include the effects of noise and damping on the polarisation tensor and we have provided an evolution equation for the tensor polarisation density.

In Part II of this work we present the results of calculations for a simple but important model.

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Appendix

In this appendix we give a pedagogical demonstration of how to arrive at the representation (3.1) for the spin-1 density matrix.

We need to write ρ as a linear combination of 3×3 matrices. There is a variety of possibilities [24, 25, 26] but we want to use the matrices \mathfrak{J} . Since eight real parameters are needed, an expansion of the form $\rho = \sum_{i=1-3} U_i \mathfrak{J}_i$ with complex U_i does not suffice. So we try an expansion of the form

$$\rho = \sum_{i,j} U_{ij} \mathfrak{J}_j \mathfrak{J}_i \quad (\text{A.1})$$

with complex U_{ij} . Then we have space for the required eight independent real parameters but their identity is not immediately evident among the eighteen real parameters defining the U_{ij} .

To come further we note that $Tr(\mathfrak{J}_j \mathfrak{J}_i) = 0$ for $i \neq j$ but that $Tr(\mathfrak{J}_1^2) = Tr(\mathfrak{J}_2^2) = Tr(\mathfrak{J}_3^2) = 2$. Then $Tr(U) = 1/2$ since $Tr(\rho) = 1$. Moreover, with the rule $\langle \hat{s}_i \hat{s}_j \rangle = Tr(\rho \mathfrak{J}_i \mathfrak{J}_j)$ we find

$$U_{ij} = \langle \hat{s}_i \hat{s}_j \rangle - \frac{1}{2} \delta_{ij} , \quad (\text{A.2})$$

which we can write in matrix form as

$$U = \langle \hat{s} \hat{s}^T \rangle - \frac{1}{2}I, \quad (\text{A.3})$$

in an obvious notation. The matrix $\langle \hat{s} \hat{s}^T \rangle$ transforms as a Cartesian tensor. This means that U transforms as a Cartesian tensor too. Thus $U^f = R U^i R^T$ in analogy with (3.5) so that $(U^T)^f = R (U^T)^i R^T$.

For the next step we write U as the sum of its symmetric and antisymmetric parts: $U = t + a$ with $t = (U + U^T)/2$ and $a = (U - U^T)/2$. Both t and a are Cartesian tensors. Furthermore, using the Hermiticity of ρ it can be shown that t is real and a is pure imaginary.

Equation (A.1) can now be written as

$$\rho = \sum_{i,j} \frac{t_{ij}}{2} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) + a_{12} (\mathfrak{J}_1 \mathfrak{J}_2 - \mathfrak{J}_2 \mathfrak{J}_1) + a_{23} (\mathfrak{J}_2 \mathfrak{J}_3 - \mathfrak{J}_3 \mathfrak{J}_2) + a_{13} (\mathfrak{J}_1 \mathfrak{J}_3 - \mathfrak{J}_3 \mathfrak{J}_1), \quad (\text{A.4})$$

and from the commutation relations among the matrices \mathfrak{J} we obtain

$$\rho = \sum_{i,j} \frac{t_{ij}}{2} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) + ia_{12} \mathfrak{J}_3 + ia_{23} \mathfrak{J}_1 - ia_{13} \mathfrak{J}_2. \quad (\text{A.5})$$

We now define a real 3-component object \vec{v} with elements $\vec{v}_1 \equiv ia_{23}$, $\vec{v}_2 \equiv -ia_{13}$ and $\vec{v}_3 \equiv ia_{12}$. Then, using the fact that a is a Cartesian tensor, we can easily show that \vec{v} transforms as a 3-vector. Thus (A.5) takes the form

$$\rho = \sum_{i,j} \frac{t_{ij}}{2} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) + \vec{v} \cdot \vec{\mathfrak{J}}. \quad (\text{A.6})$$

With the definition $C = t/2$ so that $Tr(C) = 1/4$, we rewrite (A.6) as

$$\rho = \sum_{i,j} C_{ij} (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) + \vec{v} \cdot \vec{\mathfrak{J}}. \quad (\text{A.7})$$

This, it turn, can be rearranged in terms of the traceless tensor $C - \frac{1}{12}I$ to give

$$\rho = \frac{1}{3}I + \sum_{i,j} (C_{ij} - \frac{1}{12}\delta_{ij}) (\mathfrak{J}_i \mathfrak{J}_j + \mathfrak{J}_j \mathfrak{J}_i) + \vec{v} \cdot \vec{\mathfrak{J}}. \quad (\text{A.8})$$

Then by making the identifications $\vec{P} = Tr(\rho \vec{\mathfrak{J}}) = 2\vec{v}$ and $\frac{1}{\sqrt{6}}T = C - \frac{1}{12}I$ we arrive at (3.1).

The passage from (A.1) to (A.8) is a demonstration of how to usefully decompose the tensor U into its scalar, vector and irreducible tensor parts [17]. Moreover, by explicitly isolating the scalar term, $\frac{1}{3}I$, in (A.8) we obtain a transparent form for ρ when the three spin substates are equally populated: \vec{P} and T must vanish.

The parametrisation (A.8) contains nine real constants, but of course, only eight of them are independent owing to the condition $Tr(C) = 1/4$. However, we can also begin with a

parametrisation based on the matrices \mathfrak{J} but with just eight parameters. For this we recall that the density matrix can be written in the form:

$$\rho = \frac{1}{3}I + \sum_{k=1-8} \lambda_k \mathcal{O}_k, \quad (\text{A.9})$$

where the 3×3 matrices \mathcal{O} are traceless and Hermitian and $Tr(\mathcal{O}_k \mathcal{O}_l) = \alpha_k \delta_{kl}$ so that together with $\frac{1}{3}I$ they comprise an orthogonal basis. The coefficients α are real and the components, $\lambda_k = Tr(\rho \mathcal{O}_k)/\alpha_k$, of the Bloch vector are real and mutually independent.

Then we can, for example, choose the eight assignments:

$$\begin{aligned} \mathcal{O}_1 &= \mathfrak{J}_1 & \mathcal{O}_2 &= \mathfrak{J}_2 & \mathcal{O}_3 &= \mathfrak{J}_3 \\ \mathcal{O}_4 &= \mathfrak{J}_1 \mathfrak{J}_2 + \mathfrak{J}_2 \mathfrak{J}_1 & \mathcal{O}_5 &= \mathfrak{J}_2 \mathfrak{J}_3 + \mathfrak{J}_3 \mathfrak{J}_2 & \mathcal{O}_6 &= \mathfrak{J}_1 \mathfrak{J}_3 + \mathfrak{J}_3 \mathfrak{J}_1 \\ \mathcal{O}_7 &= \mathfrak{J}_1 \mathfrak{J}_1 - \mathfrak{J}_3 \mathfrak{J}_3 & \mathcal{O}_8 &= \mathfrak{J}_2 \mathfrak{J}_2 - \frac{2}{3}I. \end{aligned} \quad (\text{A.10})$$

It is simple to show that, as required, the value of $\langle \hat{s}_1 \hat{s}_1 + \hat{s}_2 \hat{s}_2 + \hat{s}_3 \hat{s}_3 \rangle$ is 2 independently of the coefficients λ , i.e, for any mixed state. Of course, \vec{P} and T are simply related to the coefficients λ . Moreover, the parametrisation (A.10) is convenient for using the equation of motion of the density matrix as in [12, Section 1–8c], but with the commutation relations for the matrices \mathfrak{J} , to demonstrate that \vec{P} for spin–1 particles obeys the T-BMT equation. That approach also leads to the equation of motion (3.6) for T .

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