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The Bloch equation for spin dynamics in electron storage rings: Computational and theoretical aspects

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In this paper, we describe our work on spin polarization in high-energy electron storage rings which we base on the Full Bloch equation (FBE) for the polarization density and which aims towards the $e^- - e^+$ option of the proposed Future Circular Collider (FCC-ee) and the proposed Circular Electron Positron Collider (CEPC). The FBE takes into account nonspin-flip and spin-flip effects due to synchrotron radiation including the spin-diffusion effects and the Sokolov–Ternov effect with its Baier–Katkov generalization as well as the kinetic-polarization effect. This mathematical model is an alternative to the standard mathematical model based on the Derbenev–Kondratenko formulas. For our numerical and analytical studies of the FBE, we develop an approximation to the latter to obtain an effective FBE. This is accomplished by finding a third mathematical model based on a system of stochastic differential equations (SDEs) underlying the FBE and by approximating that system via the method of averaging from perturbative ODE theory. We also give an overview of our algorithm for numerically integrating the effective FBE. This discretizes the phase space using spectral methods and discretizes time via

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the additive Runge–Kutta (ARK) method which is a high-order semi-implicit method. We also discuss the relevance of the third mathematical model for spin tracking.

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1. Introduction

In this paper, we describe some analytical and numerical aspects of our work on spin polarization in high-energy electron storage rings aimed towards the $e^- - e^+$ option of the proposed Future Circular Collider (FCC-ee) and the proposed Circular Electron Positron Collider (CEPC). The main questions for high-energy rings like the FCC-ee and CEPC are: (i) Can one get polarization? (ii) What are the theoretical limits of the polarization? This paper builds on our ICAP18 papers and talks,[1,2] as well as a talk at an IAS mini-workshop on Beam Polarization.[3]

Photon emission in synchrotron radiation affects the orbital motion of electron bunches in a storage ring and can lead to an equilibrium bunch density in phase space. This is modeled by adding noise and damping to the particle motion.[4,5] The photon emission also affects the spin motion and can lead to an equilibrium bunch polarization. This is viewed as a balance of three factors: spin diffusion, the so-called Sokolov–Ternov process and the so-called kinetic polarization effect. These three factors have been modeled mathematically in two ways, the first based on Ref. 6 and the second on Ref. 7. Here, we discuss the second model and introduce a new, third, mathematical model, based on stochastic differential equations (SDEs). So far, analytical estimates of the attainable polarization have been based on the so-called *Derbenev–Kondratenko formulas*.[6,8] A recent overview is part of Ref. 3. In analogy with studies of the trajectories of single particles, this model leans towards the study of single spins and relies in part on plausible assumptions grounded in deep physical intuition. Here, the spin diffusion is viewed as a consequence of the trajectory noise feeding through to the spin motion via the spin–orbit coupling in the Thomas-BMT equation[9] and thus leading to depolarization. The Sokolov–Ternov process[10] causes a build up of the polarization because of an asymmetry in the transitions rates for spin up and spin down. The roots here are in the Dirac equation. This is sometimes referred to as "spin-flip" and relies on the introduction of a spin quantization axis. The kinetic polarization effect follows from the fact that the spin quantization axis is phase space-dependent. Thus, a third question for high-energy rings like the FCC-ee and CEPC is: Are the Derbenev–Kondratenko formulas complete?

We believe that the model based on the Derbenev–Kondratenko formulas is an approximation of the model from Ref. 7 mentioned above which is based on the so-called *polarization density* of the bunch. In the model of Ref. 7, one studies the evolution of the bunch density in phase space with the Fokker–Planck (F–P) equation (2). The corresponding equation for spin is the evolution equation (8) for the polarization density which we call the Full Bloch equation (FBE) and which generalizes the orbital F–P equation. We use the name "Bloch" to reflect the analogy with

equations for magnetization in condensed matter.[11] Each of the above three synchrotron radiation effects correspond to terms in the FBE. Thus, it takes into account effects on spin due to synchrotron radiation including the spin-diffusion effects, the Sokolov–Ternov effect with its Baier–Katkov generalization, as well as the kinetic-polarization effect.

The FBE was introduced by Derbenev and Kondratenko in 1975[7] as a generalization to the whole phase space (with its noisy trajectories) of the Baier–Katkov–Strakhovenko (BKS) equation which just describes the evolution of polarization by spin-flip along a single deterministic trajectory.[3,12] The FBE is a system of three F–P like equations for the three components of the polarization density coupled by a Thomas-BMT term and the BKS terms but uncoupled within the F–P terms. The integral of the polarization density is the polarization vector of the bunch. We remark that the polarization density is proportional to the phase space density of the spin angular momentum. See Refs. 13 and 3 for recent reviews of polarization history and phenomenology. Thus, we study the initial-value problem of the system of coupled orbital F–P equation and the FBE. The third model is based on the system of coupled spin–orbit SDEs (14) and (16) and its associated F–P equation which governs the evolution of the (joint) spin–orbit probability density. We believe that the third model is equivalent to the second model, i.e. the one based on Ref. 7, but we believe that it is also more amenable to analysis.

We proceed as follows. In Sec. 2, we present the FBE for the laboratory frame. We also introduce our newly discovered system of SDEs which underlie the whole FBE. Thus, we can model the FBE in terms of white-noise in the SDEs, thereby extending the classical treatment of spin diffusion from Ref. 14 to a classical treatment of all terms of the FBE. So we have extended the classical model of spin diffusion to a classical model which includes the Sokolov–Ternov effect, its Baier–Katkov correction and the kinetic-polarization effect. As an aside this may lead to a new Monte–Carlo approach to simulation which includes these effects, using modern techniques for integrating SDEs. Section 2 also presents the reduced Bloch equation (RBE) obtained by neglecting the spin-flip terms and the kinetic-polarization term in the FBE. The RBE approximation is sufficient for computing the physically interesting depolarization time and it shares the terms with the FBE that are most challenging to discretize. Thus, in this paper, when we consider the discretization, we only do it for the RBE. In Sec. 3, we discuss the RBE in the beam frame and the underlying SDEs. In Sec. 4, we derive an effective RBE by applying the method of averaging to the underlying SDEs. In Sec. 5, we outline our algorithm for integrating the effective RBE. This will be applied to the FBE in three degrees of freedom. Finally, in Sec. 6, we describe ongoing and future work.

2. FBE, RBE and Associated SDEs in the Laboratory Frame

In a semiclassical probabilistic description of an electron or positron bunch the spin–orbit dynamics is described by the *spin*-1/2 *Wigner function* ρ (also called the

Stratonovich function) written as

$$\rho(t,z) = \frac{1}{2}\left(f(t,z)I_{2\times 2} + \boldsymbol{\sigma}\cdot\boldsymbol{\eta}(t,z)\right), \tag{1}$$

where f is the classical phase-space density normalized by $\int f(t,z)dz = 1$ and $\boldsymbol{\eta}$ is the polarization density of the bunch. Here, $z = (\mathbf{r},\mathbf{p})$ where $\mathbf{r}$ and $\mathbf{p}$ are the position and momentum vectors of the phase space and t is the time. Also, $\boldsymbol{\sigma}$ is the vector of the three Pauli matrices. Thus, $f = \mathrm{Tr}[\rho]$ and $\boldsymbol{\eta} = \mathrm{Tr}[\rho\boldsymbol{\sigma}]$. Here and in the following, we use arrows on three-component column vectors and no arrows on other quantities. As explained in Ref. 14, $\boldsymbol{\eta}$ is proportional to the spin angular momentum density. In fact, it is given by $\boldsymbol{\eta}(t,z) = f(t,z)\mathbf{P}_{\mathrm{loc}}(t,z)$ where $\mathbf{P}_{\mathrm{loc}}$ is the local polarization vector. Then $\rho(t,z)$ is a product of $f(t,z)$ and a pure spin part with $\rho(t,z) = \frac{1}{2}f(t,z)(I_{2\times 2} + \boldsymbol{\sigma}\cdot\mathbf{P}_{\mathrm{loc}}(t,z))$. The polarization vector $\mathbf{P}(t)$ of the bunch is $\mathbf{P}(t) = \int\boldsymbol{\eta}(t,z)dz$. When the particle motion is governed just by a Hamiltonian, as in the case of protons where one neglects all synchrotron radiation effects, the phase-space density is conserved along a trajectory. Then, the polarization density obeys the Thomas-BMT equation along each trajectory. However, if the particles are subject to noise and damping due to synchrotron radiation, the evolution of the density of particles in phase space is more complicated. But as advertised above it can be handled with a F–P formalism.

Then, by neglecting collective effects and after several other approximations, the phase-space density evolves according to Ref. 7 via

$$\partial_t f = L_{\mathrm{FP}}(t,z)f. \tag{2}$$

Using the units as in Ref. 7 the F–P operator L_{FP} is defined by

$$L_{\mathrm{FP}}(t,z) := -\nabla_{\mathbf{r}}\cdot\frac{1}{m\gamma}\mathbf{p} - \nabla_{\mathbf{p}}\cdot\Bigg[e\mathbf{E}(t,\mathbf{r}) + \frac{e}{m\gamma}(\mathbf{p}\times\mathbf{B}(t,\mathbf{r})) + \mathbf{F}_{\mathrm{rad}}(t,z) + \mathbf{Q}_{\mathrm{rad}}(t,z)\Bigg] + \frac{1}{2}\sum_{i,j=1}^{3}\partial_{p_i}\partial_{p_j}\mathcal{E}_{ij}(t,z), \tag{3}$$

where

$$\mathbf{F}_{\mathrm{rad}}(t,z) := -\frac{2}{3}\frac{e^4}{m^5\gamma}|\mathbf{p}\times\mathbf{B}(t,\mathbf{r})|^2\mathbf{p}, \tag{4}$$

$$Q_{\mathrm{rad},i}(t,z) := \frac{55}{48\sqrt{3}}\sum_{j=1}^{3}\frac{\partial[\lambda(t,z)p_ip_j]}{\partial p_j}, \tag{5}$$

$$\mathcal{E}_{ij}(t,z) := \frac{55}{24\sqrt{3}}\lambda(t,z)p_ip_j, \quad \lambda(t,z) := \hbar\frac{|e|^5}{m^8\gamma}|\mathbf{p}\times\mathbf{B}(t,\mathbf{r})|^3, \tag{6}$$

$$\gamma \equiv \gamma(\mathbf{p}) = \frac{1}{m}\sqrt{|\mathbf{p}|^2 + m^2}, \tag{7}$$

and with e and m being the charge and rest mass of the electron or positron and $\mathbf{E},\mathbf{B}$ being the external electric and magnetic fields.

The parabolic F–P terms are those in the double sum of (3). The F–P operator $L_{\rm FP}(t,z)$ whose explicit form is taken from Ref. 7 is a linear second-order partial differential operator and, with some additional approximations, is commonly used for electron synchrotrons and storage rings, see Sec. 2.5.4 in Refs. 4 and 15. As usual, since it is minuscule compared to all other forces, the Stern–Gerlach effect from the spin onto the orbit is neglected in (2). The polarization density $\boldsymbol{\eta}$ evolves via Eq. (2) in Ref. 7, i.e. via the laboratory-frame FBE

$$\partial_t \boldsymbol{\eta} = L_{\rm FP}(t,z)\boldsymbol{\eta} + M(t,z)\boldsymbol{\eta} + [1+\nabla_{\mathbf{p}}\cdot\mathbf{p}]\lambda(t,z)\frac{1}{m\gamma}\frac{\mathbf{p}\times\mathbf{a}(t,z)}{|\mathbf{a}(t,z)|}f(t,z), \tag{8}$$

where

$$M(t,z) := \Omega(t,z) - \lambda(t,z)\frac{5\sqrt{3}}{8}\left[I_{3\times 3} - \frac{2}{9m^2\gamma^2}\mathbf{p}\mathbf{p}^T\right], \tag{9}$$

and with

$$\mathbf{a}(t,z) := \frac{e}{m^2\gamma^2}(\mathbf{p}\times\mathbf{B}(t,\mathbf{r})). \tag{10}$$

The skew-symmetric matrix $\Omega(t,z)$ takes into account the Thomas-BMT spin-precession effect. The quantum aspect of (2) and (8) is embodied in the factor $\hbar$ in $\lambda(t,z)$. For example $\mathbf{Q}_{\rm rad}$ is a quantum correction to the classical radiation reaction force $\mathbf{F}_{\rm rad}$. The terms $-\lambda(t,z)\frac{5\sqrt{3}}{8}\boldsymbol{\eta}$ and $\lambda(t,z)\frac{1}{m\gamma}\frac{\mathbf{p}\times\mathbf{a}(t,z)}{|\mathbf{a}(t,z)|}f(t,z)$ take into account spin-flips due to synchrotron radiation and encapsulate the Sokolov–Ternov effect. The term $\lambda(t,z)\frac{5\sqrt{3}}{8}\frac{2}{9m^2\gamma^2}\mathbf{p}\mathbf{p}^T\boldsymbol{\eta}$ encapsulates the Baier–Katkov correction, and the term $\nabla_{\mathbf{p}}\cdot\mathbf{p}\ \lambda(t,z)\frac{1}{m\gamma}\frac{\mathbf{p}\times\mathbf{a}(t,z)}{|\mathbf{a}(t,z)|}f(t,z) = \sum_1^3 \partial_{p_i}[p_i\lambda(t,z)\frac{1}{m\gamma}\frac{\mathbf{p}\times\mathbf{a}(t,z)}{|\mathbf{a}(t,z)|}f(t,z)]$ encapsulates the kinetic-polarization effect.

The Ito SDEs corresponding to (2) can be written informally as

$$\frac{d\mathbf{r}}{dt} = \frac{1}{m\gamma}\mathbf{p}, \tag{11}$$

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E}(t,\mathbf{r}) + \frac{e}{m\gamma}(\mathbf{p}\times\mathbf{B}(t,\mathbf{r})) + \mathbf{F}_{\rm rad}(t,z) + \mathbf{Q}_{\rm rad}(t,z) + \mathcal{B}^{\rm orb}(t,z)\xi(t), \tag{12}$$

where ξ is the white-noise process and

$$\mathcal{B}^{\rm orb}(t,z) := \mathbf{p}\sqrt{\frac{55}{24\sqrt{3}}\lambda(t,z)}, \tag{13}$$

or more concisely as

$$\frac{dZ}{dt} = F(t,Z) + G(t,Z)\xi(t). \tag{14}$$

More precisely, the stochastic process $Z = (\mathbf{r}, \mathbf{p})^T$ evolves according to the integral equation

$$Z(t) = Z(t_0) + \int_{t_0}^{t} F(\tau, Z(\tau))d\tau + \int_{t_0}^{t} G(\tau, Z(\tau))d\mathcal{W}(\tau), \tag{15}$$

where the second integral in (15) is the so-called Ito integral and $\mathcal{W}$ is the Wiener process. Note that in (14), and from now on, the dependent variables in the SDEs are denoted by large letters. In contrast, independent variables are denoted by small letters, as in $f(t, z)$. We note that (14) is ambiguous. It is common to interpret (14) as either an Ito system of SDEs or a Stratonovich system of SDEs, leading to different F–P equations if G depends on z. The SDEs (14) lead to (2) via Ito but not via Stratonovich. In this paper all SDEs are to be interpreted in the Ito sense. Helpful discussions about Ito SDEs can be found, for example, in Refs. 16–18.

A remarkable and perhaps unknown fact is our recent finding that the FBE can be modeled in terms of white-noise as well, i.e. we can construct a system of SDEs underlying (2) and (8). We already have (14) for the orbital motion and now introduce a vector $\mathbf{S}$ defined to obey

$$\frac{d\mathbf{S}}{dt} = M(t, Z)\mathbf{S} + \mathcal{D}^{\text{spin}}(t, Z) + \mathcal{B}^{\text{kin}}(t, Z)\xi(t), \tag{16}$$

where

$$\mathcal{D}^{\text{spin}}(t, z) := \lambda(t, z)\frac{1}{m\gamma}\frac{\mathbf{p} \times \mathbf{a}(t, z)}{|\mathbf{a}(t, z)|}, \tag{17}$$

$$\mathcal{B}^{\text{kin}}(t, z) := -\frac{1}{m\gamma}\frac{\mathbf{p} \times \mathbf{a}(t, z)}{|\mathbf{a}(t, z)|}\sqrt{\frac{24\sqrt{3}}{55}\lambda(t, z)}. \tag{18}$$

The terms $M(t, Z)$, $\mathcal{B}^{\text{kin}}(t, z)$ and $\mathcal{D}^{\text{spin}}(t, z)$ in (16) are chosen so that they deliver the required FBE (8) by the end of the path for obtaining the FPE described below. As can be expected from the discussion after (9) above, the term $\Omega(t, Z)\mathbf{S}$ will account for the Thomas-BMT spin-precession effect, the terms $-\lambda(t, Z)\frac{5\sqrt{3}}{8}\mathbf{S}$ and $\mathcal{D}^{\text{spin}}(t, Z)$ will account for spin-flips due to synchrotron radiation and encapsulate the Sokolov–Ternov effect. The term proportional to 2/9 in (9) will account for the Baier–Katkov correction, and the white-noise term $\mathcal{B}^{\text{kin}}(t, Z)\xi(t)$ will account for the kinetic-polarization effect. The latter motivates the use of the superscript "kin." As the notation suggests, the white-noise process $\xi(t)$ in (16) is the same as the white-noise process $\xi(t)$ in (12).

To show that (14) and (16) lead to (2) and (8) one proceeds as follows. The SDEs for the joint process $(Z, \mathbf{S})$ can be written as

$$\frac{d}{dt}\begin{pmatrix} Z \\ \mathbf{S} \end{pmatrix} = H(t, Z, \mathbf{S}) + N(t, Z)\xi(t), \tag{19}$$

where

$$H(t, Z, \mathbf{S}) = \begin{pmatrix} F(t, Z) \\ M(t, Z)\mathbf{S} + \mathcal{D}^{\text{spin}}(t, Z) \end{pmatrix}, \quad N(t, Z) = \begin{pmatrix} G(t, Z) \\ \mathcal{B}^{\text{kin}}(t, Z) \end{pmatrix}, \tag{20}$$

and we remind the reader that the SDE is to be interpreted as an Ito SDE. The associated F–P equation for the $(Z, \mathbf{S})$ process evolves the (joint) probability density $\mathcal{P} = \mathcal{P}(t, z, \mathbf{s})$ which is related to f and $\boldsymbol{\eta}$ via

$$f(t,z) = \int_{\mathbb{R}^3} d\mathbf{s}\mathcal{P}(t,z,\mathbf{s}), \quad \boldsymbol{\eta}(t,z) = \int_{\mathbb{R}^3} d\mathbf{s}\mathbf{s}\mathcal{P}(t,z,\mathbf{s}). \tag{21}$$

It is straightforward to show via the F–P equation for $\mathcal{P}$ that f and $\boldsymbol{\eta}$ evolve according to (2) and (8). Thus indeed (14) and (16) lead to (2) and (8).

Note that $|\mathbf{S}(t)|$ in (16) is not conserved in time. So $\mathbf{S}(t)$ in (16) is not the spin vector of a single particle. Nevertheless, $|\mathbf{S}(t)|$ can be related to familiar quantities. In fact, by (21) and since f is the phase-space density, at time t the conditional expectation of $\mathbf{S}(t)$ given $Z(t)$ is $\frac{1}{f(t,z)}\boldsymbol{\eta}(t,z)$, namely the local polarization $\mathbf{P}_{\mathrm{loc}}(t, Z(t))$.

Because $\mathbf{P}(t) = \int \boldsymbol{\eta}(t,z)dz$ it also follows from (21), that the polarization vector $\mathbf{P}(t)$ is the expectation value of the random vector $\mathbf{S}(t)$, i.e. $\mathbf{P}(t) = \langle \mathbf{S}(t) \rangle$ with $\mathbf{S}(t)$ from (16). Thus, and since $|\mathbf{P}(t)| \leq 1$, we obtain $|\langle \mathbf{S}(t) \rangle| \leq 1$, in particular the constraint on the initial condition is: $|\langle \mathbf{S}(0) \rangle| \leq 1$.

Since (2) and (8) follow from (14) and (16) one can use (14) and (16) as the basis for a Monte–Carlo spin tracking algorithm for $\mathbf{P}(t)$. Thus this would extend the standard Monte–Carlo spin tracking algorithms by taking into account all physical effects described by (8), like the Sokolov–Ternov effect, the Baier–Katkov correction, the kinetic-polarization effect and, of course, spin diffusion. A detailed paper on this is in progress.[19]

If we ignore the spin-flip terms and the kinetic-polarization term in the FBE then (8) simplifies to

$$\partial_t \boldsymbol{\eta} = L_{\mathrm{FP}}(t,z)\boldsymbol{\eta} + \Omega(t, z(t))\boldsymbol{\eta}\,. \tag{22}$$

We refer to (22) as the RBE. Accordingly the system of SDEs underlying (22) is (14) and a simplified (16), namely

$$\frac{d\mathbf{S}}{dt} = \Omega(t, Z(t))\mathbf{S}. \tag{23}$$

The RBE models spin diffusion due to the orbital motion. Note that by (23), and in contrast to (16), $|\mathbf{S}(t)|$ is conserved in time. As mentioned in Sec. 1, the RBE is sufficient for computing the depolarization time and it shares the terms with the FBE that are most challenging to discretize.

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The conventional Monte–Carlo spin tracking algorithms to compute the radiative depolarization time, e.g. SLICKTRACK by Barber, SITROS by Kewisch, Zgoubi by Meot, PTC/FPP by Forest, and Bmad by Sagan take care of the spin diffusion and they are based on the SDEs (14) and (23).[15,20–22] In contrast the Monte–Carlo spin tracking algorithm proposed above is based on the SDEs (14) and (16) taking into account spin diffusion, the Sokolov–Ternov effect, the Baier–Katkov correction and the kinetic-polarization effect.

Equations (2) and (8) can be derived from quantum electrodynamics, using the semiclassical approximation of the Foldy–Wouthuysen transformation of the Dirac Hamiltonian and finally by making a Markov approximation.[23] We stress however, that (14) and (16) provide a model for (8) which can be treated classically. In fact, in the special case where one neglects all spin-flip effects and the kinetic-polarization effect the corresponding SDEs (14) and (23) (and thus the RBE (22)) can be derived purely classically as in Ref. 14. See Sec. 3 too.

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3. RBE and SDEs in the Beam Frame

In the beam frame, i.e. in accelerator coordinates y, the RBE (22) becomes

$$\partial_\theta \boldsymbol{\eta}_Y = L_Y(\theta, y)\boldsymbol{\eta}_Y + \Omega_Y(\theta, y)\boldsymbol{\eta}_Y, \tag{24}$$

where the meaning of the subscript "Y" will become clear below. Here θ is the accelerator azimuth

$$L_Y(\theta, y) = -\sum_{j=1}^{6} \partial_{y_j}(\mathcal{A}(\theta)y)_j + \frac{1}{2} b_Y(\theta)\partial_{y_6}^2,$$

$\mathcal{A}(\theta)$ is a 6×6 matrix encapsulating radiationless motion and the deterministic effects of synchrotron radiation, $b_Y(\theta)$ encapsulates the quantum fluctuations, and $\Omega_Y(\theta, y)$ is the Thomas-BMT term. The latter is a skew-symmetric 3×3 matrix and we linearize it as in Ref. 24. Note that $\mathcal{A}(\theta)$, $\Omega_Y(\theta, y)$ and $b_Y(\theta)$ are 2π-periodic in θ. Given the beam-frame polarization density $\boldsymbol{\eta}_Y$, the beam-frame polarization vector $\mathbf{P}(\theta)$ of the bunch at azimuth θ is

$$\mathbf{P}(\theta) = \int dy \boldsymbol{\eta}_Y(\theta, y). \tag{25}$$

Our central computational focus is the RBE (24) with $\mathbf{P}(\theta)$ being a quantity of interest. To proceed with this we use the underlying system of SDEs which are

$$Y' = \mathcal{A}(\theta)Y + \sqrt{b_Y(\theta)}e_6\xi(\theta), \tag{26}$$

$$\mathbf{S}' = \Omega_Y(\theta, Y)\mathbf{S}, \tag{27}$$

where ξ is the white-noise process, $e_6 = (0, 0, 0, 0, 0, 1)^T$ and, recalling the previous section, $\mathbf{S}(\theta)$ is the local polarization vector at $Y(\theta)$. The six components of Y are defined here as in Refs. 5 and 24. Thus the sixth component of Y is $(\gamma - \gamma_r)/\gamma_r$ where γ_r is the reference value of γ. Since (26) is an Ito system of SDEs which, in the language of SDEs, is linear in the narrow sense, it defines a Gaussian process $Y(t)$ if $Y(0)$ is Gaussian. See Ref. 17. Equations (26) and (27) can be obtained by transforming (14) and (23) from the laboratory frame to the beam frame. However (26) and (27) can also be found in several expositions on spin in high-energy electron storage rings, e.g. Ref. 24. Note that these expositions make some approximations. We use Ref. 24 which involves transforming from the laboratory to the beam frame and then linearizing in the beam-frame coordinates, leading to the linear SDEs (26)

and to $\Omega_Y(\theta, Y)$ which is linear in Y. Practical calculations with the Derbenev–Kondratenko formalism make similar approximations.

The F–P equation for the density of the Gaussian process Y is

$$\partial_\theta \mathcal{P}_Y = L_Y(\theta, y)\mathcal{P}_Y. \tag{28}$$

In fact with (26) and (27) the evolution equation for the spin–orbit joint probability density $\mathcal{P}_{YS}$ is the following F–P equation

$$\partial_\theta \mathcal{P}_{YS} = L_Y(\theta, y)\mathcal{P}_{YS} - \sum_{j=1}^{3} \partial_{s_j}((\Omega_Y(\theta, y)\mathbf{s})_j \mathcal{P}_{YS}). \tag{29}$$

Note that $\mathcal{P}_Y$ is related to $\mathcal{P}_{YS}$ by

$$\mathcal{P}_Y(\theta, y) = \int_{\mathbb{R}^3} d\mathbf{s} \mathcal{P}_{YS}(\theta, y, \mathbf{s}). \tag{30}$$

Also, by integrating (29) over $\mathbf{s}$ one recovers (28). The polarization density $\boldsymbol{\eta}_Y$ corresponding to $\mathcal{P}_{YS}$ is defined by

$$\boldsymbol{\eta}_Y(\theta, y) = \int_{\mathbb{R}^3} d\mathbf{s}\ \mathbf{s}\ \mathcal{P}_{YS}(\theta, y, \mathbf{s}). \tag{31}$$

Note that (30) and (31) are analogous to (21). The RBE (24) follows from (29) by differentiating (31) w.r.t. θ. For (24) see Ref. 14 too. We recall that the relation between a system of SDEs and its F–P equation is standard, see, e.g. Refs. 16–18.

4. Approximating the Beam-Frame RBE by the Method of Averaging

Because the coefficients of $L_Y(\theta, y)$ are θ-dependent, the RBE (24) is difficult to understand analytically and difficult for a numerical method. Since the RBE is derivable from the associated SDEs (26) and (27) we can focus on these difficulties in the SDEs, rather than in the RBE, where approximation methods are better developed. For this purpose we rewrite (26) as

$$Y' = (A(\theta) + \epsilon\delta A(\theta))Y + \sqrt{\epsilon}\sqrt{b(\theta)}e_6\xi(\theta), \tag{32}$$

where $A(\theta)$ is the Hamiltonian part of $\mathcal{A}(\theta)$ and ϵ is chosen so that δA is order 1. Then b is defined by $\sqrt{\epsilon}\sqrt{b(\theta)} = \sqrt{b_Y(\theta)}$. Here $\epsilon\delta A(\theta)$ represents the part of $\mathcal{A}(\theta)$ associated with damping effects due to synchrotron radiation and cavities (see, e.g. Eq. (5.3) in Ref. 24). The term $\sqrt{\epsilon}\sqrt{b(\theta)}$ corresponds to the quantum noise and the square root is needed for the balance of damping, cavity acceleration and quantum noise (see Eq. (34)). We are interested in situations where Y has been appropriately scaled and where the synchrotron radiation has a small effect so that ϵ is small.

Equation (32) can be approximated using the method of averaging which will eliminate some of the θ-dependent coefficients and allow for a numerical method which can integrate the resultant RBE efficiently over long times. This has the added benefit of deepening our analytical understanding, as a perturbation analysis

usually does. We call the approximation of the RBE the effective RBE and we will find it by refining the averaging technique presented in Sec. 2.1.4 of the Accelerator Handbook.[5] This refinement allows us to use the method of averaging to approximate the SDEs (32). We just give a sketch here (a detailed account will be published elsewhere[25]).

Because the process Y is Gaussian, if $Y(0)$ is Gaussian, all the information is in its mean m_Y and covariance K_Y and they evolve by the ODEs

$$m_Y' = (A(\theta) + \epsilon\delta A(\theta))m_Y, \tag{33}$$

$$K_Y' = (A(\theta) + \epsilon\delta A(\theta))K_Y + K_Y(A(\theta) + \epsilon\delta A(\theta))^T + \epsilon\omega(\theta)e_6e_6^T. \tag{34}$$

In (34) the δA terms and the ω are balanced at $O(\epsilon)$ and so can be treated together in first-order perturbation theory. This is the reason for the $\sqrt{\epsilon}$ in (32). However this balance is also physical since the damping and diffusion come from the same source and the cavities replenish the energy loss. We cannot include the spin equation (27) because the joint $(Y, \mathbf{S})$ process is not Gaussian. Equation (27) has a quadratic nonlinearity since it is linear in Y and $\mathbf{S}$ so that the joint moment equations would not close. Thus here we will apply averaging to the Y process only and discuss the spin after that. However, see Remark 3 below which outlines a plan for a combined approach.

To apply the method of averaging to (33) and (34) we must transform them to a standard form for averaging. We do this by using a fundamental solution matrix X of the unperturbed $\epsilon = 0$ part of (32) and (33), i.e.

$$X' = A(\theta)X. \tag{35}$$

We thus transform Y, m_Y and K_Y into U, m_U and K_U via

$$Y = X(\theta)U, \quad m_Y = X(\theta)m_U, \quad K_Y = X(\theta)K_UX^T(\theta), \tag{36}$$

and (32), (33) and (34) are transformed to

$$U' = \epsilon\mathcal{D}(\theta)U + \sqrt{\epsilon}\sqrt{\omega(\theta)}X^{-1}(\theta)e_6\xi(\theta), \tag{37}$$

$$m_U' = \epsilon\mathcal{D}(\theta)m_U, \tag{38}$$

$$K_U' = \epsilon(\mathcal{D}(\theta)K_U + K_U\mathcal{D}^T(\theta)) + \epsilon\mathcal{E}(\theta). \tag{39}$$

Here $\mathcal{D}(\theta)$ and $\mathcal{E}(\theta)$ are defined by

$$\mathcal{D}(\theta) = X^{-1}(\theta)\delta A(\theta)X(\theta), \tag{40}$$

$$\mathcal{E}(\theta) = \omega(\theta)X^{-1}(\theta)e_6e_6^TX^{-T}(\theta). \tag{41}$$

Of course, (37)–(39) carry the same information as (32)–(34).

Now, applying the method of averaging to (38) and (39), we obtain the Gaussian process V with mean and covariance matrix

$$m_V' = \epsilon\bar{\mathcal{D}}m_V, \tag{42}$$

$$K_V' = \epsilon(\bar{\mathcal{D}}K_V + K_V\bar{\mathcal{D}}^T) + \epsilon\bar{\mathcal{E}}, \tag{43}$$

where the bar denotes θ-averaging, i.e. the operation $\lim_{T\to\infty}(1/T)\int_0^T d\theta\ldots$. For physically reasonable A each fundamental matrix X is a quasiperiodic function whence $\mathcal{D}$ and $\mathcal{E}$ are quasiperiodic functions so that their θ averages $\bar{\mathcal{D}}$ and $\bar{\mathcal{E}}$ exist. By averaging theory $|m_U(\theta) - m_V(\theta)| \le C_1(T)\epsilon$ and $|K_U(\theta) - K_V(\theta)| \le C_2(T)\epsilon$ for $0 \le \theta \le T/\epsilon$ where T is a constant (see also Refs. 26–29) and ϵ small. However, we expect to be able to show that these estimates are uniformly valid on $[0,\infty)$ so that an accurate estimate of the orbital equilibrium would be found.

The key point now is that every Gaussian process V, whose mean m_V and covariance matrix K_V satisfy the ODEs (42) and (43), also satisfies the system of SDEs

$$V' = \epsilon\bar{\mathcal{D}}V + \sqrt{\epsilon}\mathcal{B}(\xi_1,\ldots,\xi_k)^T. \tag{44}$$

Here $\xi_1,\ldots,\xi_k$ are statistically independent versions of the white-noise process and $\mathcal{B}$ is a $6\times k$ matrix which satisfies $\mathcal{B}\mathcal{B}^T = \bar{\mathcal{E}}$ with $k = \operatorname{rank}(\bar{\mathcal{E}})$. Since $m_U(\theta) = m_V(\theta) + O(\epsilon)$ and $K_U(\theta) = K_V(\theta) + O(\epsilon)$ we get $U(\theta) \approx V(\theta)$. In particular $Y(\theta) \approx X(\theta)V(\theta)$ (more details will be in Ref. 25). Conversely, the mean vector m_V and covariance matrix K_V of every V in (44) satisfy the ODEs (42) and (43).

Remark. It's likely that stochastic averaging techniques can be applied directly to (37) giving (44) as an approximation and we are looking into this (see Ref. 30 and references therein). However, because (37) is linear and defines a Gaussian process, the theory for getting to (44) from the ODEs for the moments could not be simpler, even though it is indirect. □

To proceed with an analysis of (44) and its associated F–P equation we need an appropriate X and we note that $X(\theta) = M(\theta)C$ where C is an arbitrary invertible 6×6 matrix and M is the principal solution matrix, i.e. $M' = A(\theta)M, M(0) = I$. Thus choosing X boils down to choosing a good C. As is common for spin physics in electron storage rings we emulate Chao's approach (see Sec. 2.1.4 in Ref. 5 and Refs. 31 and 32) and use the eigenvectors of $M(2\pi)$. We assume that the unperturbed orbital motion is stable. Thus $M(2\pi)$ has a full set of linearly independent eigenvectors and the eigenvalues are on the unit circle in the complex plane.[33] We further assume a nonresonant condition on the orbital frequencies. We construct C as a real matrix using the real and imaginary parts of the eigenvectors in its columns and using the fact that $M(2\pi)$ is symplectic (since $A(\theta)$ is a Hamiltonian matrix). It follows that $\bar{\mathcal{D}}$ has block diagonal form and $\bar{\mathcal{E}}$ has diagonal form. Explicitly,

$$\bar{\mathcal{D}} = \begin{pmatrix} \mathcal{D}_I & 0_{2\times 2} & 0_{2\times 2} \\ 0_{2\times 2} & \mathcal{D}_{II} & 0_{2\times 2} \\ 0_{2\times 2} & 0_{2\times 2} & \mathcal{D}_{III} \end{pmatrix}, \tag{45}$$

$$\mathcal{D}_\alpha = \begin{pmatrix} a_\alpha & b_\alpha \\ -b_\alpha & a_\alpha \end{pmatrix}, \quad (\alpha = I, II, III), \tag{46}$$

and $\bar{\mathcal{E}} = \operatorname{diag}(\mathcal{E}_I, \mathcal{E}_I, \mathcal{E}_{II}, \mathcal{E}_{II}, \mathcal{E}_{III}, \mathcal{E}_{III})$ with $a_\alpha \le 0$ and $\mathcal{E}_I, \mathcal{E}_{II}, \mathcal{E}_{III} \ge 0$.

To include the spin note that, under the transformation $Y \mapsto U$, (26) and (27) become

$$U' = \epsilon \mathcal{D}(\theta)U + \sqrt{\epsilon}\sqrt{\omega(\theta)}X^{-1}(\theta)e_6\xi(\theta), \tag{47}$$

$$\mathbf{S}' = \Omega_Y(\theta, X(\theta)U)\mathbf{S}\ , \tag{48}$$

where we have repeated (37). Now, as we just mentioned, U is well approximated by V, i.e. $U = V + O(\epsilon)$ on θ intervals of a length of $O(1/\epsilon)$ (and because of damping we may have uniform validity for $0 \leq \theta < \infty$). Thus

$$\Omega_Y(\theta, X(\theta)U) = \Omega_Y(\theta, X(\theta)V) + O(\epsilon), \tag{49}$$

and (48) becomes

$$\mathbf{S}' = \Omega_Y(\theta, X(\theta)V)\mathbf{S} + O(\epsilon). \tag{50}$$

Dropping the $O(\epsilon)$ in (50) and replacing U by V in (48) we obtain the system

$$V' = \epsilon \bar{\mathcal{D}}V + \sqrt{\epsilon}\mathcal{B}(\xi_1, \ldots, \xi_k)^T, \tag{51}$$

$$\mathbf{S}' = \Omega_Y(\theta, X(\theta)V)\mathbf{S}, \tag{52}$$

where (51) is a repeat of (44). With (51) and (52) the evolution equation for the spin–orbit probability density $\mathcal{P}_{VS} = \mathcal{P}_{VS}(\theta, \mathrm{v}, \mathbf{s})$ is the following F–P equation:

$$\partial_\theta \mathcal{P}_{VS} = L_V(v)\mathcal{P}_{VS} - \sum_{j=1}^{3} \partial_{s_j}((\Omega_Y(\theta, X(\theta)\mathrm{v})\mathbf{s})_j \mathcal{P}_{VS}), \tag{53}$$

where

$$L_V(v) = -\epsilon \sum_{j=1}^{6} \partial_{\mathrm{v}_j}(\bar{\mathcal{D}}\mathrm{v})_j + \frac{\epsilon}{2} \sum_{i,j=1}^{6} \bar{\mathcal{E}}_{ij}\partial_{\mathrm{v}_i}\partial_{\mathrm{v}_j}. \tag{54}$$

Thus the three degrees of freedom are uncoupled in L_V since, by (54),

$$L_V = L_{V,I} + L_{V,II} + L_{V,III}, \tag{55}$$

where each $L_{V,\alpha}$ is an operator in one degree of freedom (=two dimensions) and is determined by $\mathcal{D}_\alpha$ and $\mathcal{E}_\alpha$ via (54) ($\alpha = I, II, III$).

This is important for our numerical approach.

The polarization density $\boldsymbol{\eta}_V$ corresponding to $\mathcal{P}_{VS}$ is defined by

$$\boldsymbol{\eta}_V(\theta, \mathrm{v}) = \int_{\mathbb{R}^3} d\mathbf{s}\mathbf{s}\mathcal{P}_{VS}(\theta, \mathrm{v}, \mathbf{s}), \tag{56}$$

so that by (53), the effective RBE is

$$\partial_\theta \boldsymbol{\eta}_V = L_V(v)\boldsymbol{\eta}_V + \Omega_Y(\theta, X(\theta)\mathrm{v})\boldsymbol{\eta}_V. \tag{57}$$

The coefficients of $L_V(v)$ are θ-independent for every choice of X and this is necessary for our numerical method.

We now have $Y(\theta) = X(\theta)U(\theta) \approx Y_a(\theta) := X(\theta)V(\theta)$ and it follows that $\boldsymbol{\eta}_Y$ in (24) is given approximately by

$$\boldsymbol{\eta}_Y(\theta, y) \approx \boldsymbol{\eta}_{Y,a}(\theta, y) = \det(X^{-1}(0))\boldsymbol{\eta}_V(\theta, X^{-1}(\theta)\mathrm{y}). \tag{58}$$

Now (57) and the effective RBE for $\boldsymbol{\eta}_{Y,a}$ carry the same information. However in general the effective RBE for $\boldsymbol{\eta}_{Y,a}$ does not have the nice features of (57), e.g. being θ-independent, which make the latter useful for our numerical method (see below). Hence we discretize (57) rather than the effective RBE for $\boldsymbol{\eta}_{Y,a}$.

We now make several remarks on the validity of the approximation leading to (51) and (52) and thus to (57).

Remark 1. The averaging which leads to (57) affects only the orbital variables. It was justified by using the fact that (47) is linear whence it defines a Gaussian process when the initial condition is Gaussian. This allowed us to apply the method of averaging to the first and second moments rather than the SDEs themselves. □

Remark 2. We cannot extend the moment approach to the system (47) and (48) because (48) has a quadratic nonlinearity and the system of moment equations do not close. In future work, we will pursue approximating the system (47) and (48) using stochastic averaging as in Ref. 30. □

Remark 3. Because of the $O(\epsilon)$ error in (50) we a priori expect an error of $O(\epsilon\theta)$ in $\mathbf{S}$ when going from (48) to (52) and so (57) may only give a good approximation to $\boldsymbol{\eta}_Y$ on θ intervals of a length of $O(1)$. The work mentioned in Remark 2 above may shed light on this. In addition we will split Ω_Y into two pieces: $\Omega_Y(\theta, y) = \Omega_0(\theta) + \epsilon_s\omega(\theta, y)$ where Ω_0 is the closed-orbit contribution to Ω_Y and ϵ_s is chosen so that ω is $O(1)$. Then, in the case where $\epsilon_s = \epsilon$, (48) becomes $\mathbf{S}' = \Omega_0(\theta)\mathbf{S} + \epsilon\omega(\theta, X(\theta)U)\mathbf{S}$. By letting $\mathbf{S}(\theta) = \Psi(\theta)\mathbf{T}(\theta)$ where $\Psi' = \Omega_0(\theta)\Psi$ we obtain

$$\mathbf{T}' = \epsilon\mathfrak{D}(\theta, U)\mathbf{T}, \tag{59}$$

where $\mathfrak{D}(\theta, U) = \Psi^{-1}(\theta)\omega(\theta, X(\theta)U)\Psi(\theta)$. Our system is now (47) and (59) and the associated averaged system consists of (51) and of the averaged form of (59), i.e.

$$V' = \epsilon\bar{\mathcal{D}}V + \sqrt{\epsilon}\mathcal{B}(\xi_1, \ldots, \xi_k)^T, \tag{60}$$

$$\mathbf{T}'_a = \epsilon\bar{\mathfrak{D}}(V)\mathbf{T}_a. \tag{61}$$

It seems likely that $\mathbf{S}(\theta) = \Psi(\theta)\mathbf{T}_a(\theta) + O(\epsilon)$ for $0 \le \theta < O(1/\epsilon)$, which we hope to prove. □

Remark 4. We have applied the method of averaging to a 1-degree-of-freedom model (= 2 dimensions) with just one spin variable and have verified the $O(\epsilon)$ error analytically. In addition, we are working on a 2-degree-of-freedom model (=4 dimensions) with just one spin variable. These are discussed in our two ICAP18 papers.[1,2] These models will be helpful for our 3-degree-of-freedom study we outlined here. □

5. Sketch of the Numerical Approach

We now briefly sketch our numerical approach to the effective RBE (57). For more details see Ref. 2. The numerical computations are performed by using three pairs $(r_\alpha, \varphi_\alpha)$ of polar coordinates, i.e. $\mathrm{v}_1 = r_I \cos\varphi_I, \ldots, \mathrm{v}_6 = r_{III} \sin\varphi_{III}$. The angle variables are Fourier transformed whence the Fourier coefficients are functions of time and the radial variables. We discretize the radial variables by using the *collocation* method[34,35] using a Chebychev grid for each radial variable. For each Fourier mode this results in a system of linear first-order ODEs in θ which we discretize by using an implicit/explicit θ-stepping scheme. The collocation method is a minimial-residue method by which the residual of the PDE is zero at the numerical grid points. Because of (54), (45) and (46) the Fourier modes are uncoupled in $L_V \boldsymbol{\eta}_V$ so that the only coupling of Fourier modes in (57) comes via $\Omega_Y(\theta, X(\theta)\mathrm{v})\boldsymbol{\eta}_V$ and this coupling is local since $\Omega_Y(\theta, X(\theta)\mathrm{v})$ is linear in v. Thus the parabolic terms are separated from the mode coupling terms. Hence in the θ stepping $L_V \boldsymbol{\eta}_V$ is treated implicitly and $\Omega_Y(\theta, X(\theta)\mathrm{v})\boldsymbol{\eta}_V$ is treated explicitly. We exploit the decoupling by evolving the resulting ODE system with the additive Runge–Kutta (ARK) method. As described in Ref. 36, ARK methods are high-order semi-implicit methods that are constructed from a set of consistent Runge–Kutta (RK) methods. In the RBE the parabolic part of the equation is treated with a diagonally implicit RK method (DIRK) and the mode coupling part is treated with an explicit RK (ERK) method which does not require a linear solve. The ODE system can be evolved independently in time for each Fourier mode, resulting in a computational cost for each timestep that scales as $\mathcal{O}(N^{3q})$ per mode where N is the number of grid-points for each of the six dimensions and where $1 \leq q \leq 3$, depending on the algorithms used for the linear solve. However, only algorithms with $q \approx 1$ are feasible (for Gaussian elimination $q = 3$). Fortunately, the structure of the averaged equations (e.g. the parabolic terms are decoupled from mode coupling terms) allows efficient parallel implementation. We have applied this in a 1-degree-of-freedom model and have demonstrated the spectral convergence.[2]

6. Discussion and Next Steps

We are continuing our work on the second model, i.e. the one based on the Bloch-equation, by extending the averaging and numerical work from the RBE to the FBE and from one and 2 degrees-of-freedom to 3 degrees-of-freedom, aiming towards realistic FODO lattices.[25,37] This will include depolarization and polarization times and equilibrium polarization. Extending the second model from the RBE to the FBE involves averaging and thus involves the SDEs from the third model. Moreover we plan to use the third model to develop a Monte–Carlo spin tracking algorithm which is based on the SDEs (14) and (16) and which takes into account the Sokolov–Ternov effect, the Baier–Katkov correction, the kinetic-polarization effect and spin diffusion. Furthermore we continue our work on comparing the Bloch-equation

approach with Derbenev–Kondratenko-formula approach and estimating the polarization at the FCC-ee and CEPC.

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