Spin dynamics in modern electron storage rings: Computational and theoretical aspects [1]

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Outline 1

- Topic: Estimating the polarization in high energy electron storage rings
- Motivation: getting polarization in high energy electron storage rings like Future Circular Collider (FCC-ee) and proposed Circular Electron Positron Collider (CEPC)
- Ultimate questions:
  1. Is polarization possible in FCC-ee or CEPC?
  2. Are the Derbenev-Kondratenko formulas valid for FCC-ee and CEPC?
- Model of electron bunch:
  - Mesoscopic approach via phase space densities: orbital density and polarization density
- Tool 1: Bloch equation for polarization density = System of linear PDEs = three Fokker-Planck equations plus coupling terms
- Tool 2: Numerical approach to Bloch equation
- Motto: Neglect collective effects and Stern-Gerlach effect ⇒ orbital density no serious issue
- This talk: derivation of our numerical approach to compute the polarization density
- Details on numerical approach: see talk of O. Beznosov

Outline 2

- Mesoscopic approach (=phase space approach):
  - Upside: provides sufficient detail of bunch
  - Downside: curse of dimensionality = polarization density carries 7 independent variables
- A “nice” Bloch equation suggests following numerical approach:
  - Use pairs of polar coordinates on phase space
  - Discretize polar angles by Fourier transform polar angles
  - Discretize radial variables by pseudospectral method (=collocation method) MOVE for phase space discretization which is a spectral method
  - Implicit/explicit time stepping scheme for time discretization
- Numerical approach promises:
  1. Large time steps
  2. Few grid points
  3. Parallel implementation

  Nice Bloch equation obtained by analytic approximation of starting Bloch equation ⇒
- Tool 3: Get “average Bloch equation” by combining method of averaging from perturbation theory with Chao’s eigenvector approach to electron spin
- Remark: Thus apply numerical approach to average Bloch equation!

Mesoscopic description of electron bunch: orbital and polarization densities (Cartesian coordinates)

- Mesoscopic description of electron bunch by spin-$1/2$ Wigner function ρ (=Stratonovich function):

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

  - Remark 1: $\vec{\sigma}$=3-vector of Pauli matrices $\Rightarrow$ ρ is complex 2×2-matrix function of 7 arguments. Note: Arrow indicates 3-component object
  - Remark 2: $z=(r,p)$ where r and p are position/momentum vectors and t is time
  - Remark 3: ρ is not fully quantum but quasiclassical = classical plus quantum corrections
  - Remark 4: f is orbital density and $f = Tr[\rho]$ and $\int f(t,z)dz = 1$
  - Remark 5: $\vec{\eta}$ is polarization density and $\vec{\eta} = Tr[\rho\vec{\sigma}]$ and $\int \vec{\eta}(t,z)dz = \vec{P}(t)$ where $\vec{P}(t)$ is polarization vector of bunch
  - Remark 6: Time evolution of ρ results in time evolution of f and $\vec{\eta}$

Mesoscopic description of electron bunch: orbital Fokker-Planck equation (Cartesian coordinates)

- Fokker-Planck equation for orbital density:

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

- Remark 1: Explicit form of Fokker-Planck operator L_{FP} known since pioneering QED work on quantum corrections to synchrotron radiation in the early 1950s by Schwinger [2]
- Remark 2: L_{FP}=linear second-order partial differential operator entailing Lorentz force and orbital synchrotron radiation effects
- Remark 3: Data in L_{FP} commonly used to derive stochastic ODEs for orbital motion in electron storage rings - see any exposition on electron storage rings, e.g., Sands [3]
- Remark 4: If necessary L_{FP} could be modified using recent QED work on undulator fields and strong fields
- Remark 5: As common, the miniscule Stern-Gerlach effect of spin on orbit neglected in (2): would show up in (2) as term linear in $\vec{\eta}$

[2] J. Schwinger, Proc. Nat. Acad. Sci.(Washington) 40:132 (1954).

[3] M. Sands, *The physics of electron storage rings, SLAC-121, 1970*

Mesoscopic description of electron bunch: Full Bloch equation for polarization density (Cartesian coordinates)

- Full Bloch equation for polarization density:

$$\begin{aligned}\partial_t\vec{\eta} &= L_{FP}(t,z)\vec{\eta} + \Omega(t,z)\vec{\eta} + G(t,z)\vec{\eta} \\ &+\vec{g}(t,z)f + \vec{L}(t,z)f \end{aligned} \qquad (3)$$

- Remark 1: Explicit form of $G, \vec{g}$ and $\vec{L}$ derived by Derbenev and Kondratenko in 1975 [4]
- Orbital Fokker-Planck equation and full Bloch equation not fully quantum but semiclassical
- Remark 2: Ω carries Thomas-BMT spin-precession effect
- Remark 3: G, $\vec{g}$ and $\vec{L}$ carry spin flips effects due to synchrotron radiation
- Remark 4: In particular G, $\vec{g}$ and $\vec{L}$ carry Sokolov-Ternov effect. Note: G contains Baier-Katkov correction to Sokolov-Ternov effect

[4] Ya.S. Derbenev, A.M. Kondratenko, *Relaxation and equilibrium state of electrons in storage rings*, *Sov. Phys. Dokl.*, vol. 19, p. 438, 1975

Mesoscopic description of electron bunch: Reduced Bloch equation for polarization density (Cartesian coordinates)

- Neglecting spin flips, full Bloch equation (3) simplifies to reduced Bloch equation (RBE):

$$\partial_t \vec{\eta} = L_{FP}(t, z)\vec{\eta} + \Omega(t, z)\vec{\eta} \tag{4}$$

- Remark 1: The RBE takes into account effects of external fields and of orbital synchrotron radiation effects $\Rightarrow$ RBE sufficient for computing depolarization time
- Remark 2: RBE contains main numerical subtleties of the full Bloch equation (all derivative terms belong to RBE)
- Remark 3: RBE can be rederived from stochastic ODE (see below)

Mesoscopic description of electron bunch: Reduced Bloch equation for polarization density (Accelerator coordinates)

- In the beam frame, i.e., in accelerator coordinates, RBE reads as

$$\partial_\theta \vec{\eta}_Y = (L_Y + L_{Y,TBMT})\vec{\eta}_Y \tag{5}$$

$$where \qquad L_Y = -\sum_{j=1}^{6} \partial_{y_j} \left(\left(A(\theta) + \epsilon \delta A(\theta) \right) y \right)_j + \frac{1}{2}\omega(\theta)\partial^2_{y_6} \,,$$

$$L_{Y,TBMT}\vec{\eta}_Y = \Omega_Y(\theta, y)\vec{\eta}_Y$$

- Remark 1: $A(\theta) + \epsilon\delta A(\theta)$=$6 \times 6$ matrix encapsulating the Lorentz force effects and the deterministic orbital synchrotron radiation effects
- Remark 2: $A(\theta)$=Hamiltonian part of $A(\theta) + \epsilon\delta A(\theta)$
- Remark 3: $\Omega_Y(\theta, y)$=skew-symmetric T-BMT matrix linear in y
- Remark 4: RBE (5) is beam frame transform of lab frame RBE (2) + approximations
- Remark 5: Quantity of interest= polarization vector of bunch=$\vec{P}(\theta) = \int \vec{\eta}_Y(\theta, y)dy$
- Remark 6: RBE (5) is what we want solved but not "nice" because L_Y too complex for numerical computation!

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Idea 1: Replace beam frame RBE (5) by "nice" RBE via approximating L_Y analytically
- Idea 2: Approximate L_Y analytically by using Method of Averaging from ODE perturbation theory
- Remark: Approximation of L_Y possible because coefficients of L_Y are coefficients of ODEs for stochastic moments!
- ODEs for first moment vector m_Y and covariance matrix K_Y of solutions of orbital Fokker-Planck equation:

$$\partial_\theta f_Y = L_Y f_Y \tag{6}$$

- Remark 1: ODE for m_Y:

$$m_Y' = (A(\theta) + \epsilon\delta A(\theta))m_Y \ , \tag{7}$$

- Remark 2: ODE for K_Y:

$$K_Y' = (A(\theta) + \epsilon\delta A(\theta))K_Y + K_Y(A(\theta) + \epsilon\delta A(\theta))^T + \epsilon\omega(\theta)e_6 e_6^T \tag{8}$$

- Remark 3: $e_6 = (0, 0, 0, 0, 0, 1)^T$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Before we analytically approximate RBE let us reconsider it!
- System of Langevin equations underlying RBE is

$$Y' = (A(\theta) + \epsilon\delta A(\theta))Y + \sqrt{\epsilon}\sqrt{\omega(\theta)}e_6\xi(\theta) \qquad (9)$$

$$\vec{S}' = \Omega_Y(\theta, Y)\vec{S} \qquad (10)$$

- Remark 1: ξ=version of white noise process
- Remark 2: $\vec{S}$=single-particle spin expectation value
- Remark 3: (9) and (10) can be found in virtually every exposition on spin in electron storage rings [5]
- Remark 4: (9) can be viewed as Ito stochastic differential equation which is linear in narrow sense and thus defines Gaussian process Y if $Y(0)$ is Gaussian
- Remark 5: (10) not linear but quadratic $\Rightarrow$ averaging of Ω_Y is future work (see however talk by O.Beznosov on 2 and 1 orbital degrees of freedom)

[5] For example: D.P. Barber, K. Heinemann, H. Mais, G. Ripken, DESY-91-146, 1991

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Remark 6: Spin-orbit joint probability density $\mathcal{P}_{YS} = \mathcal{P}_{YS}(\theta, y, \vec{s})$ satisfies Fokker-Planck equation:

$$\partial_\theta \mathcal{P}_{YS} = L_Y \mathcal{P}_{YS} - \sum_{j=1}^{3} \partial_{s_j} \left(\left(\Omega_Y(\theta, y)\vec{s} \right)_j \mathcal{P}_{YS} \right) \qquad (11)$$

- Remark 7: $\mathcal{P}_{YS}$ related to orbital density by

$$f_Y(\theta, y) = \int_{\mathbb{R}^3} ds\, \mathcal{P}_{YS}(\theta, y, \vec{s}) \qquad (12)$$

- Remark 8: Since $\vec{s}$ normalized $\Rightarrow \mathcal{P}_{YS}$ supported on 2-sphere $|\vec{s}| = 1$ $\Rightarrow \mathcal{P}_{YS}(\theta, y, \vec{s})$ proportional to $\delta(|\vec{s}| - 1)$
- Remark 9: Polarization density $\vec{\eta}_Y$ corresponding to $\mathcal{P}_{YS}$:

$$\vec{\eta}_Y(\theta, y) = \int ds \vec{s}\, \mathcal{P}_{YS}(\theta, y, \vec{s}) \qquad (13)$$

- Remark 10: RBE (5) follows from (11) by θ-differentiating (13)

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Now let us find nice RBE, i.e., approximation of L_Y!
- Recall ODEs for moments m_Y and K_Y

$$m_Y' = (A(\theta) + \epsilon\delta A(\theta))m_Y \ ,$$
$$K_Y' = (A(\theta) + \epsilon\delta A(\theta))K_Y + K_Y(A(\theta) + \epsilon\delta A(\theta))^T + \epsilon\omega(\theta)e_6 e_6^T$$

- Recall: data in moment ODEs are coefficients of $L_Y \Rightarrow$ approximating moment ODEs results in approximation of L_Y to get "nice" RBE!
- Thus apply method of averaging:
- Step 1: Transform moment ODEs to standard form for averaging by transforming moments m_Y and K_Y into m_U and K_U via

$$m_Y = X(\theta)m_U, \quad K_Y = X(\theta)K_U X^T(\theta) \tag{14}$$

- Remark: X is fundamental solution matrix of unperturbed ($\epsilon = 0$) part of ODE for m_Y:

$$X' = A(\theta)X \tag{15}$$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Step 2: Write down transformed moment ODEs:

$$m_U' = \epsilon \mathcal{D}(\theta) m_U \ , \tag{16}$$
$$K_U' = \epsilon(\mathcal{D}(\theta) K_U + K_U \mathcal{D}^T(\theta)) + \epsilon \mathcal{E}(\theta) \tag{17}$$

- Remark 1:

$$\mathcal{D}(\theta) = X^{-1}(\theta) \delta A(\theta) X(\theta) \ , \tag{18}$$
$$\mathcal{E}(\theta) = \omega(\theta) X^{-1}(\theta) e_6 e_6^T X^{-T}(\theta) \tag{19}$$

- Remark 2: Thus L_Y transforms into L_U where coefficients of L_U are $\mathcal{D}$ and $\mathcal{E}$ hence:

$$L_U = -\epsilon \sum_{j=1}^{6} \partial_{\mathrm{v}_j} (\mathcal{D}(\theta)\mathrm{v})_j + \frac{\epsilon}{2} \sum_{i,j=1}^{6} (\mathcal{E}(\theta))_{ij} \partial_{\mathrm{v}_i} \partial_{\mathrm{v}_j} \tag{20}$$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Step 3: Average ODEs for m_U and K_U and denote their solutions by m_V and K_V:

$$m_V' = \epsilon \bar{\mathcal{D}} m_V \ , \tag{21}$$
$$K_V' = \epsilon(\bar{\mathcal{D}} K_V + K_V \bar{\mathcal{D}}^T) + \epsilon \bar{\mathcal{E}} \tag{22}$$

- Remark 1: bar denotes θ-averaging, i.e., operation $\lim_{T\to\infty}(1/T)\int_0^T d\theta \cdots$
- Remark 2: For physically reasonable lattices, A guarantees that each fundamental matrix X is quasiperiodic function $\Rightarrow$ $\bar{\mathcal{D}}$ and $\bar{\mathcal{E}}$ exist
- Remark 3: $\mathcal{D}$ and $\mathcal{E}$ are approximated by $\bar{\mathcal{D}}$ and $\bar{\mathcal{E}}$ hence L_U is approximated by

$$L_V = -\epsilon \sum_{j=1}^{6} \partial_{\mathrm{v}_j} (\bar{\mathcal{D}} \mathrm{v})_j + \frac{\epsilon}{2} \sum_{i,j=1}^{6} \bar{\mathcal{E}}_{ij} \partial_{\mathrm{v}_i} \partial_{\mathrm{v}_j} \tag{23}$$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- With L_V and X the evolution equation for spin-orbit probability density $\mathcal{P}_{VS} = \mathcal{P}_{VS}(\theta, \mathrm{v}, \vec{s})$ is Fokker-Planck equation:

$$\partial_\theta \mathcal{P}_{VS} = L_V \mathcal{P}_{VS} - \sum_{j=1}^{3} \partial_{s_j} \left(\left(\Omega_Y(\theta, X(\theta)\mathrm{v}) \vec{s} \right)_j \mathcal{P}_{VS} \right) \tag{24}$$

- Polarization density $\vec{\eta}_V$ corresponding to $\mathcal{P}_{VS}$ is defined by

$$\vec{\eta}_V(\theta, \mathrm{v}) = \int ds \vec{s}\, \mathcal{P}_{VS}(\theta, \mathrm{v}, \vec{s}) \tag{25}$$

- Thus RBE is

$$\partial_\theta \vec{\eta}_V = (L_V + L_{V,TBMT}) \vec{\eta}_V \tag{26}$$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Remark: By averaging theory $|m_U(\theta) - m_V(\theta)| \leq C_1(T)\epsilon$ and $|K_U(\theta) - K_V(\theta)| \leq C_2(T)\epsilon$ for $0 \leq \theta \leq T/\epsilon$ where T is a constant and ϵ sufficiently small
- Lets complete finding "nice" RBE!
- Step 4: Use freedom in choice of fundamental matrix X to to get simple form of L_V
- Remark:

$$X(\theta) = M(\theta)C \tag{27}$$

  where C is arbitrary invertible 6×6 matrix and M is principal solution matrix, i.e., $M' = A(\theta)M, M(0) = I$.
- To construct C we emulate Chao's approach to spin physics in electron storage rings and use the eigenvectors of $M(2\pi)$
- We assume:
  - Unperturbed orbital motion is stable, i.e., $M(2\pi)$ is diagonalizable and its eigenvalues lie on unit circle of complex plane
  - Orbital tunes non-resonant

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- We thus construct C as real matrix using real and imaginary parts of eigenvectors in its columns and using that $M(2\pi)$ is symplectic (since $A(\theta)$ is a Hamiltonian matrix).
- Thus $\bar{\mathcal{D}}$ has block diagonal form and $\bar{\mathcal{E}}$ has diagonal form:

$$\bar{\mathcal{D}} = \begin{pmatrix} \mathcal{D}_I & 0_{2\times 2} & 0_{2\times 2} \\ 0_{2\times 2} & \mathcal{D}_{II} & 0_{2\times 2} \\ 0_{2\times 2} & 0_{2\times 2} & \mathcal{D}_{III} \end{pmatrix} , \tag{28}$$

$$\mathcal{D}_\alpha = \begin{pmatrix} a_\alpha & b_\alpha \\ -b_\alpha & a_\alpha \end{pmatrix} , (\alpha = I, II, III) \tag{29}$$

and $\bar{\mathcal{E}} = diag(\mathcal{E}_I, \mathcal{E}_I, \mathcal{E}_{II}, \mathcal{E}_{II},\ \mathcal{E}_{III}, \mathcal{E}_{III})$ with $a_\alpha \leq 0$ and $\mathcal{E}_I, \mathcal{E}_{II}, \mathcal{E}_{III} \geq 0$

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Remark 1: All three degrees of freedom are uncoupled in L_V:

$$L_V = L_{V,I} + L_{V,II} + L_{V,III} \tag{30}$$

- Remark 2: Each $L_{V,\alpha}$ is an operator in one degree of freedom and is determined by $\mathcal{D}_\alpha$ and $\mathcal{E}_\alpha$ ($\alpha = I, II, III$)

Approximating reduced Bloch equation for polarization density (Accelerator coordinates)

- Now: nice feature of $\vec{\eta}_V$ helpful for finding appropriate numerical phase space domain for $\vec{\eta}_V$.
  - Orbital probability density f_V corresponding to $\mathcal{P}_{VS}$ defined by

$$f_V(\theta, \mathrm{v}) = \int ds \mathcal{P}_{VS}(\theta, \mathrm{v}, \vec{s}) \tag{31}$$

  - Thus

$$|\vec{\eta}_V(\theta, \mathrm{v})| = |\int ds \vec{s} \mathcal{P}_{VS}(\theta, \mathrm{v}, s)| \leq \int ds |\vec{s} \mathcal{P}_{VS}(\theta, \mathrm{v}, s)|$$
$$= \int ds |\vec{s}| \mathcal{P}_{VS}(\theta, \mathrm{v}, s) = \int ds \mathcal{P}_{VS}(\theta, \mathrm{v}, s) = f_V(\theta, \mathrm{v}) \tag{32}$$

  - Thus numerical phase space domain for $\vec{\eta}_V$ can be identified with numerical phase space domain for f_V
  - Numerical phase space domain for f_V is easy to find since we generally use exact expressions of f_V, e.g., the one for orbital equilibrium.

Sketch of numerical approach

- Starting point is RBE in accelerator coordinates:

$$\partial_\theta \vec{\eta}_Y = (L_Y + L_{Y,TBMT})\vec{\eta}_Y \tag{33}$$

- Averaged RBE is much simpler:

$$\partial_\theta \vec{\eta}_V = (L_V + L_{V,TBMT})\vec{\eta}_V \tag{34}$$

- 3 pairs $(r_\alpha, \varphi_\alpha)$ of polar coordinates for $\mathrm{v}_1, ..., \mathrm{v}_6$
- Fourier expansion of $\vec{\eta}_V$ results in $\vec{\eta}_k(\theta, r)$
- Discretize r by pseudospectral method using Chebychev grid
- Gives large linear first-order ODEs in θ with very special structure thanks to method of averaging and Chao eigen formalism
- Discretize ODE system by implicit/explicit θ-stepping scheme
- For details see talk by O. Beznosov in Fiesta Key at 11.45am