Higher-order effects in polarized proton dynamics

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So far, polarized proton beams have never been accelerated to energies higher than 25 GeV. During the acceleration process, the beam polarization is quite undisturbed, when the accelerator is well adjusted, except at first-order depolarizing spin orbit resonances. At some accelerators other effects have been observed but first-order resonances have always been dominant. At these resonances the spin tune plus or minus one of the orbit tunes is an integer. These beams have usually been investigated by theories which correspondingly lead to an undisturbed polarization during acceleration, except at such resonances. Therefore we speak of "first-order theories." The first frequently used first-order theory is the single resonance model, which is usually used for simulating the acceleration process. Here the equation of spin motion is simplified drastically by dropping all but the dominant Fourier component of the driving term of that differential equation. The second frequently used first-order theory, the linearized spin-orbit motion theory, is also quite crude. It is based on a linearization of the spin and orbit equation of motion with respect to the phase space coordinates and two suitably chosen spin coordinates. Because of linearization this method cannot be used close to resonances but at fixed energies it is a useful tool. It will be shown that the validity of these first-order theories is restricted at Hadron Electron Ring Accelerator (HERA) energies of up to 820 GeV. An overview of the available theories which go beyond the first-order resonances is given and we explain which of these approaches are applicable for the analysis of polarization in the HERA proton ring. Since these theories include more than one Fourier harmonic in the driving term of the equation of motion, we refer to them as "non-first-order" or "higher-order" theories. Finally, the higher-order effects observed while simulating polarized beams in HERA with these advanced methods are illustrated.

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I. INTRODUCTION

The Hadron Electron Accelerator Ring (HERA) is the only circular accelerator which utilizes longitudinally polarized high energy electrons. Currently the electrons interact with the polarized gas target of the HERMES experiment with a center of momentum energy of $E_{\text{c.m.}} = 7$ GeV. In recent years an increasing number of high energy physicists have become interested in using this unique potential for collider experiments with high energy polarized protons at $E_{\text{c.m.}} = 300$ GeV. Therefore, a feasibility study has been launched together with several collaborating international institutions to analyze HERA's potential for accelerating polarized proton beams (see list in [1]).

When accelerating the electron beam in HERA, no special precautions are necessary since the electron beam does not have to be polarized during the acceleration process. In contrast to proton beams, the electron beam polarizes itself at high energy due to spin flip synchrotron radiation [2]. Since protons do not emit an appreciable amount of synchrotron radiation, polarized beams have to be created by a polarized source and then have to be accelerated up to high energy with little loss of polarization. Accelerating protons up to 820 GeV in HERA would be achieved by the following acceleration chain: a 19 keV H^- source, a 750 keV radio frequency quadrupole, a 50 MeV proton linear accelerator, the 8 GeV proton synchrotron DESY III, the 39 GeV proton synchrotron PETRA, and the 820 GeV storage ring HERA. In each of these accelerators depolarizing effects have to be avoided.

So far, polarized proton beams have been accelerated to about 25 GeV [3]. During the acceleration of polarized beams up to that energy, the polarization was quite undisturbed except at two different classes of resonances, which are traditionally called the imperfection resonances and the intrinsic resonances. The imperfection resonances occur when the spin of a proton performs an integer number of complete rotations around some rotation axis while the particle travels once around the closed orbit of the accelerator. These resonances can be avoided by using so-called partial snakes [4,5]. When the accelerator was equipped with such an element and well adjusted, the polarization was essentially disturbed only at the so-called intrinsic resonances. At these resonances the spin tune plus or minus one of the orbit tunes is an integer and we therefore refer to them as first-order depolarizing

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spin-orbit resonances. Other destructive effects mostly due to synchrotron motion were usually less dominant than these intrinsic resonances.

Theories which correspondingly lead to an undisturbed polarization during acceleration except at such resonances have been instrumental in reaching the energies obtained to date. Two theories have been frequently used for these simulations, the single resonance model (SRM) and the linearized spin-orbit motion (SLIM) theories. They will be referred to as first-order theories, and they will be described below. In this paper, we will show up to which energy range in the HERA accelerator chain these first-order theories can be applied. We refer to theories which describe more effects than these two simple theories as higher-order theories, and we give an overview of the available theories which go beyond the first-order resonances. Then we explain which of these approaches are applicable for the analysis of polarization in the HERA proton ring. Furthermore, we will show which effects occur when this energy range is exceeded. In this paper we will not investigate measures to avoid loss of polarization due to these effects. We have described such measures in other papers [1,6,7].

II. THE EQUILIBRIUM SPIN FIELD

A polarized particle moving along a phase space trajectory $\vec{z}(l)$ parametrized by the arc length l of the ring travels through an arrangement of electromagnetic fields. During this motion the classical spin vector $\vec{s}$ changes its direction according to the Thomas-BMT equation of spin motion, which has the form

$$\frac{d\vec{s}}{dt} = \vec{\Omega}(\vec{z}(t), l(t)) \times \vec{s}\,, \tag{2.1}$$

where $\vec{\Omega}$ depends on the electric field $\vec{E}$, the magnetic field $\vec{B}$, and the energy $mc^2\gamma$ of the particle. In terms of the magnetic field components parallel and perpendicular to the particle velocity, the Thomas-BMT equation (with charge e and magnetic anomaly $G \approx 1.79$ of the proton) is

$$\vec{\Omega} = -\frac{e}{\gamma m}\left[(G\gamma + 1)\vec{B}_\perp + (1 + G)\vec{B}_\parallel + \left(G\gamma + \frac{\gamma}{\gamma + 1}\right)\frac{\vec{E} \times \vec{\beta}}{c}\right]. \tag{2.2}$$

Different particles in a beam travel through different magnetic fields during their motion around the accelerator. One particle might travel straight through the center of a quadrupole, leaving its classical spin vector unchanged in the process, but a different particle gets focused by the quadrupole and experiences a spin rotation which is $G\gamma + 1$ times as strong as the focusing kick to its orbit. Since $G\gamma + 1$ can be very big, at 820 GeV/c it is approximately 1568, the spin dynamics of two particles in the beam can be very different as they both travel around the ring.

It is therefore not surprising that a beam which is polarized to 100% at a chosen azimuth of the ring will not be completely polarized after one turn. The particles in the center of the beam will still have their initial direction of polarization. However, the particles at higher phase space amplitudes will have traveled through different magnetic fields and their classical spin vector will have changed significantly. The average polarization would therefore be strongly diminished after one turn. However, after the next turn the spin vectors of different particles will again move in different fashions, and some might rotate back in the direction of the initial polarization. Thus, the average polarization might recover somewhat during the following turns and an ongoing oscillation of the beam's polarization will result. The diminished polarization after the first turn therefore does not indicate a depolarization mechanism. A depolarization mechanism cannot be observed well with a beam in such a fluctuating polarization state. Therefore it is often not appropriate to initiate polarized beam simulations with 100% polarized beams, i.e., with a spin field $\vec{f}(\vec{z})$ which associates the same initial polarization direction $\vec{f}(\vec{z}) = \vec{f}(0)$ with all particles no matter at which phase space position $\vec{z}$ they are. A spin field has unit length $|\vec{f}(\vec{z})| = 1$ and determines the direction of polarization at a phase space point at the chosen azimuth. After one turn the spin field will be different since particles at different phase space points will have traveled through different fields. A spin field is at equilibrium if the beam comes back with the same spin field after every turn. Such a periodic spin field is usually denoted by $\vec{n}(\vec{z})$ and called an $\vec{n}$ axis. It is advisable to simulate polarized beams in a polarization state which is very close to equilibrium for the following two reasons:

(i) The equilibrium spin field yields a polarization averaged over the beam $\langle\vec{n}(\vec{z})\rangle$ which is constant from turn to turn and therefore allows for studies of small depolarizing effects due to time dependent perturbations of spin-orbit dynamics.

(ii) The average $\langle\vec{n}(\vec{z})\rangle$ describes how big the equilibrium polarization in a beam can be. In a proton beam which has been accelerated with little polarization loss to high energy the polarization measured by the detector is limited by a wide spread in the directions of $\vec{n}(\vec{z})$. This limit is not due to a dynamic depolarization mechanism which could be caused by stochastic effects but it is a fixed limit which does not vary in time.

III. SPIN TUNE AND RESONANCES

Since the absolute value of the classical spin $\vec{s}$ does not change, it can be rotated only by some angle around some rotation direction. For particles on the closed orbit, the spin's relative rotation angle (angle divided by 2π) after one turn around the ring is called the spin tune ν_0. The corresponding rotation direction is called the closed orbit spin direction $\vec{n}_0$. If a particle starts to travel along

the closed orbit with its spin parallel to $\vec{n}_0$ then the spin comes back to $\vec{n}_0$ just as the closed orbit comes back to its starting point after one turn. For this reason $\vec{n}_0$ is sometimes called the spin closed orbit. $\vec{n}_0$ should never be confused with the equilibrium spin field $\vec{n}(\vec{z})$ which is a function of phase space. On the closed orbit we have $\vec{n}_0 = \vec{n}(0)$. Particles on the closed orbit have to be polarized in this direction in order to have the same polarization direction after every turn. In a ring without horizontal magnetic fields on the closed orbit, spins rotate $\nu_0 = G\gamma$ times around a vertical direction $\vec{n}_0$ while the particle travels along the closed orbit. The magnetic anomaly, $G = 1.79$ for protons, causes the spin to rotate rapidly approximately 1567 times during one revolution around HERA at 820 GeV.

A particle with phase space amplitudes and a particle on the closed orbit travel through slightly different fields, and the rotation vector differs by

$$\vec{\omega}(\vec{z}, l) = \vec{\Omega}(\vec{z}, l) - \vec{\Omega}(0, l). \tag{3.1}$$

This causes a coupling of the spin motion to the phase space motion. If there were no such amplitude dependent fields perturbing the spin motion, particles with nonzero phase space amplitudes would also have their spins rotated by ν_0 around $\vec{n}_0$. However, in reality spins can rotate around a vastly different phase space dependent vector by a phase space dependent angle since the small perturbations can have an accumulating effect over many turns. The most perturbing are the components of $\vec{\omega}(\vec{z}(l), l)$ which rotate spins away from their closed orbit direction $\vec{n}_0$. In a coordinate system in which the 3rd direction is parallel to $\vec{n}_0$, these are the 1st and 2nd components of $\vec{\omega}(\vec{z}(l), l)$. Such disturbing rotations often average out since spins rotate quickly around $\vec{n}_0$. However, when $\vec{\omega}(\vec{z}(l), l)$ itself rotates around $\vec{n}_0$ with the frequency ν_0, even small perturbations caused by $\vec{\omega}$ cannot average out. Then the small perturbation rotates spins away from the closed orbit spin direction $\vec{n}_0$ during every turn, an effect which will accumulate to large amounts even when the perturbation is very small. The amplitude of the corresponding Fourier frequency

$$\varepsilon = \lim_{L\to\infty} \frac{1}{L} \int_0^L [\omega_1(\vec{z}(l), l) + i\omega_2(\vec{z}(l), l)] \times e^{-i(2\pi/L_0)\nu_0 l}\, dl\, \frac{L_0}{2\pi} \tag{3.2}$$

is referred to as the resonance strength of spin motion. L_0 is the circumference of the ring.

A warning is needed. The picture of perturbing effects which add up coherently suggests that the beam is slowly depolarized after it has been injected with 100% polarization. In fact the spins get deflected from their initial polarization direction $\vec{n}_0$ during one turn only because the equilibrium direction $\vec{n}(\vec{z})$ is tilted far away from the closed orbit spin direction $\vec{n}_0$. If the spins had started parallel to the equilibrium direction, no net deflection due to the perturbing fields and no depolarization would have occurred. However, since $\vec{n}(\vec{z})$ is tilted far away from $\vec{n}_0$, the average polarization $|\langle\vec{n}(\vec{z})\rangle|$ for such an initial distribution is very small to start with.

IV. THE SINGLE RESONANCE MODEL (SRM) AND THE LINEARIZED SPIN-ORBIT MOTION (SLIM)

One begins by linearizing the equation of motion for a particle's phase space coordinates $\vec{z}$. Then the Fourier harmonics of the phase space trajectories are $\frac{2\pi P}{L_0}(m \pm \check{q}_i)$. Here P is the superperiod of the ring, m is any integer, and $\check{q}_i$ is the fractional betatron phase advance of one superperiod. The vector $\vec{\omega}(\vec{z}, l)$ causes the perturbing spin rotations described above and is periodic in l. In a first approximation it is a linear function of the phase space coordinates. Therefore it also has only Fourier harmonics $\frac{2\pi P}{L_0}(m \pm \check{q}_i)$ and the perturbing effects can in a first approximation accumulate coherently at so-called first-order spin-orbit resonances, where the fractional spin phase advance of one superperiod is $\check{\nu}_0 = m \pm \check{q}_i$. With the ring's full (integer and rational part) orbit tune Q_i and the full spin tune ν_0, one can write this resonance condition as $\nu_0 = Pm \pm Q_i$. Here it has to be noted that the integer part of the spin tune in a nonflat ring is often not known and therefore the resonance condition for one superperiod containing $\check{\nu}_0$ and $\check{q}_i$ is in general more useful. The resonance strength ε is nonzero only at these resonance conditions. In general, one speaks of a spin-orbit resonance when $\nu_0 + \vec{k} \cdot \vec{Q}$ is integer for some vector of integers $\vec{k}$. When the sum of coefficients $\sum_j |k_j|$ is larger than one, we speak of a higher-order resonance. In this case, where $\vec{\omega}(\vec{z}, l)$ is approximated by a linear phase space function, only first-order resonances ($\nu_0 \pm Q_i$ is integer) occur in the integral (3.2).

The simplest model that can be used to describe the spin motion was introduced in [8] and proved to be very successful. In this model one approximates the linearized phase space function $\vec{\omega}$ by simply neglecting all but the dominant Fourier amplitude of $\vec{\omega}(\vec{z}(l), l)$. This model is called the single resonance model, since only a single resonance strength given by the integral (3.2) is taken into account. For all accelerators which accelerated polarized proton beams so far, this method proved to be very helpful for predicting polarization losses at resonances and to find means to avoid these losses. The theory could be applied so successfully for the following two reasons: (i) the resonances were so weak that they were very well separated, and (ii) when the accelerator was not close to a first-order resonance, the spin perturbations were so weak that they could be neglected.

In the next section we will analyze in which energy regime of the proton acceleration chain at DESY the SRM can be applied safely and in which region it cannot.

A similarly simple theory introduced in [9] represents spins in terms of two small angles α and β describing the spin's tilt away from $\vec{n}_0$. The final spin direction after one turn is described by α_f and β_f and is linearly related to the initial phase space point $\vec{z}_i$ and the initial spin direction α_i, β_i by

$$\begin{pmatrix} \alpha_f \\ \beta_f \end{pmatrix} = \underline{G}_{2\times 6}\vec{z}_i + \begin{pmatrix} \cos 2\pi\nu_0 & \sin 2\pi\nu_0 \\ -\sin 2\pi\nu_0 & \cos 2\pi\nu_0 \end{pmatrix}\begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix}. \tag{4.1}$$

The six-dimensional phase space position is transported around the ring by $\vec{z}_f = \underline{M}\vec{z}_i$. This formalism was first implemented in the program SLIM [9] and is often called SLIM theory.

In order to analyze the polarization in a beam, one investigates the equilibrium spin field $(n_\alpha(\vec{z}), n_\beta(\vec{z}))$. Such a distribution gets transported to itself after one turn,

$$\begin{pmatrix} n_\alpha(\vec{z}_f) \\ n_\beta(\vec{z}_f) \end{pmatrix} = \underline{G}_{2\times 6}\vec{z}_i + \begin{pmatrix} \cos 2\pi\nu_0 & \sin 2\pi\nu_0 \\ -\sin 2\pi\nu_0 & \cos 2\pi\nu_0 \end{pmatrix}\begin{pmatrix} n_\alpha(\vec{z}_i) \\ n_\beta(\vec{z}_i) \end{pmatrix}. \tag{4.2}$$

From this periodicity condition the equilibrium spin field $(n_\alpha(\vec{z}), n_\beta(\vec{z}))$ can be computed [10]. At the phase space point $\vec{z}$, it yields the spin component $1/\sqrt{1 + n_\alpha(\vec{z})^2 + n_\beta(\vec{z})^2}$ in the direction parallel to $\vec{n}_0$. Since this theory is based on a linearization with respect to the angles α and β, this polarization has to be close to one in order to justify the approximation. To show that the phase space average of the equilibrium polarization diminishes in the vicinity of resonances, we use action-angle variables $\vec{J}$ and $\vec{\phi}$ of the linear phase space motion. The initial phases $\vec{\phi}$ are increased by the tunes $\vec{Q}$ times 2π during one turn around the ring to $\vec{\phi} + 2\pi\vec{Q}$. Introducing the complex notation $\hat{n}(\vec{J}, \vec{\phi}) = n_\alpha(\vec{J}, \vec{\phi}) + i n_\beta(\vec{J}, \vec{\phi})$ and using the Fourier expansion $\hat{n}(\vec{J}, \vec{\phi}) = \sum_{\vec{k}} \hat{n}_{\vec{k}}(\vec{J}) e^{i\vec{k}\cdot\vec{\phi}}$ with respect to the angle variables leads to the periodicity condition

$$\hat{n}_{\vec{k}} e^{i2\pi\vec{k}\cdot\vec{Q}} = (\underline{G}\vec{z}_i)_1 + i(\underline{G}\vec{z}_i)_2 + \hat{n}_{\vec{k}} e^{-i2\pi\nu_0}. \tag{4.3}$$

Close to a spin-orbit resonance, where $e^{i2\pi\vec{k}\cdot\vec{Q}} \approx e^{-i2\pi\nu_0}$, the Fourier coefficient $\hat{n}_{\vec{k}}$ becomes very big and $\vec{n}(\vec{z})$ deviates strongly from $\vec{n}_0$.

The resonance analysis has traditionally been used for polarized proton accelerators whereas the equilibrium spin field technique for the linearized spin-orbit equation of motion has traditionally been used for polarized electron storage.

V. RELIABILITY OF THE FIRST-ORDER THEORIES

The resonance strength describes how phase space dependent fields cause spins to be deflected from the closed orbit spin direction $\vec{n}_0$ during one turn. As mentioned above, this is only an indication for the fact that the equilibrium spin field $\vec{n}(\vec{z})$ can be tilted strongly away from $\vec{n}_0$. The SRM can therefore be used to compute the average polarization of a polarized beam in equilibrium whenever the underlying approximations are valid. This model leads to the average polarization $|\langle\vec{n}(\vec{z})\rangle| = |\nu_0 - Q_i|/\sqrt{(\nu_0 - Q_i)^2 + |\varepsilon|^2}$ [10]. This approximation requires the resonances to be well separated. When a ring has no exact superperiod, as for HERA, the resonances appear when $\nu_0 \pm Q_i$ is any integer. In a flat ring particles with only vertical phase space amplitude travel through horizontal magnetic fields and therefore resonances appear only when ν_0 plus or minus the vertical orbit tune Q_y is integer. With a vertical orbit tune of approximately $1/3$, the variation of ν_0 between resonances is $1/3$ or $2/3$. To justify a single resonance approach, the resonance strength should therefore be significantly less than $1/3$. HERA is not flat, but after installing so-called flattening snakes, introduced in [1,11], the first-order spin motion is very similar to that of a flat ring.

The SLIM theory can be applied even when the resonances are not well separated. However, the SLIM theory is based on a linearization in the opening angle. Therefore, when computing the average polarization of a polarized beam in equilibrium, the average opening angle of the equilibrium spin field must be small enough to justify the underlying approximation. If we accept an opening angle up to $\langle\angle(\vec{n}(\vec{z}), \vec{n}_0)\rangle \approx |\frac{\varepsilon}{\nu_0 - Q_i}| \leq 0.5$, the average polarization computed with the SLIM approach is trustworthy only as long as it is above about 87%.

The average polarization computed with either of these two models is accurate only if there are no effects which are not dominated by first-order resonances. Effects which are not related to first-order resonances cannot be simulated by either the SRM or the SLIM theory and therefore the first-order theories cannot be used to decide whether non-first-order effects are small or not. In general, therefore, a higher-order extension is needed to decide about the validity of the first-order theories. Before introducing the techniques which include non-first-order effects, we demonstrate that the SRM and SLIM theories are not generally applicable in HERA. In order to find out up to which energy the first-order formalisms can be used to analyze polarization dynamics in the proton accelerators at DESY, we will present these comparisons for the three accelerators DESY III, PETRA, and HERA.

In SLIM theory the opening angle between $\vec{n}(\vec{z})$ and $\vec{n}_0$ is given by $\sqrt{\alpha^2 + \beta^2}$ for small angles; for big angles we use $\arctan(\sqrt{\alpha^2 + \beta^2})$ to avoid that the SLIM theory leads to opening angles which are greater than

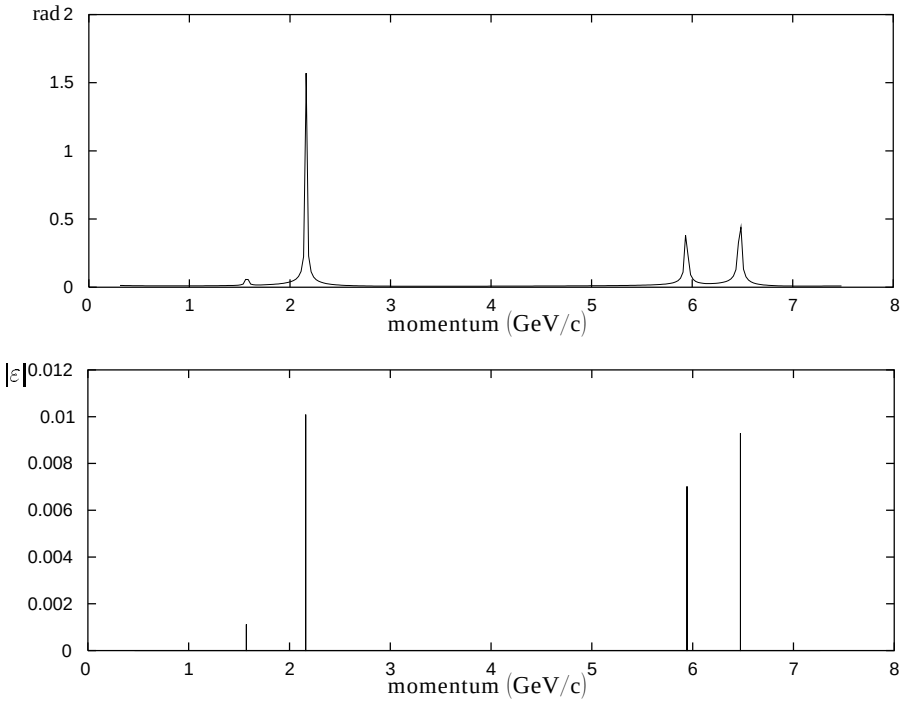

FIG. 1. SLIM opening angles of $\vec{n}(\vec{z})$ (top) and resonance strength (bottom) for a beam with normalized vertical emittance of 4π mm mrad in DESY III.

$\pi/2$. In Fig. 1 the peaks in the resonance strength (bottom) are located exactly at the peaks of the big opening angles of $\vec{n}(\vec{z})$ computed with the SLIM formalism (top); furthermore, the widths of the peaks in the opening angle are correlated with the resonance strengths. The resonances are well separated, and in DESY III first-order theories for analyzing polarization dynamics along with classical means of controlling depolarizing effects [1] are therefore applicable as long as perturbing effects are not strong at higher-order resonances. This is the case for realistic emittances as will be shown below.

Figure 2 is the corresponding picture for PETRA and shows again that broad opening angle peaks of the SLIM theory are correlated with large resonance strength. However, the first-order resonances are getting so close at the high energy end of 39 GeV that several pairs of resonances are close to overlapping. The resonance strengths are still far away from $1/3$ and therefore also in this energy regime classical means of controlling depolarizing first-order resonances can be applied.

In HERA the situation changes. The first resonance which is stronger than $1/3$ for a normalized vertical emittance of 4π mm mrad appears at about 150 GeV/c and resonances start to overlap. Since there are over 3000 first-order resonances on the ramp of HERA from 39 to 820 GeV/c, this effect can be seen only when looking at a smaller energy range as in Fig. 3. The resonances are strongly overlapping and the average opening angles of the equilibrium spin field are so big that the first-order methods are not trustworthy anymore. Therefore methods which include higher-order spin effects have to be applied.

VI. METHODS TO SIMULATE HIGHER-ORDER EFFECTS

Several methods have been suggested for the computation of the averaged polarization of the equilibrium spin field. We now give an explanation of the various methods along with a short evaluation of their applicability to polarization analysis in high energy storage rings.

A. Fourier expansion with SODOM

As mentioned above, the equilibrium spin field $\vec{n}(\vec{z})$ is a periodic vector field of the one turn spin-orbit motion. An initial spin $\vec{s}_i$ is transported to a final spin $\vec{s}_f = \underline{A}(\vec{z}_i)\vec{s}_i$ during one turn around the storage ring. The matrix $\underline{A}(\vec{z}_i)$ describes a rotation which depends on the initial phase space position of the particle. The equilibrium spin field which has to be calculated is defined by the periodicity condition

$$\vec{n}(\vec{z}_f) = \underline{A}(\vec{z}_i)\vec{n}(\vec{z}_i)\,, \tag{6.1}$$

which has to be satisfied for all initial phase space positions. It is sometimes useful to formulate the rotation of spins in a spinor formalism using the Cayley-Klein SU(2) formulation for rotations. Spins $\vec{s} \in \mathbb{R}^3$ with

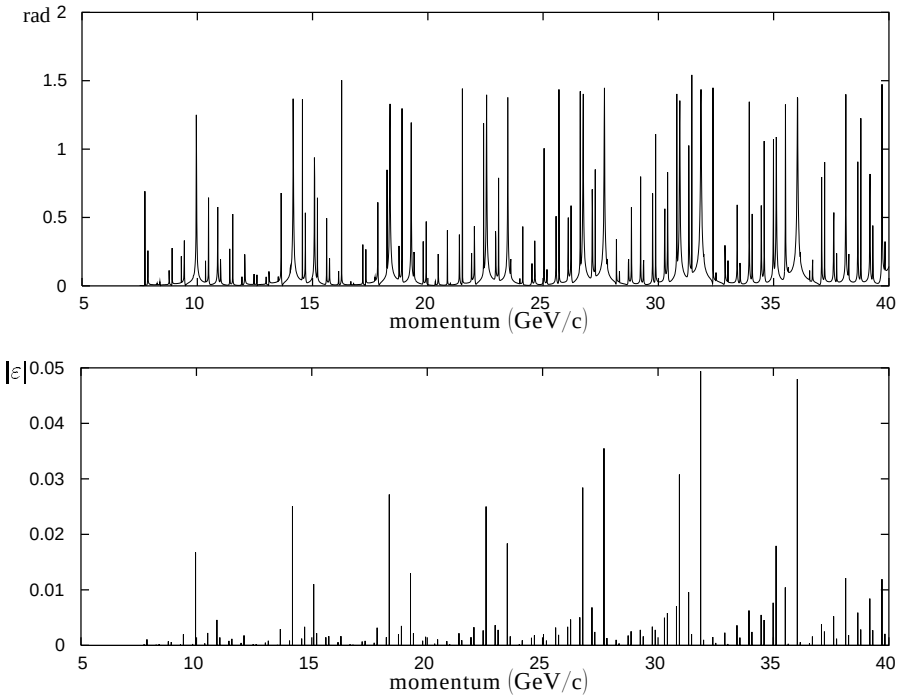

FIG. 2. SLIM opening angles of $\vec{n}(\vec{z})$ (top) and resonance strength (bottom) for a beam with normalized vertical emittance of 4π mm mrad in PETRA.

$|\vec{s}| = 1$ are then represented by spinors $\Psi \in \mathbb{C}^2$ with $|\Psi_1|^2 + |\Psi_2|^2 = 1$. Ψ_1 and Ψ_2 have an arbitrary common phase. Here it is assumed that the orbit motion can be represented by action angle coordinates $\vec{J}, \vec{\phi}$. Since the actions are constant during the motion along a particle trajectory, we will not indicate $\vec{J}$ any longer when

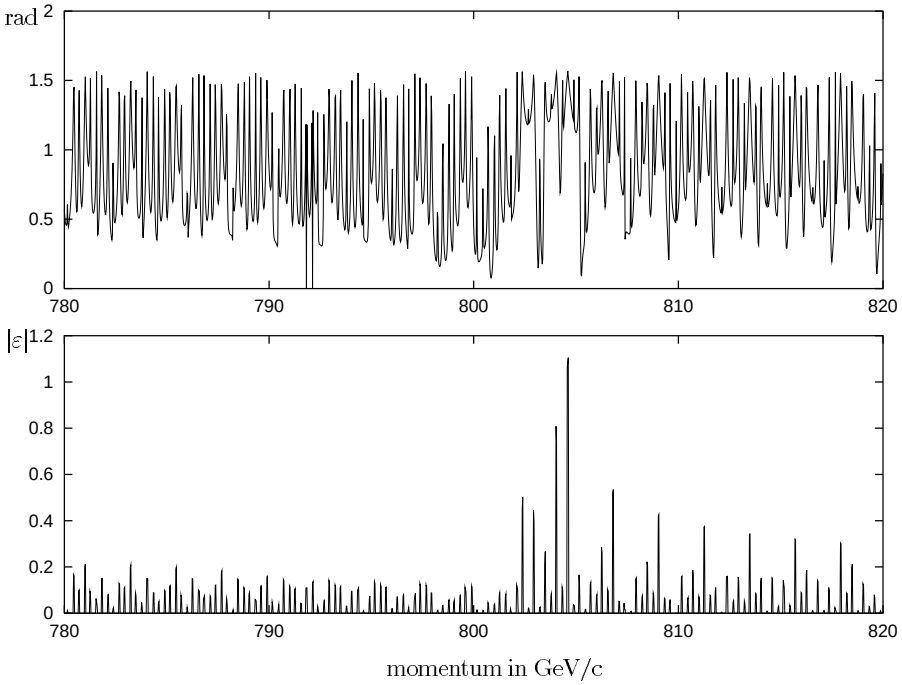

FIG. 3. SLIM opening angles of $\vec{n}(\vec{z})$ (top) and resonance strength (bottom) for a beam with normalized vector emittance of 4π mm mrad in HERA.

specifying a phase space coordinate. During one turn around the ring, the angle variables $\vec{\phi}$ change by the orbit tunes to $\vec{\phi} + 2\pi\vec{Q}$. In this representation the periodicity condition for the equilibrium spin field is expressed with the SU(2) rotation matrix $\underline{U}(\vec{\phi})$ which corresponds to the SO(3) rotation matrix $\underline{A}(\vec{z})$,

$$e^{i\theta(\vec{\phi})}\Psi_{\vec{n}}(\vec{\phi} + 2\pi\vec{Q}) = \underline{U}(\vec{\phi})\Psi_{\vec{n}}(\vec{\phi}), \qquad (6.2)$$

with a phase θ which is arbitrary since $\Psi_{\vec{n}}$ and $e^{i\theta(\vec{\phi})}\Psi_{\vec{n}}$ represent the same $\vec{n}$ axis. For simplification one uses a coordinate system in which the rotation direction $\vec{n}_0$ on the closed orbit is expressed by the spinor $\Psi_0 = (1, 0)$. For small phase space amplitudes one expects small deviation from this vector and writes

$$\Psi_{\vec{n}} = \begin{pmatrix} 1 \\ \zeta \end{pmatrix} \frac{1}{\sqrt{1 + |\zeta|^2}}, \qquad \underline{U} = \begin{pmatrix} -ig & -if^* \\ -if & ig^* \end{pmatrix}, \qquad |f|^2 + |g|^2 = 1. \qquad (6.3)$$

The periodicity condition is then written as

$$e^{i\theta(\vec{\phi})}\begin{pmatrix} 1 \\ \zeta(\vec{\phi} + 2\pi\vec{Q}) \end{pmatrix} \frac{1}{\sqrt{1 + |\zeta(\vec{\phi} + 2\pi\vec{Q})|^2}} = \begin{pmatrix} -ig - if^*\zeta(\vec{\phi}) \\ -if + ig^*\zeta(\vec{\phi}) \end{pmatrix} \frac{1}{\sqrt{1 + |\zeta(\vec{\phi})|^2}}. \qquad (6.4)$$

One eliminates the phase θ and the denominators by building the product of the top component on the left-hand side with the bottom component of the right-hand side and equating it with the product of the other two components; the result is the following difference equation for ζ:

$$\zeta(\vec{\phi})g^*(\vec{\phi}) + \zeta(\vec{\phi} + 2\pi\vec{Q})g(\vec{\phi}) = f(\vec{\phi}) - f^*(\vec{\phi})\zeta(\vec{\phi})\zeta(\vec{\phi} + 2\pi\vec{Q}). \qquad (6.5)$$

When the Fourier expansions $f(\vec{\phi}) = \sum_{\vec{k}} f_{\vec{k}} e^{i\vec{k}\cdot\vec{\phi}}$ and $g(\vec{\phi}) = \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{\phi}}$ are known, the periodicity condition entails a condition for the Fourier coefficients of ζ,

$$\sum_{\vec{l}} \zeta_{\vec{l}}(g^*_{\vec{l}-\vec{k}} + g_{\vec{k}-\vec{l}} e^{i2\pi\vec{l}\cdot\vec{Q}}) = f_{\vec{k}} - \sum_{\vec{l},\vec{m}} f^*_{\vec{m}+\vec{l}-\vec{k}} e^{i2\pi\vec{l}\cdot\vec{Q}} \zeta_{\vec{l}}\zeta_{\vec{m}}. \qquad (6.6)$$

This equation is solved by restriction to a finite number M of Fourier coefficients and by a perturbation expansion in $\zeta_{\vec{k}} \ll 1$. In the first step one neglects parts nonlinear in ζ and solves the linear equation for the coefficients $\zeta_{\vec{k}}$. This can be done for example by inverting the $M \times M$ dimensional matrix $[g^*_{\vec{l}-\vec{k}} + g_{\vec{k}-\vec{l}} \exp(i2\pi\vec{l}\cdot\vec{Q})]$. In the next step one uses the coefficients obtained in the first step to compute the nonlinear parts and again solves the resulting linear equation for a second iteration of the coefficients $\zeta_{\vec{k}}$. This perturbation procedure is repeated until the Fourier coefficients have converged. For particles on the closed orbit the one turn transformation $\underline{U}$ describes the rotation by the spin tune ν_0,

$$\underline{U} = \begin{pmatrix} e^{-i\pi\nu_0} & 0 \\ 0 & e^{i\pi\nu_0} \end{pmatrix}. \qquad (6.7)$$

Therefore $g_0 = ie^{-i\pi\nu_0}$ and, for small phase space amplitudes, the other Fourier components $g_{\vec{k}}$ are small. The matrix to be inverted is dominated by the diagonal elements $g^*_0 + g_0 e^{i2\pi\vec{l}\cdot\vec{Q}}$ since the elements $g^*_{\vec{l}-\vec{k}} + g_{\vec{k}-\vec{l}} e^{i2\pi\vec{l}\cdot\vec{Q}}$ for $\vec{k} \neq \vec{l}$ are small at small phase space amplitudes. Close to a spin-orbit resonance, one of the diagonal elements also becomes small and therefore the inverse matrix contains big elements. These lead to big absolute values for $\zeta_{\vec{k}}$ which describes big opening angles of the equilibrium spin field. This shows that the SODOM formalism leads to a drop of the equilibrium polarization at higher-order resonances. However, the computational procedure starts with small deviations of $\vec{n}(\vec{z})$ from $\vec{n}_0$ and therefore might not converge when the equilibrium spin field has a large opening angle (see note added in proof).

In the case of high energy polarized electrons (e.g., at HERA or at the 27 km CERN e^+e^- collider LEP), the opening angle of $\vec{n}(\vec{z})$ is rather small and the Fourier expansion as implemented in the program SODOM [12] converges. For polarized protons at HERA energies it is not so promising.

B. The differential algebra (DA) normal form method

With programs using differential algebra (DA) for computing polynomial expansions, one can compute a polynomial expansion of $\Psi_{\vec{n}}(\vec{z})$ from the periodicity condition. This procedure is similar to computing normal form transformations of phase space dynamics which is nonlinear in the phase space coordinates $\vec{z}$. There one introduces a change of the coordinate system which depends nonlinearly on $\vec{z}$ to obtain mth-order polynomial expansions of action variables $\vec{J}(\vec{z})$ and angle variables $\vec{\phi}(\vec{z})$. This theory is well known [13,14] and well implemented [15], and we do not want to dwell on it here. Therefore we use linearized orbit motion for our short explanation of computing the polynomial expansion of $\Psi_{\vec{n}}(\vec{z})$. The extension to nonlinear orbit motion is nearly obvious and is covered in [16]. We represent the orbit motion in the eigenvector basis of the one turn transport matrix. Therefore an initial phase space coordinate $\vec{z}_i$ is transported once around the ring by

$\vec{z}_f = (z_{i,1}^+ e^{i2\pi Q_1}, z_{i,1}^- e^{-i2\pi Q_1}, \ldots)$, which leads to the actions $J_i = z_i^+ z_i^-$. With the vector $\vec{q} = (Q_1, -Q_1, \ldots)$ the monomial $\vec{z}_f^{\vec{k}} = \prod_j (z_{f,j})^{k_j}$ is equal to $\vec{z}_i^{\vec{k}} e^{i2\pi \vec{k}\cdot\vec{q}}$. In the DA approach of computing the polynomial expansion of the equilibrium spin field $\vec{n}(\vec{z})$ to some order m one starts by computing the polynomial expansion $\underline{U}(\vec{z})$ of the spin transport matrix introduced in Sec. VI A, which can be done using DA integration of the equation of motion. Then one computes a coordinate transformation $\underline{C}(\vec{z})$ which depends nonlinearly on the phase space coordinates and simplifies the spin motion in the new coordinate system

$$\begin{aligned} \Psi_f &= \underline{C}(\vec{z}_f)\underline{U}(\vec{z}_i)\underline{C}^{-1}(\vec{z}_i)\Psi_i\,, \\ \underline{\tilde{U}}(\vec{z}_i) &= \underline{C}(\vec{z}_f)\underline{U}(\vec{z}_i)\underline{C}^{-1}(\vec{z}_i)\,. \end{aligned} \tag{6.8}$$

The SU(2) transformation matrix $\underline{C}$ is computed in an order by order procedure as $\underline{C} = \exp(\underline{C}_n) \times \cdots \times \exp(\underline{C}_1)$, where the anti-Hermitian matrix $\underline{C}_m(\vec{z})$ is a polynomial in $\vec{z}$ with contributions of order m only. The spin basis has initially been chosen to let $\vec{n}_0$ be parallel to the third coordinate direction, which makes the spin transport matrix on the closed orbit equivalent to

$$\underline{U}_0 = \begin{pmatrix} e^{-i\pi\nu_0} & 0 \\ 0 & e^{i\pi\nu_0} \end{pmatrix}. \tag{6.9}$$

If $\underline{U}(\vec{z})$ has been transformed to the simplifying coordinate system up to order $m-1$ by $\underline{\tilde{U}} = \exp(\underline{C}_{m-1}) \cdots \underline{U} \cdots \exp(-\underline{C}_{m-1})$, then in the next step one looks for a $\underline{C}_m(\vec{z})$ which further simplifies the spin transport matrix. Up to order m the transformed SU(2) matrix has the form $\underline{\tilde{U}}(\vec{z}_i) + \underline{C}_m(\vec{z}_f)\underline{U}_0 - \underline{U}_0\underline{C}_m(\vec{z}_i)$. To simplify $\underline{\tilde{U}}$, one tries to eliminate all mth-order polynomial coefficients. To eliminate the coefficient matrix $\underline{\tilde{U}}_{\vec{k}}$ of the expansion of $\underline{\tilde{U}} = \sum_{\vec{k}} \underline{\tilde{U}}_{\vec{k}} \vec{z}^{\vec{k}}$, one chooses the coefficient matrices of $\underline{C}_m(\vec{z}_i) = \sum_{\vec{k}} \underline{C}_{m,\vec{k}} \vec{z}_i^{\vec{k}}$ and of $\underline{C}_m(\vec{z}_f) = \sum_{\vec{k}} \underline{C}_{m,\vec{k}} \vec{z}_i^{\vec{k}} e^{i2\pi\vec{k}\cdot\vec{q}}$ to be

$$\underline{C}_{m,\vec{k}} = \underline{U}_0^{-1} \begin{pmatrix} \frac{\tilde{U}_{\vec{k}1,1}}{1-\exp i2\pi\vec{k}\cdot\vec{q}} & \frac{\tilde{U}_{\vec{k}1,2}}{1-\exp i2\pi(\vec{k}\cdot\vec{q}+\nu_0)} \\ \frac{\tilde{U}_{\vec{k}2,1}}{1-\exp i2\pi(\vec{k}\cdot\vec{q}-\nu_0)} & \frac{\tilde{U}_{\vec{k}2,2}}{1-\exp i2\pi\vec{k}\cdot\vec{q}} \end{pmatrix} \tag{6.10}$$

whenever the denominators do not vanish. When a denominator vanishes, the coefficient is set to zero. This eliminates all coefficients of $\tilde{U}_{\vec{k}}$ except those where the coefficient of $\underline{C}_{m,\vec{k}}$ was set to zero. Since the eigenvalues of the symplectic orbit transport map always come in pairs of $e^{i2\pi Q_j}$ and $e^{-i2\pi Q_j}$, the factor $\vec{k}\cdot\vec{q} = \sum_i (k_i^+ - k_i^-) Q_i$ is always zero when the corresponding k_j^+ and k_j^- are equal. The polynomial coefficients corresponding to such a $\vec{k}$ cannot be eliminated. Since $z_j^+ z_j^-$ is an action variable of linear orbit motion, only those terms of the polynomial expansion cannot be eliminated which depend only on the action variables, and these terms occur only on the diagonal of $\underline{\tilde{U}}$. We assume that all other coefficients of $\tilde{U}_{\vec{k}}$ can be eliminated. This is possible if there are no orbit resonances, i.e., no other vectors $\vec{k}$ which lead to integer values of $\vec{k}\cdot\vec{q}$ and if there are no spin-orbit resonances where $\nu_0 + \vec{k}\cdot\vec{q}$ would be integer. Therefore, close to spin-orbit resonances $\underline{C}_m$ contains big polynomial coefficients. After the complete transformation $\underline{C}$ has been applied up to order m, we are left with a diagonal SU(2) matrix of order m,

$$\underline{\tilde{U}}(\vec{J}) = \begin{pmatrix} e^{-i\pi\nu(\vec{J})} & 0 \\ 0 & e^{i\pi\nu(\vec{J})} \end{pmatrix}. \tag{6.11}$$

This matrix contains the amplitude dependent spin tune $\nu(\vec{J})$ in a polynomial expansion up to order m, and one obtains the equilibrium spin field $\Psi_{\vec{n}}(\vec{z}) = \underline{C}(\vec{z})\binom{1}{0}$ since this spinor satisfies the periodicity condition

$$\begin{aligned} \underline{U}(\vec{z}_i)\Psi_{\vec{n}}(\vec{z}_i) &= \underline{U}(\vec{z}_i)\underline{C}(\vec{z}_i)\begin{pmatrix}1\\0\end{pmatrix} = \underline{C}(\vec{z}_f)\underline{\tilde{U}}(\vec{J})\begin{pmatrix}1\\0\end{pmatrix} \\ &= e^{-i\pi\nu(\vec{J})}\Psi_{\vec{n}}(\vec{z}_f)\,. \end{aligned} \tag{6.12}$$

Since spinors have a free phase, the right-hand side is a spinor representation of $\vec{n}(\vec{z}_f)$. Since the polynomial expansion of $\vec{n}(\vec{z})$ contains big coefficients close to spin-orbit resonances, the DA method leads to a drop of $|\langle\vec{n}(\vec{z})\rangle|$ at first-order and at higher-order resonances. This approach is very elegant, but, unfortunately, it uses polynomial expansions of the spin motion with respect to the phase space coordinates. At high energies in HERA the spin rotates $G\gamma = 1567$ times $\Delta\Theta$ when the orbit is tilted by $\Delta\Theta$ in a transverse magnetic field and the spin motion is therefore extremely strongly dependent on the phase space variables. This strong dependence cannot be approximated well at all by a polynomial expansion of relatively low orders and the DA approach, so far, did not turn out to be very useful for analyzing higher-order effects in the HERA spin dynamics.

Two short comments are needed. Sometimes the phase space dependent spin tune is computed as the angle of the rotation generated by $\underline{A}(\vec{z})$ [17,18]. However, this is not the spin tune $\nu(\vec{J})$ since spins are not rotated around the rotation vector of the matrix $\underline{A}(\vec{z})$ but around $\vec{n}(\vec{z})$. Furthermore [18], the polynomial expansion of $\vec{n}(\vec{z})$ cannot simply be computed from $\vec{n}(\vec{z}_f) = \underline{A}(\vec{z}_i)\vec{n}(\vec{z}_i)$ by using the mth-order polynomial expansion $\underline{A}_m(\vec{z})$, separating $\vec{n}(\vec{z})$ into one part $\vec{n}_m$ of order m and another part $\vec{n}_{<m}$ of order lower than m, and solving for the polynomial coefficients of $\vec{n}_m$ in

$$\vec{n}_m(\vec{z}_f) - \underline{A}(0)\vec{n}_m(\vec{z}_i) =_m - \vec{n}_{<m}(\vec{z}_f) + \underline{A}_m(\vec{z}_i)\vec{n}_{<m}(\vec{z}_i)\,. \tag{6.13}$$

The index on the equivalence sign indicates that the polynomials on the right-hand side and the left-hand side should agree up to order m. The determination of all the polynomial coefficients of $\vec{n}_m$ is not possible since some of the coefficients with equivalent k_j^+ and k_j^- cannot be determined in this way. These coefficients can, in principle, be determined by considering the polynomial

coefficients which appear on the right-hand side in higher order than m, but this procedure becomes more intricate.

C. The SMILE formalism

The first fully fledged formalism to compute the nonlinear dependence of the $\vec{n}$ axis on phase space coordinates was the basis of the computer code SMILE [19]. It is an analytical way of computing the polynomial expansion $\vec{n}_m(\vec{z})$, and therefore the limitations of the DA method, which performs this expansion automatically, also apply to the SMILE formalism; therefore, this formalism is not appropriate for an analysis of polarized proton beams in HERA. Nevertheless, for historical reasons and for completeness we describe this formalism. Since $\vec{n}(\vec{z})$ is a spin field, it is propagated by the Thomas-BMT equation (2.1),

$$\frac{d}{dl}\,\vec{n}(\vec{z},l) = [\vec{\Omega}(0,l) + \vec{\omega}(\vec{z},l)] \times \vec{n}(\vec{z},l)\,. \tag{6.14}$$

This equation can be simplified by choosing an orthonormal coordinate system $(\vec{m}_0, \vec{l}_0, \vec{n}_0)$ which rotates around $\vec{n}_0$ according to the Thomas-BMT equation on the closed orbit, $\frac{d}{dl}\vec{m}_0 = \vec{\Omega}(0,l) \times \vec{m}_0$, $\frac{d}{dl}\vec{l}_0 = \vec{\Omega}(0,l) \times \vec{l}_0$. In this coordinate system a spin field satisfies

$$\vec{n} = \begin{pmatrix} \vec{n}\cdot\vec{m}_0 \\ \vec{n}\cdot\vec{l}_0 \\ \vec{n}\cdot\vec{n}_0 \end{pmatrix}, \qquad \frac{d}{dl}\,\vec{n}(\vec{z},l) = \underline{\omega}(\vec{z},l)\vec{n}(\vec{z},l)\,,$$
$$\underline{\omega} = \begin{pmatrix} 0 & -\vec{\omega}\cdot\vec{n}_0 & \vec{\omega}\cdot\vec{l}_0 \\ \vec{\omega}\cdot\vec{n}_0 & 0 & -\vec{\omega}\cdot\vec{m}_0 \\ -\vec{\omega}\cdot\vec{l}_0 & \vec{\omega}\cdot\vec{m}_0 & 0 \end{pmatrix}, \tag{6.15}$$

where the matrix $\underline{\omega}$ is chosen to let the matrix product $\underline{\omega}\vec{n}$ describe the vector product $\vec{\omega} \times \vec{n}$ in the new coordinate system. To compute the propagator of spin fields, we first introduce the phase space trajectory $\hat{\vec{z}}$ which ends at the final phase space point $\vec{z}_f$ when the particle has reached the azimuth l_f of the accelerator, $\vec{z}_f = \hat{\vec{z}}(l_f)$. The propagator from l_0 to l of the ordinary differential equation can now formally be written as the time ordered product indicated by the time ordering operator T,

$$\vec{n}(\vec{z}_f, l_f) = T[e^{\int_{l_0}^{l_f} \underline{\omega}(\hat{\vec{z}}(l),l)\,dl}]\vec{n}(\hat{\vec{z}}(l_0), l_0) \tag{6.16}$$

$$= \left[1 + \int_{l_0}^{l_f} \underline{\omega}(\hat{\vec{z}}(l), l)\,dl + \int_{l_0}^{l_f} \underline{\omega}(\hat{\vec{z}}(l), l) \int_{l_0}^{l} \underline{\omega}(\hat{\vec{z}}(l'), l')\,dl'\,dl + \ldots\right]\vec{n}(\hat{\vec{z}}(l_0), l_0)\,. \tag{6.17}$$

The $\vec{n}$ axis is a spin field which satisfies the periodicity property $\vec{n}(\vec{z},l) = \vec{n}(\vec{z}, l + L_0)$. It can formally be expressed by

$$\tilde{\vec{n}}(\vec{z}_f, l_f) = \lim_{\epsilon\to+0} T[e^{\int_{-\infty}^{l_f} e^{\epsilon l}\underline{\omega}(\hat{\vec{z}}(l),l)\,dl}]\vec{e}_3 \tag{6.18}$$

$$= \lim_{\epsilon\to+0}\left[1 + \int_{-\infty}^{l_f} e^{\epsilon l}\underline{\omega}(\hat{\vec{z}}(l), l)\,dl + \int_{-\infty}^{l_f} e^{\epsilon l}\underline{\omega}(\hat{\vec{z}}(l), l) \int_{-\infty}^{l} e^{\epsilon l'}\underline{\omega}(\hat{\vec{z}}(l'), l')\,dl'\,dl + \cdots\right]\vec{e}_3\,. \tag{6.19}$$

On the closed orbit we have $\vec{\omega}(0,l) = 0$ and one obtains $\vec{n}(0,l) = \vec{e}_3$ since the periodic spin direction $\vec{n}_0$ was chosen to be the third coordinate direction $\vec{e}_3$ in the new coordinate system. The vector $\tilde{\vec{n}}$ in Eq. (6.19) is a spin field, due to the propagation by the time order product. Furthermore, it is periodic since $\underline{\omega}(\vec{z},l) = \underline{\omega}(\vec{z}, l + L_0)$ and due to the l independent starting point of the integration.

Now we assume that $\underline{\omega}(\vec{z},l)$ is a linear function of the phase space coordinates; furthermore, only linear orbit motion is considered. This is often a good approximation, since $\underline{\omega}$ contains a big $a\gamma$ factor and therefore the higher powers of $\underline{\omega}$ in Eq. (6.19) contribute more to one order in $\tilde{\vec{n}}$ than the nonlinear phase space dependence of $\underline{\omega}$ itself. However, sextupole fields, for example, cannot be taken into account in this approximation. In principle one could, however, extend the SMILE formalism to nonlinear terms in $\underline{\omega}$ but the procedure would become rather involved.

Equation (6.19) can now be rewritten in iterative form. First, one writes the power expansion $\vec{n}_m$ of the $\vec{n}$ axis as a sum of terms $\vec{n}^j$ which are homogeneous of order j in the phase space coordinates $\vec{z}$. These terms can then be computed iteratively by

$$\vec{n}^0 = \vec{e}_3, \qquad \vec{n}^{j+1}(\hat{\vec{z}}(l), l) = \lim_{\epsilon\to+0}\int_{-\infty}^{l} e^{\epsilon l'}\underline{\omega}(\hat{\vec{z}}(l'), l')\vec{n}^j(\hat{\vec{z}}(l'), l')\,dl', \qquad \vec{n}_m = \sum_{j=0}^{m}\vec{n}^j\,. \tag{6.20}$$

Using a complex notation, this can be rewritten with $\breve{\omega} = \vec{\omega}\cdot(\vec{m}_0 + i\vec{l}_0)$, $\breve{n} = \vec{n}\cdot(\vec{m}_0 + i\vec{l}_0)$ as

$$\breve{n}^{j+1} = \lim_{\epsilon\to+0} i\int_{-\infty}^{l} e^{\epsilon l'}(\omega_3\breve{n}^j - n_3^j\breve{\omega})\,dl', \qquad n_3^{j+1} = \lim_{\epsilon\to+0}\int_{-\infty}^{l} e^{\epsilon l'}\Im\{\breve{\omega}^*\breve{n}^j\}\,dl'. \tag{6.21}$$

The integral over the infinite range $(-\infty, l)$ cannot be evaluated numerically but it can be written as an infinite sum of one turn integrals. To sum up these one turn integrals analytically, one has to take advantage of the symmetry properties of the integrands in Eq. (6.21). Symmetry properties of the orbital motion are especially obvious when the eigenvector basis of the linear motion is used. This basis was already introduced for the DA method in Sec. VI B. To compute the polynomial coefficients $\vec{n}_{\vec{k}}$ of $\vec{n}(\vec{z}, l) = \sum_{\vec{k}} \vec{n}_{\vec{k}}(l)\vec{z}^{\vec{k}}$, we introduce the corresponding polynomial coefficients of $\vec{\omega}$ and the operator $P_{\vec{k}}$ which projects the coefficient with exponent $\vec{k}$ from a polynomial. The recursion formula then reads

$$\breve{n}_{\vec{k}}\vec{z}^{\vec{k}} = \lim_{\epsilon \to +0} \int_{-\infty}^{l} e^{\epsilon l'} \vec{z}^{\vec{k}} P_{\vec{k}} \left[\sum_{|\vec{j}|=|\vec{k}|-1} (\omega_{\vec{k}-\vec{j},3}\vec{n}_{\vec{j}} - n_{\vec{j},3}\vec{\omega}_{\vec{k}-\vec{j}}) \right] \cdot (\vec{m}_0 + i\vec{l}_0)\, dl', \tag{6.22}$$

$$n_{\vec{k},3}\vec{z}^{\vec{k}} = \lim_{\epsilon \to +0} \int_{-\infty}^{l} e^{\epsilon l'} \vec{z}^{\vec{k}} P_{\vec{k}} \left[\Re \left\{ \sum_{|\vec{j}|=|\vec{k}|-1} [\vec{\omega}_{\vec{j}-\vec{k}} \cdot (\vec{m}_0 + i\vec{l}_0)]^* [\vec{n}_{\vec{j}} \cdot (\vec{m}_0 + i\vec{l}_0)] \right\} \right] dl'. \tag{6.23}$$

In the second equation we used the property $(\vec{z}^{\vec{k}})^* = \vec{z}^{-\vec{k}}$ of coordinates in the orbital eigenvector basis. The factors of the integrands have the following periodicity properties:

(i) In the basis of orbital eigenvectors, the phase space position after one turn is $\vec{z}(l + L_0) = [\vec{z}_1^{+}(l)e^{i2\pi Q_1}, \vec{z}_1^{-}(l)e^{-i2\pi Q_1}, \ldots]$ and a monomial $\vec{z}^{\vec{k}}$ has the property $\vec{z}(l + L_0)^{\vec{k}} = \vec{z}(l)^{\vec{k}} e^{i2\pi \vec{k}\cdot\vec{q}}$ with $\vec{q} = (Q_1, -Q_1, \ldots)$.

(ii) Since the basis vectors $\vec{m}_0$ and $\vec{l}_0$ rotate around $\vec{n}_0$ according to the Thomas-BMT equation on the closed orbit, the vectors rotate by the spin tune ν_0 during one turn giving

$$\vec{m}_0(l + L_0) + i\vec{l}_0(l + L_0) = e^{-i2\pi\nu_0}(\vec{m}_0(l) + i\vec{l}_0(l)). \tag{6.24}$$

(iii) The polynomial coefficients $\vec{\omega}_{\vec{k}}(l)$ and $\vec{n}_{\vec{k}}(l)$ are periodic with period L_0 since $\vec{\omega}(\vec{z}, l + L_0) = \vec{\omega}(\vec{z}, l)$ and $\vec{n}(\vec{z}, l + L_0) = \vec{n}(\vec{z}, l)$. Therefore, the complete factors $P_{\vec{k}}[\cdots]$ are periodic with L_0.

The complete integrands $I_+(l) = e^{\epsilon l}\vec{z}^{\vec{k}} P_{\vec{k}} \times [\sum_{|\vec{j}|=|\vec{k}|-1}(\omega_{\vec{k}-\vec{j},3}\vec{n}_{\vec{j}} - n_{\vec{j},3}\vec{\omega}_{\vec{k}-\vec{j}})] \cdot (\vec{m}_0 + i\vec{l}_0)$ and $I_0(l) = \vec{e}^{\epsilon l} z^{\vec{k}} P_{\vec{k}}[\Re\{\sum_{|\vec{j}|=|\vec{k}|} ([\vec{\omega}_{\vec{j}-\vec{k}} \cdot (\vec{m}_0 + i\vec{l}_0)]^* [\vec{n}_{\vec{j}} \cdot (\vec{m}_0 + i\vec{l}_0)])\}]$ therefore have the symmetry property

$$\begin{aligned} I_+(l + L_0) &= e^{i\vec{q}\cdot\vec{k}} e^{\epsilon L_0} e^{i\nu_0} I_+(l), \\ I_0(l + L_0) &= e^{i\vec{q}\cdot\vec{k}} e^{\epsilon L_0} I_0(l). \end{aligned} \tag{6.25}$$

Now we can compute the integral from $-\infty$ to l by evaluating a one turn integral,

$$\int_{-\infty}^{l} I_+(l')\, dl' = \int_{l-L_0}^{l} I_+(l')\, dl' + \int_{l-2L_0}^{l-L_0} I_+(l')\, dl' + \int_{l-3L_0}^{l-2L_0} I_+(l')\, dl' + \cdots \tag{6.26}$$

$$= \int_{l-L_0}^{l} I_+(l')\, dl' (1 + e^{-\epsilon L_0 + i(\nu_0 - \vec{q}\cdot\vec{k})} + e^{-2\epsilon L_0 + i2(\nu_0 - \vec{q}\cdot\vec{k})} + \cdots) \tag{6.27}$$

$$= \int_{l-L_0}^{l} I_+(l')\, dl' \frac{1}{1 - e^{-\epsilon L_0 + i(\nu_0 - \vec{q}\cdot\vec{k})}}, \tag{6.28}$$

$$\int_{-\infty}^{l} I_0(l')\, dl' = \int_{l-L_0}^{l} I_0(l')\, dl' + \int_{l-2L_0}^{l-L_0} I_0(l')\, dl' + \int_{l-3L_0}^{l-2L_0} I_0(l')\, dl' + \cdots \tag{6.29}$$

$$= \int_{l-L_0}^{l} I_0(l')\, dl' (1 + e^{-\epsilon L_0 - i\vec{q}\cdot\vec{k}} + e^{-2\epsilon L_0 - i2\vec{q}\cdot\vec{k}} + \cdots) \tag{6.30}$$

$$= \int_{l-L_0}^{l} I_0(l')\, dl' \frac{1}{1 - e^{-\epsilon L_0 - i\vec{q}\cdot\vec{k}}}. \tag{6.31}$$

The remaining one turn integrals are computed numerically. In the limit $\lim_{\epsilon \to +0}$, spin-orbit and pure orbit resonance denominators appear, and the average equilibrium polarization thus drops close to first-order and higher-order resonances. However, if $\vec{k} = (k_1, k_1, k_2, k_2, k_3, k_3)$, then a small divisor problem occurs since $\vec{k} \cdot \vec{q}$ vanishes. It can be shown that the numerators are of order ϵ for all such vectors $\vec{k}$. However, special care has to be taken in the numerical calculation, as described in [19,20]. This formalism was also adopted in the framework of canonical spin-orbit motion in [21,22].

D. Stroboscopic averaging with SPRINT

The methods described in the two previous sections were the only procedures for including higher-order effects into the computation of the equilibrium spin field which were known up to two years ago. Both turned out to be not applicable at HERA's proton energies. A new method has then been developed in [10] called stroboscopic averaging.

Suppose that initially the phase space distribution of particles in the beam is polarized in the direction $\vec{f}(\vec{z})$. The stroboscopic average of this initial spin field $\vec{f}(\vec{z})$ can then be viewed as the time average of a pointlike polarimeter measurement of the polarization at a phase space point $\vec{z}$. Initially, the pointlike polarimeter measures $\vec{f}(\vec{z})$. After one turn it measures $\underline{A}(\vec{z}_{-1})\vec{f}(\vec{z}_{-1})$, where $\vec{z}_{-k}$ is the phase space point which is transported to $\vec{z}$ after k turns around the ring. Similarly, after N turns the pointlike polarimeter measures $\underline{A}(\vec{z}_{-1})\cdots\underline{A}(\vec{z}_{-N})\vec{f}(\vec{z}_{-N})$. The stroboscopic average $\vec{n}_N(\vec{z})$ at $\vec{z}$ is defined to be the average polarization measured in the pointlike polarimeter,

$$\vec{n}_N(\vec{z}) = \frac{1}{N}\sum_{j=1}^{N}[\underline{A}(\vec{z}_{-1})\cdots\underline{A}(\vec{z}_{-j})]\vec{f}(\vec{z}_{-j}) = \frac{1}{N}\sum_{j=1}^{N}\left[\prod_{k=1}^{j}\underline{A}(\vec{z}_{-k})\right]\vec{f}(\vec{z}_{-j})\,. \tag{6.32}$$

It is obvious that this quantity is very relevant for the high energy experiments since this time average of polarization has to be high to perform polarization experiments effectively. It is less obvious that this stroboscopic average converges to a vector parallel to $\vec{n}(\vec{z})$ if an equilibrium spin field exists and if $\vec{n}_N(\vec{z})$ does not converge to zero. Convergence properties, variations of this method for increasing the convergence speed, and properties of the field $\vec{n}(\vec{z})$ are derived in [10] and we do not want to mention these here. Here we want to illustrate only that $\vec{n}_N(\vec{z})$ satisfies the periodicity condition for the equilibrium spin field $\vec{n}(\vec{z})$ up to a small error which decreases with N. The periodicity condition can be written as $\vec{n}(\vec{z}) = \underline{A}(\vec{z}_{-1})\vec{n}(\vec{z}_{-1})$,

$$\begin{aligned}\vec{n}_N(\vec{z}) - \underline{A}(\vec{z}_{-1})\vec{n}_N(\vec{z}_{-1}) &= \frac{1}{N}\left\{\sum_{j=1}^{N}\left[\prod_{k=1}^{j}\underline{A}(\vec{z}_{-k})\right]\vec{f}(\vec{z}_{-j}) - \underline{A}(\vec{z}_{-1})\sum_{j=1}^{N}\left[\prod_{k=1}^{j}\underline{A}(\vec{z}_{-k-1})\right]\vec{f}(\vec{z}_{-j-1})\right\}\\ &= \frac{1}{N}\left\{\sum_{j=1}^{N}\left[\prod_{k=1}^{j}\underline{A}(\vec{z}_{-k})\right]\vec{f}(\vec{z}_{-j}) - \sum_{j=2}^{N+1}\left[\prod_{k=1}^{j}\underline{A}(\vec{z}_{-k})\vec{f}(\vec{z}_{-j})\right]\right\} \qquad (6.33)\\ &= \frac{1}{N}\left\{\underline{A}(\vec{z}_{-1})\vec{f}(\vec{z}_{-1}) - \left[\prod_{k=1}^{N+1}\underline{A}(\vec{z}_{-k})\right]\vec{f}(\vec{z}_{-N-1})\right\}. \qquad (6.34)\end{aligned}$$

The right-hand side is a vector of length smaller than $2/N$. This method of computing $\vec{n}(\vec{z})$ contains all higher-order effects since it uses only tracking data and does not perform any expansion in small quantities. It works well for large phase space amplitudes as well as for large angles between the equilibrium spin direction $\vec{n}(\vec{z})$ and the closed orbit spin direction $\vec{n}_0$. The method of stroboscopic averaging was implemented in the spin dynamics code SPRINT and it has been seen in several examples that stroboscopic averaging can be used well in the vicinity of resonances. Therefore, we have adopted this method for analyzing higher-order spin dynamics in HERA at high energies. And it was this method of stroboscopic averaging which led to the establishment of the following technique which is currently under development and investigation.

E. Adiabatic antidamping or adiabatic spin-orbit coupling

It has been observed in numerical simulations that a spin field which is parallel to $\vec{n}(\vec{z})$ stays parallel to this equilibrium direction when parameters of the accelerator are adiabatically changed. This suggests that the angle between $\vec{n}(\vec{z})$ and the spin $\vec{s}$ carried by a particle at phase space point $\vec{z}$ is an adiabatic invariant. There has also been theoretical work associating this angle with an action variable of a Hamiltonian theory, which also indicates that this angle can be an adiabatic invariant [23]. Further theoretical work has been initiated and we believe that the conditions for adiabaticity of the angle $\angle(\vec{n}(\vec{z}),\vec{s})$ will be established soon in a separate paper.

Assuming for now that this angle is an adiabatic invariant, one can envision three procedures of computing the field $\vec{n}(\vec{z})$.

(a) One could start a tracking computation with a spin aligned parallel to $\vec{n}_0$ at a low energy far away from any resonance where the equilibrium polarization is essentially parallel to $\vec{n}_0$ in all of the relevant phase space. Then one would accelerate the particles adiabatically up to the energy under investigation. The disadvantage of this approach is that at HERA one would essentially have to ramp the particle all the way from 39 to 820 GeV/c in an adiabatic manner, which would take a lot of computation

time. And in any case several 1000 resonances would have to be crossed and this cannot always be done adiabatically. Therefore the adiabatic acceleration is not a suitable method of computing the equilibrium spin field. Nevertheless, this method shows well what actually happens to the polarized beam when it is slowly accelerated in HERA.

(b) One could start a tracking computation with a particle on the closed orbit polarized parallel to $\vec{n}_0 = \vec{n}(0)$. When the phase space amplitude is increased adiabatically the spin will stay parallel to $\vec{n}(\vec{z})$ during the complete tracking run until the phase space amplitude of interest is reached. The energy is not changed during this process. This method has been tested and can be performed with practical speed. It has the advantage over the other methods presented so far that one obtains the field $\vec{n}(\vec{z})$ at many phase space amplitudes. One can therefore easily compute the dependence of the averaged equilibrium polarization on phase space amplitude.

(c) A third method which has been tested with success starts a tracking run with a particle at the phase space point $\vec{z}_{-N}$ and a spin parallel to $\vec{n}_0$. In order to make $\vec{n}_0$ parallel to the equilibrium field $\vec{n}(\vec{z})$, the spin-orbit coupling is switched off, i.e., particles all over phase space have the same spin motion as a particle on the closed orbit. Finally, the spin-orbit coupling is switched on adiabatically while tracking the particle for N turns until it arrives at the phase space point $\vec{z}$. This procedure is especially helpful when analyzing the influence of resonance strength on the average polarization since one obtains this polarization for a variation of resonance strength from zero to a final value, allowing one to compute the maximally allowed resonance strength for a required average polarization.

The mathematical concepts involved in the three adiabatic methods are very similar. These three methods are implemented in the code SPRINT and we now show examples of the higher-order effects which were observed with these methods while studying polarized proton beams at high energy in HERA.

VII. HIGHER-ORDER RESONANCES

As mentioned earlier, the SRM and SLIM theories can only compute the effects of first-order resonances, i.e., where $\nu_0 \pm Q_j$ is integer. However, resonance effects can appear whenever $\nu_0 + \vec{k} \cdot \vec{Q}$ is integer for any vector $\vec{k}$ of integers. As mentioned above, when the sum of the components $\sum_j |k_j|$ is larger than 1, one then speaks of a higher-order resonance. Even at low energy in DESY III, higher-order resonances can be observed at phase space amplitudes of 32π mm mrad. The first-order theories presented in Fig. 1 do not show the small resonance peaks of Fig. 4.

At high energy in HERA the first-order resonances are spaced so densely that higher-order resonances are not as clearly visible. So to examine higher order resonances, we suppress the first-order resonances by including Siberian snakes. These fix the spin tune to $\nu_0 = \frac{1}{2}$. Therefore, no resonance peak can be seen in the lower curve of Fig. 5 for a small emittance. However, with increasing phase space amplitude higher-order resonances appear in the upper curve.

VIII. AMPLITUDE DEPENDENT SPIN TUNE

In the first-order analysis the average opening angle of $\vec{n}(\vec{z})$ is approximated by $|\frac{\varepsilon}{\nu_0 - Q_i}|$. The resonance strength ε given in Eq. (3.2) is the Fourier coefficient of a linear function of phase space variables $\vec{\omega}(\vec{z}, l)$ and it therefore increases with the square root of the action variable, $\langle \angle(\vec{n}(\vec{z}), \vec{n}_0) \rangle \propto \sqrt{J_i}$. When more than only the first-order effects are taken into account, the polarization depends on the orbital amplitudes in a more complex fashion. In some cases (an example is shown in Fig. 6), the average opening angle decreases with amplitude after it had previously increased. This is an indication for an amplitude dependent spin tune $\nu(\vec{J})$. While the amplitude changes, a resonance is crossed which causes the average equilibrium polarization to drop at some intermediate phase space amplitude. In Fig. 6 it was not the orbit tune which crossed the resonance since we simulated linear orbit motion, where $\vec{Q}$ does not depend on the phase space amplitude.

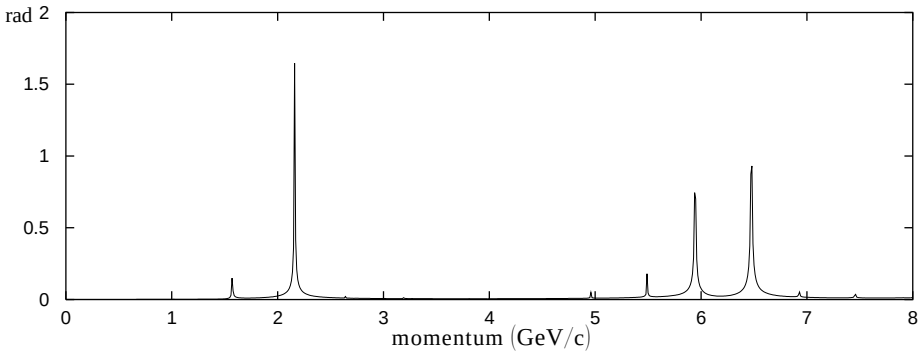

FIG. 4. SPRINT opening angles for a beam with normalized vertical emittance of 32π mm mrad in DESY III.

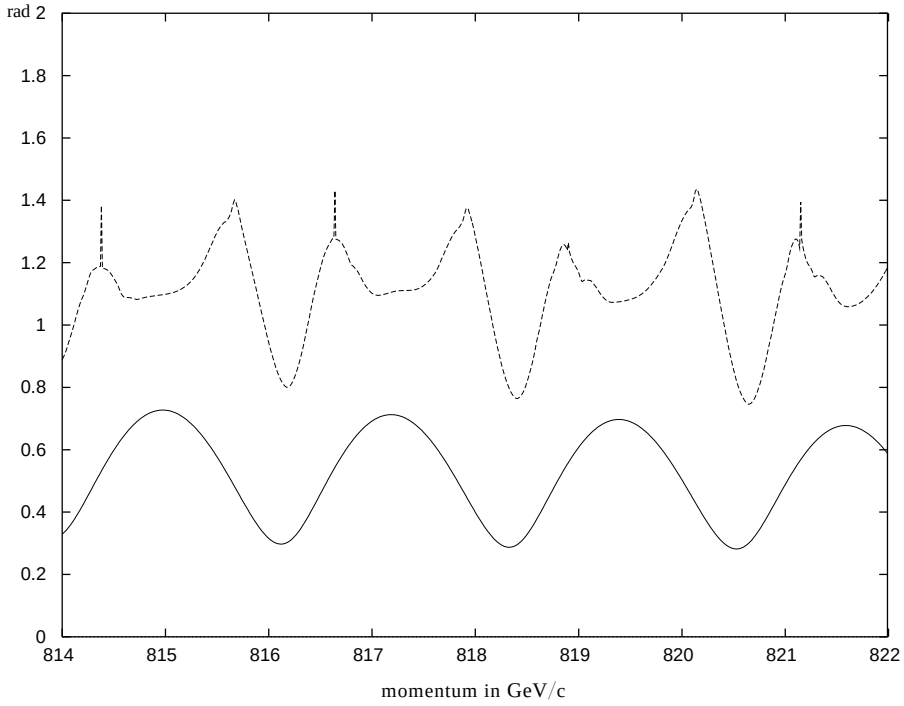

FIG. 5. SPRINT opening angles for a beam with normalized vertical emittance of 32π mm mrad in HERA (dashed line) and 4π mm mrad (solid line). Higher-order resonance peaks appear with increasing emittance. First-order resonance peaks were avoided by fixing the spin tune to $\nu_0 = 1/2$ with Siberian snakes.

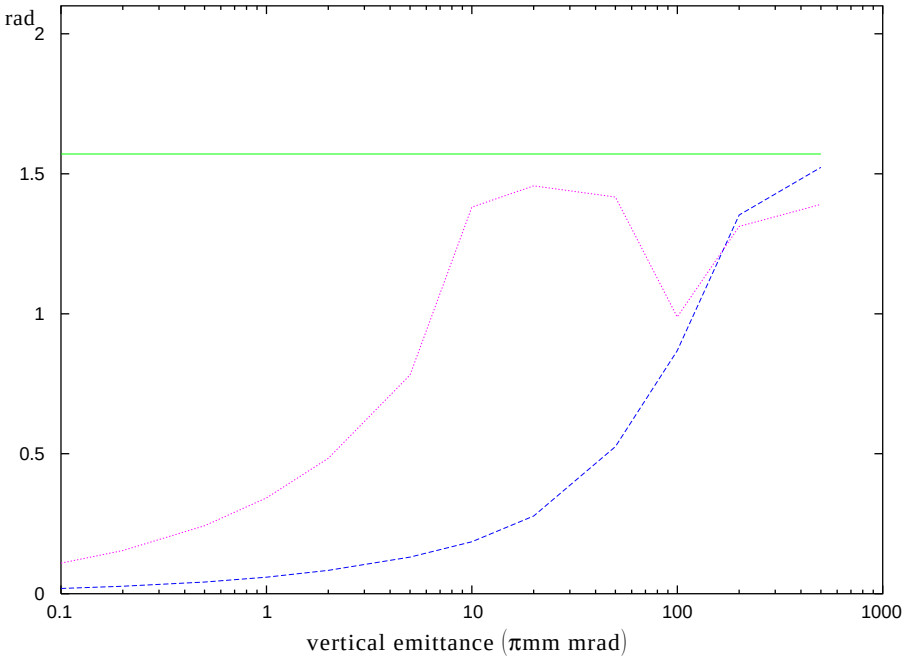

FIG. 6. (Color) SPRINT opening angles for a beam with normalized vertical emittance of up to 400π mm mrad in HERA at 803.9 GeV/c (purple dotted line) and at 819 GeV/c (blue dashed line). The green horizontal line indicates an average opening angle of $\pi/2$ and therefore zero average polarization.

To study such amplitude dependent depolarizing effects, it is advantageous to have a method which quickly leads to $\vec{n}(\vec{z})$ at various amplitudes. The antidamping method described above has this feature and was implemented into SPRINT for that purpose. In fact the technique of antidamping the spin-orbit coupling is already contained in the SMILE formalism [19]. There it was not exploited numerically but used for deriving a formalism which leads to the required periodicity in azimuth.

IX. IRREGULAR INVARIANTS OF SPIN-ORBIT MOTION

If only one phase space amplitude is excited, a particle moves on an invariant ellipse. Turn after turn the particle has a different phase space coordinate $\vec{z}$ but it is always located on a one parametric closed curve in phase space corresponding to the invariant ellipse. We parametrize this curve as $\vec{z}(\varphi)$ with $\varphi \in [0, 2\pi)$. When the particle is initially polarized parallel to $\vec{n}(\vec{z}_i)$, the transported spins change from turn to turn but they are always located on the one parametric closed curve $\vec{n}(\vec{z}(\varphi))$. If the initial spin was not parallel to the equilibrium spin field, the transported spins would not all be located on a one parametric closed curve but could point in other directions. Such closed curves $\vec{n}(\vec{z}(\varphi))$ on the unit sphere are invariant curves of spin-orbit motion. Figure 7 displays an example of such a curve which was computed for HERA with a proton energy of 820 GeV and a vertical phase space amplitude of 16π mm mrad. The first-order theories lead to invariant curves on the unit sphere which are ellipses around the vertical direction. Obviously, the irregularity of the invariant curves of spin-oribt motion at high energy illustrates effects which go beyond first-order resonances.

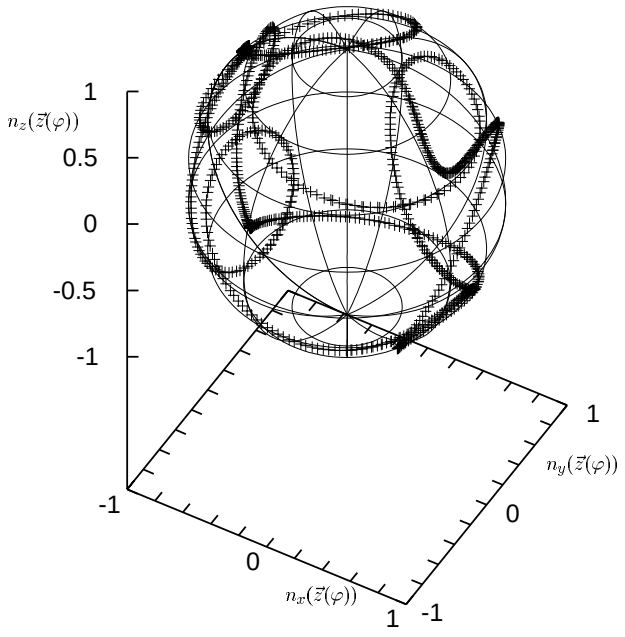

FIG. 7. An invariant curve of spin-orbit motion in HERA at 820 GeV/c for a normalized vertical emittance of 16π mm mrad.

X. CROSSTALK BETWEEN DEGREES OF FREEDOM

So far, only vertical motion has been considered since in a flat ring only particles with vertical phase space amplitude travel through horizontal magnetic fields. In the first-order theories the horizontal and the longitudinal phase space amplitudes therefore do not cause any depolarization. When higher-order effects are included, the spin motion does depend on the horizontal and longitudinal phase space amplitude. When a particle has no vertical phase space amplitude and observes only vertical fields, the equilibrium spin field will still be vertical all over the horizontal phase space. However, when a vertical amplitude is excited then the fields through which a particle is propagating change depending on the horizontal and longitudinal amplitude, and therefore the average polarization of the equilibrium spin field changes. In the spin motion one thus observes crosstalk between the degrees of freedom, even when the orbital motion is completely decoupled (linearly as well as nonlinearly). Figure 8 shows an invariant spin curve $\vec{n}(\vec{z}(\varphi))$ on the unit sphere for a relatively large vertical emittance (left). The average polarization is already strongly reduced. When the particle also has a horizontal phase space amplitude, the phase space coordinates $\vec{z}$ are no longer on a closed curve, and therefore the invariant curves on the unit sphere get washed out. The average polarization is reduced to zero (right). Since the first-order theories neglect any influence of the horizontal motion on the invariant closed curves, Fig. 8 is far out of the range of validity of these theories.

XI. CONCLUSION

Spin dynamics can be described rather well by first-order theories when the energy is low. When studying polarized proton beams in the DESY accelerators we observed that this first-order regime extends up to about 150 GeV/c in HERA. At higher energies, non-first-order effects become relevant. The effects which we observed with customized tools are overlapping resonances, higher-order resonances, amplitude dependent spin tune shifts, very distorted invariant curves of spin-orbit motion, and a coupling between the effects on the spin motion of the orbital degrees of freedom.

While similar concepts are well known for nonlinear orbit motion, they are not so well known for spin motion since all polarized proton beams produced so far operated in an energy regime which is dominated by first-order effects.

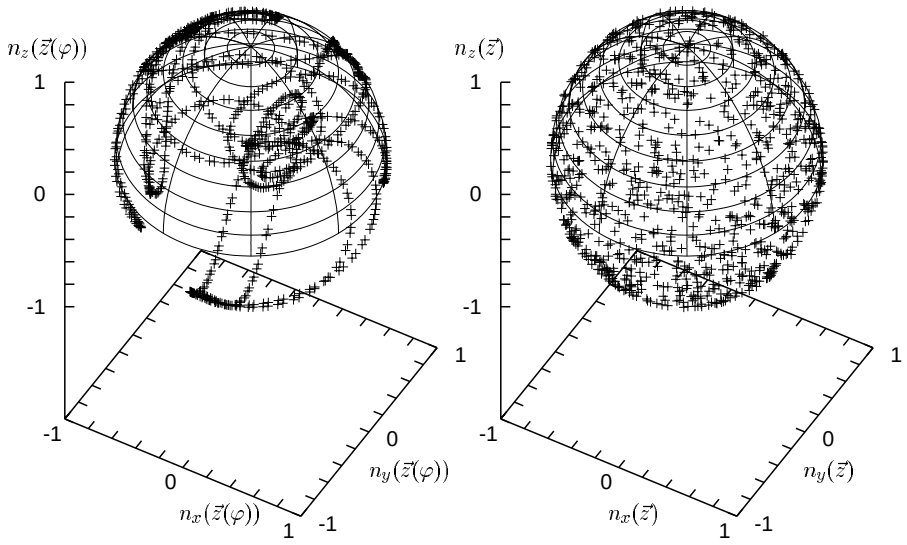

FIG. 8. Invariant curves of spin-orbit motion on the unit sphere for a beam in HERA with normalized vertical emittance of 64π mm mrad and no horizontal emittance (left) and with an additional normalized horizontal emittance of 4π mm mrad (right).

Note added in proof.—A new version of the SODOM algorithm has now been provided by Yokoya which also works for large opening angles [24].

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