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BEAM OPTICS OF THE DIRAC PARTICLE WITH ANOMALOUS MAGNETIC MOMENT

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Beam optics of a spin-$\frac{1}{2}$ particle with anomalous magnetic moment is studied in the monoenergetic and paraxial approximations based on the Dirac equation; the treatment is at the level of single-particle dynamics, considers the electromagnetic field as classical and disregards radiation aspects. The general theory, developed for any magnetic optical element with straight axis, describes the quantum mechanics of the orbital dynamics, the Stern-Gerlach kicks and the Thomas-Bargmann-Michel-Telegdi (Thomas-BMT) spin evolution, up to the paraxial approximation. To illustrate the general theory, the first order transfer maps for the spin components and the transverse phase-space, including the transverse Stern-Gerlach kicks, are computed for a normal magnetic quadrupole lens. The longitudinal Stern-Gerlach kick in a general inhomogeneous magnetic field is also discussed briefly.

Keywords: Beam optics; magnetic moment; polarization.

1 INTRODUCTION

We present an approach to the quantum theory of accelerator optics for a spin-$\frac{1}{2}$ particle with anomalous magnetic moment, including the spin evolution, at the level of single-particle dynamics and disregarding radiation aspects, based, *ab initio*, on the Dirac equation. Here, we are concerned only with monoenergetic and paraxial beams. The electromagnetic field is treated as classical.

As is well known, the present understanding of accelerator beam optics is based mainly on classical mechanics and electrodynamics (see, *e.g.*,[1] and references therein). The main framework for studying the spin dynamics and beam polarization is essentially based on the well known quasiclassical Thomas-Bargmann-Michel-Telegdi (Thomas-BMT) equation (see, *e.g.*,[2]), though quantum fluctuations of the trajectory of an electron (or a positron) and the radiative polarization are understood using the quantized nature of radiation and solutions of the Dirac equations (see, *e.g.*,[3–6]). The Thomas-BMT equation has been understood on the basis of the Dirac equation, independent of the beam optics, in different ways (see, *e.g.*,[3,7,8] and references therein). Understanding the orbital motion in an axially symmetric focusing magnetic field by solving the Dirac equation has also been attempted.[3] Quantum mechanical implications for low energy polarized (anti)proton beams in a spin-splitter device,[9–13] using the transverse Stern-Gerlach kicks, have been analysed on the basis of the nonrelativistic Schrödinger equation.[14,15] For a single spin-$\frac{1}{2}$ particle, it is possible to transform the Dirac Hamiltonian using the Foldy-Wouthuysen theory[16] leading to its expansion as the nonrelativistic part plus relativistic correction terms and thereby obtain a quasiclassical effective Hamiltonian accounting for the orbital motion, the Stern-Gerlach effect and the Thomas-BMT spin evolution[17] (see also [18,19] and references therein; see [20] for the justification of the same quasiclassical effective Hamiltonian using a Pauli reduction of the Dirac theory). Based on such a quasiclassical Hamiltonian a completely classical approach to beam optics has also been developed[18,19] in which an extended classical canonical formalism is used by adding to the classical phase-space variables two new real canonical variables describing all the three components of spin. But, so far, in the realm of accelerator optics there does not seem to have been any attempt, even at the level of single-particle dynamics, to develop the quantum theory of the orbital motion and spin dynamics of spin-$\frac{1}{2}$ particle *beam* leading to a single unified framework based on the standard Dirac theory; note that a beam, though considered to be just a collection of noninteracting particles in motion, is characterized by the property that all its constituent particles move predominantly along a design trajectory. The main aim of this paper is to initiate the development of such an approach in which a beam optical quantum Hamiltonian, valid for any energy, nonrelativistic or relativistic, is obtained from first principles, starting from the Dirac equation, and the transfer maps for the beam observables across an optical block can be computed systematically up to any order of approximation starting with the first order, or paraxial, approximation.

Independently, an algebraic approach to the quantum theory of electron optics (or charged-particle optics, in general) has been under systematic development using the Dirac, Klein-Gordon and the nonrelativistic Schrödinger equations[21–26] (see also [27] for a formal scalar quantum theory of electron optics with a Schrödinger-like basic equation in which the beam emittance plays the role of Planck's constant $\hbar$, and [28] for a path integral approach to the optics of Dirac particles). In Refs. [21–24], developing the spinor theory of electron optics mainly with applications to high voltage micro-electron-beam devices in mind (see [29] for the traditional approach to the quantum mechanics of electron optics), the spin dynamics has not been explicitly considered. Here, in developing the quantum mechanical approach to the beam optics of the Dirac particle, as mentioned above, we follow closely the Refs. [21–24].

In Section 2 we present the general framework of our theory for any arbitrary magnetic optical element with straight axis; details are given for the paraxial approximation. In Section 3 we illustrate the general theory by computing the first order transfer maps for the spin components and the transverse phase-space, including the transverse Stern-Gerlach kicks, in the case of a normal magnetic quadrupole lens and also discuss briefly the longitudinal Stern-Gerlach kick[30] in a general inhomogeneous magnetic field.

2 BEAM OPTICS OF THE DIRAC PARTICLE: GENERAL THEORY FOR A MAGNETIC OPTICAL ELEMENT WITH STRAIGHT AXIS

We are interested in studying the spin dynamics and optics of a monoenergetic paraxial Dirac-particle beam transported through a magnetic optical element with straight axis comprising the static field $\mathbf{B} = \text{ curl } \mathbf{A}$ associated with a vector potential $\mathbf{A}$. Let us consider the Dirac particle to have mass m, charge q and anomalous magnetic moment μ_a. The beam propagation is governed by the stationary Dirac equation

$$H_D \left|\psi_D\right\rangle = E \left|\psi_D\right\rangle \, , \tag{2.1}$$

where $\left|\psi_D\right\rangle$ is the time-independent 4-component Dirac spinor, E is the energy of the beam particle and the Hamiltonian H_D, including the Pauli term is given by

$$H_D = \beta mc^2 + c\boldsymbol{\alpha} \cdot (-\mathrm{i}\,\hbar\boldsymbol{\nabla} - q\mathbf{A}) - \mu_a \beta \boldsymbol{\Sigma} \cdot \mathbf{B}\,,$$

$$\beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\sigma} \end{pmatrix},$$

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathbf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.2}$$

It should be noted that we are dealing with the scattering states of the time-independent Hamiltonian H_D with conserved positive energy

$$E = +\sqrt{m^2c^4 + c^2p^2}\,, \qquad p = |\mathbf{p}|\,, \tag{2.3}$$

where $\mathbf{p}$ is the momentum of the beam particle entering the system from the field-free input region. Let the system have its straight optic axis along the z-direction. We shall consider the beam to be paraxial and moving along the positive z-direction such that for any constituent particle of the beam

$$p \approx p_z > 0\,, \quad |p_x| \ll p\,, \quad |p_y| \ll p\,. \tag{2.4}$$

We shall use the right handed Cartesian coordinate system with z pointing along the design trajectory, y as the vertical coordinate and x as the horizontal transverse coordinate.

Since we want to know the changes in the beam parameters along the optic axis of the system (*i.e.*, the $+z$-direction) we have to study the Dirac equation (2.1) rewritten as

$$\mathrm{i}\,\hbar\frac{\partial}{\partial z}\,|\psi_D\rangle = \mathcal{H}_D\,|\psi_D\rangle\,. \tag{2.5}$$

In effect, we want to know how the Dirac wavefunction satisfying (2.1) evolves with z. If we assume that for any constituent particle of the beam, scattered by the static field of the optical element, the probability of location at the transverse plane at z, namely $\int d^2\mathbf{r}_\perp \sum_{i=1}^{4} |\psi_{Di}(\mathbf{r}_\perp, z)|^2$, is almost a constant in the region of interest, then, one can consider $(\psi_{D1}(\mathbf{r}_\perp, z), \psi_{D2}(\mathbf{r}_\perp, z), \psi_{D3}(\mathbf{r}_\perp, z), \psi_{D4}(\mathbf{r}_\perp, z))$, apart from a common normalization factor, as the components of a spinor wavefunction in the transverse plane at z, and regard z as a parameter evolving along the optic axis of the system. Bearing this in mind, we multiply (2.1) from left by α_z/c and rearrange the terms to get the desired form (2.5): The result is that

$$
\begin{aligned}
\mathcal{H}_D &= -p\beta\chi\alpha_z - qA_z\mathbb{1} + \alpha_z\boldsymbol{\alpha}_\perp \cdot \hat{\boldsymbol{\pi}}_\perp + (\mu_a/c)\beta\alpha_z\boldsymbol{\Sigma}\cdot\mathbf{B}\,, \\
\chi &= \begin{pmatrix} \xi\mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\xi^{-1}\mathbf{1} \end{pmatrix}, \quad \mathbb{1} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}, \quad \xi = \sqrt{\frac{E+mc^2}{E-mc^2}}\,, \\
\hat{\boldsymbol{\pi}}_\perp &= (-\,\mathrm{i}\,\hbar\boldsymbol{\nabla}_\perp - q\mathbf{A}_\perp) = (\hat{\mathbf{p}}_\perp - q\mathbf{A}_\perp)\,.
\end{aligned} \tag{2.6}
$$

Noting that, with

$$
M = \frac{1}{\sqrt{2}}(\mathbb{1} + \chi\alpha_z)\,, \quad M^{-1} = \frac{1}{\sqrt{2}}(\mathbb{1} - \chi\alpha_z)\,, \tag{2.7}
$$

one has

$$
M(\beta\chi\alpha_z)M^{-1} = \beta\,, \tag{2.8}
$$

we define

$$
|\psi_D\rangle = M^{-1}\left|\psi'\right\rangle. \tag{2.9}
$$

This turns (2.5) into

$$
\mathrm{i}\,\hbar\frac{\partial}{\partial z}\left|\psi'\right\rangle = \mathcal{H}'\left|\psi'\right\rangle, \quad \mathcal{H}' = M\mathcal{H}_D M^{-1} = -p\beta + \hat{\mathcal{E}} + \hat{\mathcal{O}}\,, \tag{2.10}
$$

with the matrix elements of $\hat{\mathcal{E}}$ and $\hat{\mathcal{O}}$ given by

$$
\begin{aligned}
\hat{\mathcal{E}}_{11} &= -qA_z\mathbf{1} - (\mu_a/2c)\left\{\left(\xi + \xi^{-1}\right)\boldsymbol{\sigma}_\perp\cdot\mathbf{B}_\perp + \left(\xi - \xi^{-1}\right)\sigma_z B_z\right\}, \\
\hat{\mathcal{E}}_{12} &= \hat{\mathcal{E}}_{21} = \mathbf{0}\,, \\
\hat{\mathcal{E}}_{22} &= -qA_z\mathbf{1} - (\mu_a/2c)\left\{\left(\xi + \xi^{-1}\right)\boldsymbol{\sigma}_\perp\cdot\mathbf{B}_\perp - \left(\xi - \xi^{-1}\right)\sigma_z B_z\right\},
\end{aligned} \tag{2.11}
$$

and

$$\hat{\mathcal{O}}_{11} = \hat{\mathcal{O}}_{22} = \mathbf{0}\,,$$

$$\hat{\mathcal{O}}_{12} = \xi\left[\boldsymbol{\sigma}_\perp \cdot \hat{\boldsymbol{\pi}}_\perp - (\mu_a/2c)\left\{\mathrm{i}\,\left(\xi - \xi^{-1}\right)\left(B_x\sigma_y - B_y\sigma_x\right)\right.\right.$$
$$\left.\left. - \left(\xi + \xi^{-1}\right) B_z\mathbf{1}\right\}\right],$$

$$\hat{\mathcal{O}}_{21} = -\xi^{-1}\left[\boldsymbol{\sigma}_\perp \cdot \hat{\boldsymbol{\pi}}_\perp + (\mu_a/2c)\left\{\mathrm{i}\,\left(\xi - \xi^{-1}\right)\left(B_x\sigma_y - B_y\sigma_x\right)\right.\right.$$
$$\left.\left. + \left(\xi + \xi^{-1}\right) B_z\mathbf{1}\right\}\right]. \tag{2.12}$$

The significance of the transformation (2.9) is that for a paraxial Dirac spinor propagating in the $+z$-direction $\left|\psi'\right\rangle$ is such that its lower spinor components are very small compared to the upper spinor components. To see this, let us consider the standard free Dirac plane-wave associated with positive energy E, namely,

$$\begin{pmatrix} \psi_{FD1}(\mathbf{r}_\perp, z) \\ \psi_{FD2}(\mathbf{r}_\perp, z) \\ \psi_{FD3}(\mathbf{r}_\perp, z) \\ \psi_{FD4}(\mathbf{r}_\perp, z) \end{pmatrix} = \frac{1}{4}\sqrt{\frac{\xi cp}{\pi^3\hbar^3 E}} \begin{pmatrix} s_+ \\ s_- \\ \{s_-p_- + s_+p_z\}/\xi p \\ \{s_+p_+ - s_-p_z\}/\xi p \end{pmatrix}$$
$$\times\ \exp\left\{\frac{\mathrm{i}}{\hbar}\,(\mathbf{p}_\perp \cdot \mathbf{r}_\perp + p_z z)\right\}, \tag{2.13}$$
$$\mathbf{r}_\perp = (x, y)\,, \quad |s_+|^2 + |s_-|^2 = 1\,,$$
$$p_+ = p_x + \mathrm{i}\,p_y\,, \quad p_- = p_x - \mathrm{i}\,p_y\,.$$

Correspondingly,

$$\begin{pmatrix} \psi'_{F1}(\mathbf{r}_\perp, z) \\ \psi'_{F2}(\mathbf{r}_\perp, z) \\ \psi'_{F3}(\mathbf{r}_\perp, z) \\ \psi'_{F4}(\mathbf{r}_\perp, z) \end{pmatrix} = \frac{1}{4}\sqrt{\frac{\xi cp}{2\pi^3\hbar^3 E}} \begin{pmatrix} \{s_+(p + p_z) + s_-p_-\}/p \\ \{s_-(p + p_z) - s_+p_+\}/p \\ -\{s_+(p - p_z) - s_-p_-\}/\xi p \\ \{s_-(p - p_z) + s_+p_+\}/\xi p \end{pmatrix} \tag{2.14}$$
$$\times\ \exp\left\{\frac{\mathrm{i}}{\hbar}\,(\mathbf{p}_\perp \cdot \mathbf{r}_\perp + p_z z)\right\},$$

and for a paraxial plane-wave moving in the positive z-direction, satisfying the condition (2.4), the upper spinor components of $\left|\psi'\right\rangle_F$, namely, $\left|\psi'_1\right\rangle_F$ and $\left|\psi'_2\right\rangle_F$, are obviously very large compared to its lower spinor components $\left|\psi'_3\right\rangle_F$ and $\left|\psi'_4\right\rangle_F$. We can take this to be generally true for any paraxial beam. Then, in the paraxial situation, the even operator $\hat{\mathcal{E}}$ in (2.11) does not couple the large upper components and the small lower components while the odd operator $\hat{\mathcal{O}}$ in (2.12) couples them. This is exactly the same as in the nonrelativistic situation obtained in the standard Dirac theory with respect to time evolution. This, and the striking resemblance of (2.10) with the standard Dirac equation (2.1) make us turn to the Foldy-Wouthuysen (FW) transformation technique[16] (see also, *e.g.*, [31]) to analyse (2.10) further; note that in (2.10) the analogue of mc^2 is $-p$ since $\mathrm{i}\,\hbar\frac{\partial}{\partial z}$ corresponds to $-\hat{p}_z$.

Let us recall that the FW-technique is useful in analysing the Dirac equation systematically as a sum of the nonrelativistic part and a series of relativistic correction terms. The FW-technique is essentially based on the fact that β commutes with any even operator with off-diagonal 2×2 block elements equal to $\mathbf{0}$, and anticommutes with any odd operator with diagonal 2×2 block elements equal to $\mathbf{0}$. So, applying this technique to (2.10) should help us analyse it as a sum of the paraxial part and a series of nonparaxial (aberration) correction terms. To this end, we substitute in (2.10)

$$\left|\psi'\right\rangle = \exp\left(\frac{1}{2p}\beta\hat{\mathcal{O}}\right)\left|\psi^{(1)}\right\rangle . \qquad (2.15)$$

The resulting equation for $\left|\psi^{(1)}\right\rangle$ is

$$\begin{aligned}
\mathrm{i}\,\hbar\frac{\partial}{\partial z}\left|\psi^{(1)}\right\rangle &= \mathcal{H}^{(1)}\left|\psi^{(1)}\right\rangle , \\
\mathcal{H}^{(1)} &= \exp\left(-\frac{1}{2p}\beta\hat{\mathcal{O}}\right)\mathcal{H}'\exp\left(\frac{1}{2p}\beta\hat{\mathcal{O}}\right) \\
&\quad - \mathrm{i}\,\hbar\exp\left(-\frac{1}{2p}\beta\hat{\mathcal{O}}\right)\frac{\partial}{\partial z}\left\{\exp\left(\frac{1}{2p}\beta\hat{\mathcal{O}}\right)\right\} \\
&= -p\beta + \hat{\mathcal{E}}^{(1)} + \hat{\mathcal{O}}^{(1)} ,
\end{aligned}$$

$$\hat{\mathcal{E}}^{(1)} = \hat{\mathcal{E}} - \frac{1}{2p}\beta\hat{\mathcal{O}}^2 + \cdots ,$$
$$\hat{\mathcal{O}}^{(1)} = -\frac{1}{2p}\beta\left\{\left[\hat{\mathcal{O}}, \hat{\mathcal{E}}\right] + \mathrm{i}\,\hbar\frac{\partial}{\partial z}\hat{\mathcal{O}}\right\} + \cdots . \tag{2.16}$$

The effect of this transformation is to eliminate from the odd part of $\mathcal{H}'$ the terms of zeroth order in $1/p$; note that $\hat{\mathcal{O}}^{(1)}$ of $\mathcal{H}^{(1)}$ contains only terms of first and higher orders in $1/p$ (not shown explicitly above). By a series of successive transformations with the same recipe (2.15) one can eliminate odd parts up to any desired order in $1/p$. We shall stop with the above first step which would correspond to the paraxial approximation. Let us write down explicitly, for later use, the 11-block element of $\mathcal{H}^{(1)}$:

$$\begin{aligned}
\mathcal{H}_{11}^{(1)} &= -p\mathbf{1} + \hat{\mathcal{E}}_{11}^{(1)} \\
&= \left\{-p - qA_z + \frac{1}{2p}\hat{\pi}_{\perp}^{2} - \frac{\epsilon\hbar^2}{4p^2}(\,\mathrm{curl}\ \mathbf{B})_z + \frac{\epsilon^2\hbar^2}{8p^3}\left(B_{\perp}^2 + \gamma^2 B_z^2\right)\right\}\mathbf{1} \\
&\quad - \frac{1}{p}\{(q+\epsilon)B_z S_z + \gamma\epsilon\mathbf{B}_{\perp}\cdot\mathbf{S}_{\perp}\} \\
&\quad + \frac{\epsilon}{2p^2}\left\{\gamma\left(B_z\mathbf{S}_{\perp}\cdot\hat{\boldsymbol{\pi}}_{\perp} + \mathbf{S}_{\perp}\cdot\hat{\boldsymbol{\pi}}_{\perp}B_z\right) - \left(\mathbf{B}_{\perp}\cdot\hat{\boldsymbol{\pi}}_{\perp} + \hat{\boldsymbol{\pi}}_{\perp}\cdot\mathbf{B}_{\perp}\right)S_z\right\} ,
\end{aligned}$$
$$\hat{\pi}_{\perp}^2 = \hat{\pi}_x^2 + \hat{\pi}_y^2 , \quad \epsilon = 2m\mu_a/\hbar , \quad \gamma = E/mc^2 , \quad \mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma} . \tag{2.17}$$

Before proceeding further, let us find out the nature of $\left|\psi^{(1)}\right\rangle$ by looking at the field-free case again. For $|\psi\rangle_F$ in (2.13)

$$\begin{aligned}
\left|\psi^{(1)}\right\rangle_F &= \exp\left(-\frac{1}{2p}\beta\chi\boldsymbol{\alpha}_{\perp}\cdot\mathbf{p}_{\perp}\right)|\psi'\rangle_F \\
&\approx \left(\mathbb{1} - \frac{1}{2p}\beta\chi\boldsymbol{\alpha}_{\perp}\cdot\mathbf{p}_{\perp}\right)|\psi'\rangle_F ,
\end{aligned}$$

$$
\begin{aligned}
\begin{pmatrix}
\psi_{F1}^{(1)}(\mathbf{r}_\perp, z) \\
\psi_{F2}^{(1)}(\mathbf{r}_\perp, z) \\
\psi_{F3}^{(1)}(\mathbf{r}_\perp, z) \\
\psi_{F4}^{(1)}(\mathbf{r}_\perp, z)
\end{pmatrix} \approx & \frac{1}{4}\sqrt{\frac{\xi c p}{2\pi^3 \hbar^3 E}} \\
& \times \begin{pmatrix}
s_+ \left\{1 + \frac{p_z}{p} - \frac{p_\perp^2}{2p^2}\right\} + \frac{1}{2} s_- \left\{\left(1 + \frac{p_z}{p}\right) \frac{p_-}{p}\right\} \\
s_- \left\{1 + \frac{p_z}{p} + \frac{p_\perp^2}{2p^2}\right\} - \frac{1}{2} s_+ \left\{\left(1 + \frac{p_z}{p}\right) \frac{p_+}{p}\right\} \\
-\frac{1}{\xi}\left[s_+ \left\{1 - \frac{p_z}{p} - \frac{p_\perp^2}{2p^2}\right\} + \frac{1}{2} s_- \left\{\left(1 - \frac{p_z}{p}\right) \frac{p_-}{p}\right\}\right] \\
\frac{1}{\xi}\left[s_- \left\{1 - \frac{p_z}{p} - \frac{p_\perp^2}{2p^2}\right\} + \frac{1}{2} s_+ \left\{\left(1 - \frac{p_z}{p}\right) \frac{p_+}{p}\right\}\right]
\end{pmatrix} \\
& \times \exp\left\{\frac{\mathrm{i}}{\hbar} \left(\mathbf{p}_\perp \cdot \mathbf{r}_\perp + p_z z\right)\right\} ,
\end{aligned} \tag{2.18}
$$

showing clearly that the transformation (2.15) keeps the upper spinor components of $\left|\psi^{(1)}\right\rangle$ large compared to its lower spinor components.

Since the lower pair of components of $\left|\psi^{(1)}\right\rangle$ $\left(\left|\psi_3^{(1)}\right\rangle \text{ and } \left|\psi_4^{(1)}\right\rangle\right)$ are almost vanishing compared to the the upper pair $\left(\left|\psi_1^{(1)}\right\rangle \text{ and } \left|\psi_2^{(1)}\right\rangle\right)$ and the odd part of $\mathcal{H}^{(1)}$ is negligible compared to its even part we can effectively introduce a Pauli-like two-component spinor formalism based on the representation (2.16). Naming the two-component spinor comprising the upper pair of components of $\left|\psi^{(1)}\right\rangle$ as $\left|\tilde{\psi}\right\rangle$ and calling $\mathcal{H}_{11}^{(1)}$ as $\tilde{\mathcal{H}}$ it is clear from (2.16) and (2.17) that we can write

$$
\begin{aligned}
& \mathrm{i}\hbar\frac{\partial}{\partial z}\left|\tilde{\psi}\right\rangle = \tilde{\mathcal{H}}\left|\tilde{\psi}\right\rangle , \qquad \left|\tilde{\psi}\right\rangle = \begin{pmatrix} \left|\tilde{\psi}_1\right\rangle \\ \left|\tilde{\psi}_2\right\rangle \end{pmatrix} , \\
& \tilde{\mathcal{H}} \approx \left(-p - qA_z + \frac{1}{2p}\hat{\pi}_\perp^2\right) \\
& \qquad - \frac{1}{p}\left\{(q+\epsilon)B_z S_z + \gamma\epsilon \mathbf{B}_\perp \cdot \mathbf{S}_\perp\right\} ,
\end{aligned} \tag{2.19}
$$

where $\tilde{\mathcal{H}}$ has been approximated by keeping only terms up to first order in $1/p$ (see (2.17)), consistent with the assumption of paraxiality condition (2.4) for the beam. Throughout the paper we shall approximate the various expressions by keeping only up to the lowest order nontrivial terms consistent with the paraxiality condition for the beam and the approximation symbol ($\approx$) will usually imply this, whenever relevant, even if not stated explicitly.

Up to now, all the observables, the field components, time, etc., are defined with reference to the laboratory frame. But, as is well known, in the covariant description the spin of the Dirac particle has simple operator representation in terms of the Pauli matrices only in a frame at which the particle is at rest. So, as is usual, we shall prefer to define spin with reference to the instantaneous rest frame of the particle while keeping the other observables, field components, time, etc., defined with reference to the laboratory frame. To this end, we transform the two-component $\left|\tilde{\psi}\right\rangle$ to an 'accelerator optics representation' $\left|\psi^{(A)}\right\rangle$ defined by

$$\left|\tilde{\psi}\right\rangle = \exp\left\{\frac{\mathrm{i}}{2p}\left(\hat{\pi}_x\sigma_y - \hat{\pi}_y\sigma_x\right)\right\}\left|\psi^{(A)}\right\rangle . \tag{2.20}$$

The reason for the choice of this transformation will become clear shortly. Now, the z-evolution equation for $|\psi^{(A)}\rangle$ is

$$\begin{aligned}
&\mathrm{i}\,\hbar\frac{\partial}{\partial z}\left|\psi^{(A)}\right\rangle = H^{(A)}\left|\psi^{(A)}\right\rangle , \\
&\qquad H^{(A)} \approx \left(-p - qA_z + \frac{1}{2p}\hat{\pi}_\perp^2\right) + \frac{\gamma m}{p}\underline{\mathbf{\Omega}}_s\cdot\mathbf{S}, \\
&\qquad \text{with }\ \underline{\mathbf{\Omega}}_s = -\frac{1}{\gamma m}\left\{q\mathbf{B} + \epsilon\left(\mathbf{B}_\parallel + \gamma\mathbf{B}_\perp\right)\right\} ,
\end{aligned} \tag{2.21}$$

where $\mathbf{B}_\parallel$ and $\mathbf{B}_\perp$ are the components of $\mathbf{B}$ along the z-axis and perpendicular to it. When $q = \pm e$ we can write $\epsilon = qa = q(g-2)/2$ where g and a are, respectively, the gyromagnetic ratio and the magnetic anomaly of the particle; for the neutron $\epsilon = g|e|/2$. It may be noted that the accelerator optical quantum Hamiltonian $H^{(A)}$ is hermitian though $\mathcal{H}_D$ in (2.6) is nonhermitian. The nonunitary similarity transformations we have made have resulted in this change and the hermiticity of $H^{(A)}$ implies the approximate constancy of the total intensity of the beam in any transverse plane along the optic axis. It should be realized that the spin part of $H^{(A)}$ corresponds to the beam optical and paraxial version of the Thomas-BMT spin Hamiltonian : note that $\mathbf{B}_{\|}$ and $\mathbf{B}_{\perp}$ in the usual Thomas-BMT vector $\mathbf{\Omega}_s$ refer to the parallel and the perpendicular components with respect to the instantaneous velocity of the particle whereas in $\underline{\mathbf{\Omega}}_s$ in (2.21) they refer to the parallel and perpendicular components with respect to the predominant direction of propagation of the particle. The Thomas-BMT part of $H^{(A)}$ is also valid up to first order in $\hbar$. To get higher order corrections, in terms of $\hat{\boldsymbol{\pi}}_{\perp}/p$ and $\hbar$, we have to go beyond the first FW-like transformation (2.15).

Since the z-evolution of $\left|\psi^{(A)}\right\rangle$ is unitary we can associate the beam with a wavefunction normalized in such a way that, at any z,

$$\left\langle\psi^{(A)}(z)\left|\psi^{(A)}(z)\right.\right\rangle = \sum_{i=1}^{2} \int d^2\mathbf{r}_{\perp} \left|\psi_i^{(A)}(\mathbf{r}_{\perp}, z)\right|^2 = 1 . \tag{2.22}$$

When the beam is described by a 2×2 statistical (density) matrix

$$\rho^{(A)} = \begin{pmatrix} \rho_{11}^{(A)} & \rho_{12}^{(A)} \\ \rho_{21}^{(A)} & \rho_{22}^{(A)} \end{pmatrix} , \tag{2.23}$$

with the normalization

$$\mathrm{Tr}\left(\rho^{(A)}(z)\right) = \sum_{i=1}^{2} \int d^2\mathbf{r}_{\perp} \left\langle\mathbf{r}_{\perp}\left|\rho_{ii}^{(A)}(z)\right|\mathbf{r}_{\perp}\right\rangle = 1 , \tag{2.24}$$

at any z, the accelerator optical z-evolution equation is

$$\mathrm{i}\,\hbar\frac{\partial}{\partial z}\rho^{(A)} = \left[H^{(A)} , \rho^{(A)}\right] . \tag{2.25}$$

If the beam can be described as a pure state we would have $\rho^{(A)} = \left|\psi^{(A)}\right\rangle\left\langle\psi^{(A)}\right|$.

Let us now define the average of any observable O at the transverse plane at z to be given by

$$\left\langle\hat{O}^{(A)}\right\rangle(z) = \mathrm{Tr}\left(\rho^{(A)}(z)\hat{O}^{(A)}\right) \tag{2.26}$$

$$= \sum_{i,j=1}^{2} \int\int d^2\mathbf{r}_{\perp}d^2\mathbf{r}'_{\perp} \left\langle\mathbf{r}_{\perp}\left|\rho_{ij}^{(A)}(z)\right|\mathbf{r}'_{\perp}\right\rangle\left\langle\mathbf{r}'_{\perp}\left|\hat{O}_{ji}^{(A)}\right|\mathbf{r}_{\perp}\right\rangle ,$$

where $\hat{O}^{(A)}$ is the operator representing O in the accelerator optical representation.

For any observable O, associated with the operator $\hat{O}_D$ in the standard Dirac representation (2.1) the corresponding $\hat{O}^{(A)}$ can be obtained as follows:

$$
\begin{aligned}
\hat{O}^{(A)} = {} & \text{the hermitian part of the 11-block element of} \\
& \left(\exp\left\{ -\frac{\mathrm{i}}{2p}\left(\hat{\pi}_x \Sigma_y - \hat{\pi}_y \Sigma_x\right)\right\} \right. \\
& \times \exp\left(-\frac{1}{2p}\beta\hat{\mathcal{O}}\right) M \hat{O}_D M^{-1} \exp\left(\frac{1}{2p}\beta\hat{\mathcal{O}}\right) \\
& \left. \times \exp\left\{ \frac{\mathrm{i}}{2p}\left(\hat{\pi}_x \Sigma_y - \hat{\pi}_y \Sigma_x\right)\right\} \right) .
\end{aligned}
\tag{2.27}
$$

In the Dirac representation the operator for the spin unit vector corresponding to the spin as defined in the instantaneous rest frame of the particle (see [3]) is given by

$$
\mathbf{S}_R = \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} - \frac{c^2(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\cdot\boldsymbol{\sigma})}{2E(E+mc^2)} & \frac{c\hat{\boldsymbol{\pi}}}{E} \\ \frac{c\hat{\boldsymbol{\pi}}}{E} & -\boldsymbol{\sigma} + \frac{c^2(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\cdot\boldsymbol{\sigma})}{2E(E+mc^2)} \end{pmatrix} . \tag{2.28}
$$

If we now compute the corresponding operator $\mathbf{S}_R^{(A)}$ in the accelerator optical representation, using the formula (2.27), it is found that up to first order (paraxial) approximation

$$
\mathbf{S}_R^{(A)} \approx \frac{\hbar}{2}\boldsymbol{\sigma} \tag{2.29}
$$

as is desired. In the Dirac representation the position operator in free space can be taken to be given by the mean position operator as indicated by the FW-theory (or what is same as the Newton-Wigner position operator). In presence of the magnetic field we can extend this position operator by the replacement $\hat{\mathbf{p}} \longrightarrow \hat{\boldsymbol{\pi}}$ and symmetrization (to make it hermitian). Then, the operator for the transverse position coordinate in the accelerator optical representation becomes just the canonical position operator $\mathbf{r}_\perp$ in the first order approximation. From these considerations it is clear that in the accelerator optical evolution Equation (2.21) $\mathbf{S}$ represents the spin as defined in the instantaneous rest frame of the particle; the field components and other operators are all defined with respect to the laboratory frame. It should be noted that in this formalism, with z as the evolution parameter (analogous to time t), $-H^{(A)}$ corresponding to $-\mathrm{i}\,\hbar\frac{\partial}{\partial z}$, will represent $\hat{p}_z$, the z-component of canonical momentum operator (analogous to the energy operator); hence, the operator $-(H^{(A)}+qA_z)$ will represent π_z the z-component of the kinetic momentum.

If we now work out the equations of motion for the average values of $\mathbf{r}_\perp$ using (2.25), they have to be consistent, *à la* Ehrenfest, with the traditional transfer map for the phase-space, including the transverse Stern-Gerlach kicks (see, *e.g.*, [11,30]), in the paraxial approximation. The transfer map for the averages of spin components, in the lowest order approximation, has to be consistent with the Thomas-BMT equation. This is confirmed easily by a preliminary analysis as follows. From (2.25) and (2.26) we have, in general,

$$\frac{d}{dz}\left\langle \hat{O}^{(A)}\right\rangle(z) = -\frac{\mathrm{i}}{\hbar}\left\langle\left[\hat{O}^{(A)}\,,\,H^{(A)}\right]\right\rangle(z) + \left\langle\frac{\partial}{\partial z}\hat{O}^{(A)}\right\rangle(z)\,. \tag{2.30}$$

To compare (2.30) with the time evolution of classical O we can use the correspondence

$$\frac{d}{dt}O \longrightarrow \frac{d}{dt}\left\langle \hat{O}^{(A)}\right\rangle \approx v_z\frac{d}{dz}\left\langle \hat{O}^{(A)}\right\rangle \approx \frac{p}{\gamma m}\frac{d}{dz}\left\langle \hat{O}^{(A)}\right\rangle, \tag{2.31}$$

since

$$\begin{aligned} v_z &= \frac{1}{\gamma m}\langle\hat{\pi}_z\rangle = -\frac{1}{\gamma m}\left\langle H^{(A)}+qA_z\right\rangle \\ &= \frac{p}{\gamma m} - \frac{1}{2\gamma m p}\left\langle\hat{\pi}_\perp^2\right\rangle - \frac{1}{p}\left\langle \underline{\mathbf{\Omega}}_s\cdot\mathbf{S}\right\rangle \approx \frac{p}{\gamma m}\,. \end{aligned} \tag{2.32}$$

Then, for $\mathbf{r}_\perp$ we get

$$\frac{d}{dz}\langle\mathbf{r}_\perp\rangle \approx -\frac{\mathrm{i}}{\hbar}\left\langle\left[\mathbf{r}_\perp\,,\,H^{(A)}\right]\right\rangle(z) = \frac{1}{p}\langle\hat{\boldsymbol{\pi}}_\perp\rangle\,, \tag{2.33}$$

and hence from (2.31),

$$\frac{d}{dt}\langle \mathbf{r}_\perp \rangle \approx -\frac{\mathrm{i}}{\hbar}\frac{p}{\gamma m}\left\langle \left[\mathbf{r}_\perp \, , \, H^{(A)} \right] \right\rangle (z) = \frac{1}{\gamma m}\langle \hat{\boldsymbol{\pi}}_\perp \rangle \, , \tag{2.34}$$

identifying $\hat{\boldsymbol{\pi}}_\perp$ as the transverse kinetic momentum. From (2.33) it is clear that $\langle \mathbf{r}_\perp \rangle$ and $\langle \hat{\boldsymbol{\pi}}_\perp \rangle / p$ ($\langle \hat{\mathbf{p}}_\perp \rangle / p$ in the field-free regions) can be identified with the transverse position and slope of the classical ray corresponding to the wavepacket represented by $\rho^{(A)}$. For $\hat{\boldsymbol{\pi}}_\perp$, we have, with $\hat{\pi}_z \approx p$,

$$\begin{aligned}
\frac{d}{dz}\langle \hat{\boldsymbol{\pi}}_\perp \rangle &\approx -\frac{\mathrm{i}}{\hbar}\left\langle \left[\hat{\boldsymbol{\pi}}_\perp \, , \, H^{(A)} \right] \right\rangle - q\left\langle \frac{\partial}{\partial z}\mathbf{A}_\perp \right\rangle \\
&\approx \frac{q}{p}\left\langle \frac{1}{2}\left(\hat{\boldsymbol{\pi}} \times \mathbf{B} - \mathbf{B} \times \hat{\boldsymbol{\pi}} \right)_\perp \right\rangle - \frac{\gamma m}{p}\left\langle \boldsymbol{\nabla}_\perp \left(\underline{\boldsymbol{\Omega}}_s \cdot \mathbf{S} \right) \right\rangle \\
&= \frac{q}{p}\left\langle \frac{1}{2}\left(\hat{\boldsymbol{\pi}} \times \mathbf{B} - \mathbf{B} \times \hat{\boldsymbol{\pi}} \right)_\perp \right\rangle \\
&\qquad + \frac{1}{p}\left\langle \boldsymbol{\nabla}_\perp \left\{ (q+\epsilon) B_z S_z + (q+\gamma\epsilon) \mathbf{B}_\perp \cdot \mathbf{S}_\perp \right\} \right\rangle \, ,
\end{aligned} \tag{2.35}$$

and hence

$$\begin{aligned}
\frac{d}{dt}\langle \hat{\boldsymbol{\pi}}_\perp \rangle &= \frac{q}{\gamma m}\left\langle \frac{1}{2}\left(\hat{\boldsymbol{\pi}} \times \mathbf{B} - \mathbf{B} \times \hat{\boldsymbol{\pi}} \right)_\perp \right\rangle \\
&\qquad + \frac{1}{\gamma m}\left\langle \boldsymbol{\nabla}_\perp \left\{ (q+\epsilon) B_z S_z + (q+\gamma\epsilon) \mathbf{B}_\perp \cdot \mathbf{S}_\perp \right\} \right\rangle \, .
\end{aligned} \tag{2.36}$$

Equation (2.36) is just in accordance with the quasiclassical equation for motion under the Lorentz and Stern-Gerlach forces up to the approximations considered. In the case of spin

$$\frac{d}{dz}\langle \mathbf{S} \rangle \approx -\frac{\mathrm{i}}{\hbar}\left\langle \left[\mathbf{S} \, , \, H^{(A)} \right] \right\rangle = -\frac{\mathrm{i}}{\hbar}\frac{\gamma m}{p}\left\langle \left[\mathbf{S} \, , \, \underline{\boldsymbol{\Omega}}_s \cdot \mathbf{S} \right] \right\rangle = \frac{\gamma m}{p}\left\langle \underline{\boldsymbol{\Omega}}_s \times \mathbf{S} \right\rangle \, , \tag{2.37}$$

and thus,

$$\frac{d}{dt}\langle \mathbf{S} \rangle \approx -\frac{\mathrm{i}}{\hbar}\frac{p}{\gamma m}\left\langle \left[\mathbf{S} \, , \, H^{(A)} \right] \right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle \left[\mathbf{S} \, , \, \underline{\boldsymbol{\Omega}}_s \cdot \mathbf{S} \right] \right\rangle = \left\langle \underline{\boldsymbol{\Omega}}_s \times \mathbf{S} \right\rangle \, , \tag{2.38}$$

as should be expected from the Thomas-BMT equation, of course up to the approximation we are concerned with. The vector $\mathbf{P}$ characterizing the polarization of the beam is given by the relation

$$\langle \mathbf{S} \rangle = \frac{\hbar}{2} \langle \boldsymbol{\sigma} \rangle = \frac{\hbar}{2} \mathbf{P} . \tag{2.39}$$

To obtain the required maps for transfer of the averages $(\langle \mathbf{r}_\perp \rangle, \langle \hat{\boldsymbol{\pi}}_\perp \rangle, \langle \mathbf{S} \rangle)$ across an optical element we can employ the quantum mechanical version[24] of the technique developed by Dragt *et al.* (see [32,33] and references therein) in the context of classical accelerator optics. We shall explain this in the next section through the example of a normal quadrupolar magnetic lens. Though we have taken $\langle \hat{\pi}_z \rangle \approx p$ in the above preliminary analysis, following (2.32), to understand the small variations in the longitudinal kinetic momentum, including the Stern-Gerlach kicks[30], a more careful analysis of the evolution of $\langle \hat{\pi}_z \rangle (z)$ along the z-axis is needed. We shall discuss this in the next section by examining the case of a general inhomogeneous magnetic field.

Before closing this section let us note that the Pauli-like two-component spinor formalism developed above is valid for all p, from the nonrelativistic to the extreme relativistic case; it becomes Pauli's two-component formalism in the nonrelativistic case when we can take $p \approx \sqrt{2m(E - mc^2)}$.

3 TRANSFER MAPS FOR PHASE-SPACE AND SPIN

First, let us consider an ideal normal magnetic quadrupole lens field given by

$$\mathbf{B} = (-Gy, -Gx, 0), \tag{3.1}$$

associated with the vector potential

$$\mathbf{A} = \left(0, 0, \frac{1}{2} G \left(x^2 - y^2\right)\right) , \tag{3.2}$$

where G is assumed to be a constant in the lens region and zero outside. Let the z-coordinates of the xy-planes at the entrance and exit of the quadrupole magnet of length ℓ be z_{n} and z_{x} (the subscripts 'n' and 'x' denoting e'n'trance and e'x'it, respectively, and $\ell = z_{\mathrm{x}} - z_{\mathrm{n}}$). Throughout the present section we shall be working with the accelerator optical representation and shall omit the superscript (A).

Now, the basic accelerator optical Hamiltonian of the system is

$$H(z) = \begin{cases} H_F = -p + \frac{1}{2p}\hat{p}_\perp^2 , & \text{for } z < z_\mathrm{n} \text{ and } z > z_\mathrm{x} , \\ H_L(z) = -p + \frac{1}{2p}\hat{p}_\perp^2 - \frac{1}{2}qG\left(x^2 - y^2\right) + \frac{\eta p}{\ell}\left(y\sigma_x + x\sigma_y\right) , \\ \qquad \text{for } z_\mathrm{n} \leq z \leq z_\mathrm{x} , \\ \qquad \text{with } \eta = (q + \gamma\epsilon)G\ell\hbar/2p^2 . \end{cases} \tag{3.3}$$

The subscripts F and L indicate, respectively, the field-free and the lens regions. Let us write H as a core part $\bar{H}$ plus a perturbation part $\tilde{H}$:

$$H(z) = \bar{H}(z) + \tilde{H}(z) ,$$

$$\bar{H}(z) = \begin{cases} \bar{H}_F \equiv H_F , & \text{for } z < z_\mathrm{n} \text{ and } z > z_\mathrm{x} , \\ \bar{H}_L(z) = -p + \frac{1}{2p}\hat{p}_\perp^2 - \frac{1}{2}qG\left(x^2 - y^2\right) , & \text{for } z_\mathrm{n} \leq z \leq z_\mathrm{x} . \end{cases}$$

$$\tilde{H}(z) = \begin{cases} \tilde{H}_F = 0 , & \text{for } z < z_\mathrm{n} \text{ and } z > z_\mathrm{x} , \\ \tilde{H}_L(z) = \frac{\eta p}{\ell}\left(y\sigma_x + x\sigma_y\right) , & \text{for } z_\mathrm{n} \leq z \leq z_\mathrm{x} . \end{cases} \tag{3.4}$$

A formal integration of the basic z-evolution equation (2.25) for ρ leads, in general, to

$$\rho(z) = U(z, z_0)\,\rho(z_0)U^\dagger(z, z_0) , \quad z \geq z_0 , \tag{3.5}$$

with the unitary z-propagator U given by

$$U(z, z_0) = \wp\left[\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{z_0}^{z} d\zeta\, H(\zeta)\right\}\right] , \tag{3.6}$$

where $\wp$ indicates the path-ordering of the exponential. Further, U is such that

$$\mathrm{i}\,\hbar\frac{\partial}{\partial z}U(z, z_0) = H(z)U(z, z_0) , \quad U(z_0, z_0) = I , \tag{3.7}$$

where I is the identity operator and for any set of points $\{z_1, z_2, \cdots, z_j\}$ in the interval $[z_0, z]$ with $z > z_j > z_{j-1} > \cdots > z_2 > z_1 > z_0$,

$$U(z, z_0) = U(z, z_j)U(z_j, z_{j-1})\cdots U(z_2, z_1)U(z_1, z_0) . \tag{3.8}$$

A convenient expression for U is given by the Magnus formula[34]: for any $z'' \geq z'$,

$$
\begin{aligned}
U(z'', z') = \exp \Bigg\{ & -\frac{i}{\hbar} \int_{z'}^{z''} d\zeta \, H(\zeta) \\
& + \frac{1}{2} \left(-\frac{i}{\hbar}\right)^2 \int_{z'}^{z''} d\zeta_2 \int_{z'}^{\zeta_2} d\zeta_1 \, [H(\zeta_2), H(\zeta_1)] \\
& + \frac{1}{6} \left(-\frac{i}{\hbar}\right)^3 \int_{z'}^{z''} d\zeta_3 \int_{z'}^{\zeta_3} d\zeta_2 \int_{z'}^{\zeta_2} d\zeta_1 \, \{[[H(\zeta_3), H(\zeta_2)], H(\zeta_1)] \\
& + [[H(\zeta_1), H(\zeta_2)], H(\zeta_3)]\} \cdots \Bigg\} . \qquad (3.9)
\end{aligned}
$$

Let us now compute $\rho(z)$ *via* an interaction picture, adapting the approach developed by Dragt *et al.* in the context of classical accelerator optics (see [32,33]). Defining

$$
\bar{U}\,(z, z_0) = \wp \left[\exp \left\{ -\frac{i}{\hbar} \int_{z_0}^{z} d\zeta \, \bar{H}(\zeta) \right\} \right] , \qquad (3.10)
$$

we have

$$
i\,\hbar \frac{\partial}{\partial z} \rho_i = [\tilde{H}_i \, , \, \rho_i] \, , \qquad \tilde{H}_i = \bar{U}^\dagger \, (z, z_0) \, \tilde{H} \bar{U} \, (z, z_0) \; . \qquad (3.11)
$$

Then, since $\rho_i(z_0) = \rho(z_0)$,

$$
\begin{aligned}
\rho_i(z) &= \tilde{U}_i \, (z, z_0) \, \rho_i(z_0) \tilde{U}_i^\dagger \, (z, z_0) = \tilde{U}_i \, (z, z_0) \, \rho(z_0) \tilde{U}_i^\dagger \, (z, z_0) \, , \\
\tilde{U}_i \, (z, z_0) &= \wp \left[\exp \left\{ -\frac{i}{\hbar} \int_{z_0}^{z} d\zeta \, \tilde{H}_i(\zeta) \right\} \right] . \qquad (3.12)
\end{aligned}
$$

Now, from (3.10) and (3.12), we see that

$$\rho(z) = \bar{U}\,(z, z_0)\,\tilde{U}_i\,(z, z_0)\,\rho(z_0)\tilde{U}_i^\dagger\,(z, z_0)\,\bar{U}^\dagger\,(z, z_0)\ . \tag{3.13}$$

Hence, for the average of any observable O we have

$$\begin{aligned}\left\langle\hat{O}\right\rangle(z) &= \operatorname{Tr}\left\langle\rho(z)\hat{O}\right\rangle \qquad (3.14)\\ &= \operatorname{Tr}\left\langle\bar{U}\,(z, z_0)\,\tilde{U}_i\,(z, z_0)\,\rho(z_0)\tilde{U}_i^\dagger\,(z, z_0)\,\bar{U}^\dagger\,(z, z_0)\,\hat{O}\right\rangle\\ &= \operatorname{Tr}\left\langle\rho(z_0)\left\{\tilde{U}_i^\dagger\,(z, z_0)\,\bar{U}^\dagger\,(z, z_0)\,\hat{O}\bar{U}\,(z, z_0)\,\tilde{U}_i\,(z, z_0)\right\}\right\rangle .\end{aligned}$$

This equation (3.14) provides the general basic formula to compute the transfer map for $\left\langle\hat{O}\right\rangle$ across the system as will be seen below in the case of the present example.

Let us take z_0 and z to be respectively in the field-free input and output regions of the quadrupole magnet : $z_0 < z_{\mathrm{n}}$, $z > z_{\mathrm{x}}$. Using (3.8) and (3.9), and after some straightforward algebra we get

$$\begin{aligned}&\bar{U}\,(z, z_0) = \bar{U}_F(z, z_{\mathrm{x}})\bar{U}_L(z_{\mathrm{x}}, z_{\mathrm{n}})\bar{U}_F(z_{\mathrm{n}}, z_0)\,,\\ &\tilde{U}_i\,(z, z_0) = \tilde{U}_{i,F}(z, z_{\mathrm{x}})\tilde{U}_{i,L}(z_{\mathrm{x}}, z_{\mathrm{n}})\tilde{U}_{i,F}(z_{\mathrm{n}}, z_0) \equiv \tilde{U}_{i,L}(z_{\mathrm{x}}, z_{\mathrm{n}})\,,\\ &\bar{U}_F(z, z_{\mathrm{x}}) = \exp\left\{\frac{\mathrm{i}}{\hbar}\Delta z_>\left(p - \frac{1}{2p}\hat{p}_\perp^2\right)\right\}\,, \qquad \text{with} \ \ \Delta z_> = z - z_{\mathrm{x}}\,,\\ &\bar{U}_L(z_{\mathrm{x}}, z_{\mathrm{n}}) = \exp\left\{\frac{\mathrm{i}}{\hbar}\ell\left[\left(p - \frac{1}{2p}\hat{p}_\perp^2\right) + \frac{1}{2}pK(x^2 - y^2)\right]\right\}\,,\\ &\qquad\qquad\qquad \text{with} \ \ K = qG/p\,,\\ &\bar{U}_F(z_{\mathrm{n}}, z_0) = \exp\left\{\frac{\mathrm{i}}{\hbar}\Delta z_<\left(p - \frac{1}{2p}\hat{p}_\perp^2\right)\right\}\,, \qquad \text{with} \ \ \Delta z_< = z_{\mathrm{n}} - z_0\,,\end{aligned}$$

$$\tilde{U}_{i,L}(z_{\mathrm{x}}, z_{\mathrm{n}})$$

$$= \exp\left\{ -\frac{\mathrm{i}}{\hbar}\eta \left[\left(\left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) px + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K\ell} \right) \hat{p}_x \right) \sigma_y \right.\right.$$

$$\left.\left. + \left(\left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) py - \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K\ell} \right) \hat{p}_y \right) \sigma_x \right] \right\}. \tag{3.15}$$

Now, using (3.14) and (3.15) the transfer maps for $\langle \mathbf{r}_\perp \rangle$ and $\langle \hat{\mathbf{p}}_\perp \rangle$ ($\equiv \langle \hat{\boldsymbol{\pi}}_\perp \rangle$ in this case) are obtained as follows : with $\lambda = h/p$, the de Broglie wavelength,

$$\begin{pmatrix} \langle x \rangle (z) \\ \langle \hat{p}_x \rangle (z)/p \\ \langle y \rangle (z) \\ \langle \hat{p}_y \rangle (z)/p \end{pmatrix} \approx \begin{pmatrix} T_{11}^x & T_{12}^x & 0 & 0 \\ T_{21}^x & T_{22}^x & 0 & 0 \\ 0 & 0 & T_{11}^y & T_{12}^y \\ 0 & 0 & T_{21}^y & T_{22}^y \end{pmatrix} \left(\begin{pmatrix} \langle x \rangle (z_0) \\ \langle \hat{p}_x \rangle (z_0)/p \\ \langle y \rangle (z_0) \\ \langle \hat{p}_y \rangle (z_0)/p \end{pmatrix} \right.$$

$$\left. + \eta \begin{pmatrix} \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K\ell} \right) \langle \sigma_y \rangle (z_0) \\ - \left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle \sigma_y \rangle (z_0) \\ - \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K\ell} \right) \langle \sigma_x \rangle (z_0) \\ - \left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle \sigma_x \rangle (z_0) \end{pmatrix} \right),$$

$$\begin{pmatrix} T^x_{11} & T^x_{12} \\ T^x_{21} & T^x_{22} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \Delta z_> \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cosh\left(\sqrt{K}\,\ell\right) & \frac{1}{\sqrt{K}} \sinh\left(\sqrt{K}\,\ell\right) \\ \sqrt{K}\, \sinh\left(\sqrt{K}\,\ell\right) & \cosh\left(\sqrt{K}\,\ell\right) \end{pmatrix} \begin{pmatrix} 1 & \Delta z_< \\ 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} T^y_{11} & T^y_{12} \\ T^y_{21} & T^y_{22} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \Delta z_> \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\left(\sqrt{K}\,\ell\right) & \frac{1}{\sqrt{K}} \sin\left(\sqrt{K}\,\ell\right) \\ -\sqrt{K}\, \sin\left(\sqrt{K}\,\ell\right) & \cos\left(\sqrt{K}\,\ell\right) \end{pmatrix} \begin{pmatrix} 1 & \Delta z_< \\ 0 & 1 \end{pmatrix},$$

$$\langle S_x \rangle (z) \approx \langle S_x \rangle (z_0) + \frac{4\pi\eta}{\lambda} \left(\left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle x S_z \rangle (z_0) + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K \ell p} \right) \left\langle \hat{p}_x S_z \right\rangle (z_0) \right),$$

$$\left\langle S_y \right\rangle (z) \approx \left\langle S_y \right\rangle (z_0) - \frac{4\pi\eta}{\lambda} \left(\left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle y S_z \rangle (z_0) - \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K \ell p} \right) \left\langle \hat{p}_y S_z \right\rangle (z_0) \right),$$

$$\begin{aligned}
\langle S_z \rangle (z) \approx \langle S_z \rangle (z_0) - & \\
& \frac{4\pi\eta}{\lambda} \left\{ \left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle x S_x \rangle (z_0) \right. \\
& - \left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \left\langle y S_y \right\rangle (z_0) \\
& + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K\ell p} \right) \left\langle \hat{p}_x S_x \right\rangle (z_0) \\
& \left. + \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K\ell p} \right) \left\langle \hat{p}_y S_y \right\rangle (z_0) \right\} . \qquad (3.16)
\end{aligned}$$

So, we have got a fully quantum mechanical derivation of the traditional transfer map for the transverse phase-space, including the Stern-Gerlach effect (see [11]), in the case of a spin-$\frac{1}{2}$ particle beam propagating through a normal magnetic quadrupole lens : the lens is focusing (defocusing) in the yz-plane and defocusing (focusing) in the xz-plane when $K > 0\,(K < 0)$. The transverse Stern-Gerlach kicks to the trajectory slope $\left(\delta \langle \hat{\mathbf{p}}_\perp \rangle / p \sim \eta\right)$ are seen to disappear at relativistic energies, varying like $\sim 1/\gamma$. At nonrelativistic energies, with $\gamma \approx 1$, the kicks are $\sim G\ell\mu/mv^2$ where μ is the total magnetic moment. These results are in general agreement with the conclusions reached earlier[11,30] based on semiclassical treatments. The spin map obtained above is seen to contain the paraxial Thomas-BMT map including the lowest order terms depending on $\mathbf{p}_\perp/p$. It should be also noted that the polarization transfer map is linear in the polarization components only when there is no spin-space correlation, i.e., for the classical behaviour to result one should have $\langle x S_z \rangle = \langle x \rangle \langle S_z \rangle$, $\langle y S_z \rangle = \langle y \rangle \langle S_z \rangle$, $\langle p_x S_z \rangle = \langle p_x \rangle \langle S_z \rangle$, etc..

Using the general theory, let us now understand the longitudinal Stern-Gerlach kicks[30] in a general inhomogeneous magnetic field. For $\hat{\pi}_z = -(H^{(A)} + qA_z)$ we get, from (2.30),

$$
\begin{aligned}
\frac{d}{dz}\langle\hat{\pi}_z\rangle &= \left\{\frac{\mathrm{i}}{\hbar}\left\langle\left[H^{(A)}+qA_z\,,\,H^{(A)}\right]\right\rangle - \left\langle\frac{\partial}{\partial z}\left(H^{(A)}+qA_z\right)\right\rangle\right\} \\
&= \left\langle\frac{\mathrm{i}}{\hbar}\left[qA_z\,,\,H^{(A)}\right] - \frac{1}{2p}\frac{\partial}{\partial z}\hat{\pi}_\perp^2\right\rangle - \frac{\gamma m}{p}\left\langle\frac{\partial}{\partial z}\left(\underline{\boldsymbol{\Omega}}_s\cdot\mathbf{S}\right)\right\rangle \\
&= \frac{q}{p}\left\langle\frac{1}{2}\left(\hat{\boldsymbol{\pi}}\times\mathbf{B}-\mathbf{B}\times\hat{\boldsymbol{\pi}}\right)_z\right\rangle - \frac{\gamma m}{p}\left\langle\frac{\partial}{\partial z}\left(\underline{\boldsymbol{\Omega}}_s\cdot\mathbf{S}\right)\right\rangle \\
&= \frac{q}{p}\left\langle\frac{1}{2}\left(\hat{\boldsymbol{\pi}}\times\mathbf{B}-\mathbf{B}\times\hat{\boldsymbol{\pi}}\right)_z\right\rangle \\
&\qquad + \frac{1}{p}\left\langle\frac{\partial}{\partial z}\left\{(q+\epsilon)B_zS_z+(q+\gamma\epsilon)\mathbf{B}_\perp\cdot\mathbf{S}_\perp\right\}\right\rangle .
\end{aligned}
\tag{3.17}
$$

The first term of the r.h.s. of (3.17) corresponds to the Lorentz force and the rest of it corresponds to the Stern-Gerlach force due to the longitudinal gradient of the field (*i.e.*, gradient in the z-direction). This is easily recognized by multiplying both sides of (3.17) by $v_z \approx p/\gamma m$ and comparing the resulting equation for $\frac{d}{dt}\langle\hat{\pi}_z\rangle$ with the classical equation of motion for π_z as is done in the case of $\hat{\boldsymbol{\pi}}_\perp$ in (2.36). Collecting together (2.35) and (3.17) we get for the z-evolution of $\langle\hat{\boldsymbol{\pi}}\rangle$

$$
\begin{aligned}
\frac{d}{dz}\langle\hat{\boldsymbol{\pi}}\rangle &\approx \frac{q}{p}\left\langle\frac{1}{2}\left(\hat{\boldsymbol{\pi}}\times\mathbf{B}-\mathbf{B}\times\hat{\boldsymbol{\pi}}\right)\right\rangle \\
&\qquad + \frac{1}{p}\left\langle\boldsymbol{\nabla}\left\{(q+\epsilon)B_zS_z+(q+\gamma\epsilon)\mathbf{B}_\perp\cdot\mathbf{S}_\perp\right\}\right\rangle .
\end{aligned}
\tag{3.18}
$$

For any given field configuration $\mathbf{B}$, with a specified $\mathbf{A}$, the solution of this equation (3.18) is given by

$$
\langle\hat{\boldsymbol{\pi}}\rangle(z) = \mathrm{Tr}\left\langle\rho(z_0)U^\dagger(z,z_0)\hat{\boldsymbol{\pi}}U(z,z_0)\right\rangle , \quad \text{for any } z > z_0 , \tag{3.19}
$$

and hence the spin-dependent Stern-Gerlach kick to the kinetic momentum and the resultant spin-dependent splitting of the kinetic energy at any $z > z_0$ can be calculated.

Multiplying both sides of (3.18) by $v_z \approx p/\gamma m$, it follows that

$$\begin{aligned}\frac{d}{dt}\langle\hat{\boldsymbol{\pi}}\rangle &\approx \frac{q}{\gamma m}\left\langle\frac{1}{2}\left(\hat{\boldsymbol{\pi}} \times \mathbf{B} - \mathbf{B} \times \hat{\boldsymbol{\pi}}\right)\right\rangle \\ &\qquad + \frac{1}{\gamma m}\left\langle\boldsymbol{\nabla}\left\{q\mathbf{B}\cdot\mathbf{S} + \epsilon\left(B_z S_z + \gamma \mathbf{B}_\perp \cdot \mathbf{S}_\perp\right)\right\}\right\rangle \\ &= \frac{q}{\gamma m}\left\langle\frac{1}{2}\left(\hat{\boldsymbol{\pi}} \times \mathbf{B} - \mathbf{B} \times \hat{\boldsymbol{\pi}}\right)\right\rangle - \left\langle\boldsymbol{\nabla}\left(\underline{\boldsymbol{\Omega}}_s \cdot \mathbf{S}\right)\right\rangle , \end{aligned} \tag{3.20}$$

in which the first term represents the Lorentz force and the second term represents the Stern-Gerlach force. This equation (3.20) for orbital motion of a Dirac particle moving predominantly along the z-direction is seen to account, under the paraxial approximation, for both the Lorentz and the Stern-Gerlach forces. It may be noted that our formalism facilitates the computation of the transfer maps for the beam observables over any interval (z_0, z) along the axis by the use of direct z-evolution formulae, like in (3.19), and we are considering the time evolution equations such as (3.20) only for the sake of comparison with the classical equations of motion. In the instantaneous rest frame of the particle with $\gamma = 1$ the second term in (3.20) is seen to correspond to the familiar Stern-Gerlach force

$$\mathbf{F}_{SG} = -\boldsymbol{\nabla} U\,, \quad U = -\mu\boldsymbol{\sigma}\cdot\mathbf{B}\,, \tag{3.21}$$

where μ is the total magnetic moment of the particle; note that in (3.21), apart from the spin, the field components, the coordinates, etc., are also defined in the rest frame of the particle.

It is of interest to know the relative merits and demerits of spin-splitter devices employing the transverse and longitudinal Stern-Gerlach kicks. When the fields **B** in such devices are known explicitly one can directly use the formula (3.19) for such a study. But, to have an idea of the situation in a general context, one can use the standard classical relativistic dynamics[35,36] starting with the form of the Stern-Gerlach force (3.21) which has been understood on the basis of the Dirac equation; the result has to agree with the classical limit of the quantum mechanical computation. Such a study[30] based on classical relativistic dynamics seems to suggest that, at high energies, devices employing the longitudinal kick are more favourable than those employing the transverse kick. To be more precise, with G_z denoting the longitudinal magnetic gradient $\frac{\partial B_z}{\partial z}$ active over a region of length L in a device employing the longitudinal kick, the fractional increase in the longitudinal momentum, $\delta p_z/p$, turns out to be $G_z\mu L/mv^2$, which becomes almost independent of energy as γ increases (see [30] for details of the calculation). In the case of a device employing the transverse kick, the fractional increase in the transverse momentum varies like $\sim 1/\gamma$ and thus decreases as γ increases, as we have seen above in the example of the quadrupolar magnetic field (see [30] for details of the calculation based on classical relativistic dynamics). Thus, one can conclude generally that at high energies a spin splitter with longitudinal kick should be more favourable than one with transverse kick, leaving aside all technical details such as the practical realization of the required longitudinal magnetic gradient and the way of exploiting the attained spin-dependent energy spread. At lower energies, the kicks are larger in both the cases.

4 CONCLUSION

In summary, we have demonstrated how one can obtain a fully quantum mechanical understanding of the accelerator beam optics for a spin-$\frac{1}{2}$ particle, with anomalous magnetic moment, starting *ab initio* from the Dirac-Pauli equation. To this end, we have used a beam optical representation of the Dirac theory, following[21–24], and have shown that such an approach, in the lowest order approximation, leads naturally to a picture of orbital and spin dynamics based on the Lorentz force, the Stern-Gerlach force and the Thomas-BMT equation for spin evolution, as is to be expected. Only the lowest order (paraxial) approximation has been considered in detail. To illustrate the general theory we have considered the computation of the transfer maps for the spin components and the transverse phase-space, including the transverse Stern-Gerlach kicks, in the case of a normal magnetic quadrupole lens, and a brief understanding of the longitudinal Stern-Gerlach kicks in a general inhomogeneous magnetic field. It is found that the above theory supports the spin-splitter concepts based on transverse and longitudinal Stern-Gerlach kicks.[9–15,30] It is clear from the general theory, presented briefly here, that the approach is suitable to handle any magnetic optical element with straight axis and computations can be carried out to any order of accuracy desired by easily extending the order of approximation. In fact, even the lowest order approximation reveals the nature of deviations from the classical behaviour for spin evolution, namely, the dependence on differences $\langle xS_z\rangle - \langle x\rangle\langle S_z\rangle$, $\langle yS_z\rangle - \langle y\rangle\langle S_z\rangle$, $\langle p_xS_z\rangle - \langle p_x\rangle\langle S_z\rangle$, etc..

In this paper, we have restricted ourselves to the treatment of propagation of a monoenergetic paraxial beam through a single optical block with a static magnetic field and straight axis. Thus, it is obvious that there are several open problems related to the issues concerning the extension of the present formalism to more complicated situations. Leaving aside the problems of including the effects of multiparticle dynamics, quantum nature of the electromagnetic field, interaction with radiation, etc., for the present, the immediate concern should be about the extension of the formalism taking into account the chromatic effects, curvature of the optic axis, global analysis of systems like storage rings, and time dependence of fields.

When the beam entering the time-independent system from the field-free input region is not monochromatic, as is in general, the wavefunction of the beam propagating through the system in the $+z$-direction can be written, in the Dirac representation, as

$$\Psi_D(\mathbf{r}, t) = \int_{p_0-\frac{1}{2}\Delta p}^{p_0+\frac{1}{2}\Delta p} dp\, \psi_D(\mathbf{r}; p) \exp\left(-\,\mathrm{i}\, E(p)t/\hbar\right) , \quad \Delta p \ll p_0 , \tag{4.1}$$

where p_0 is the design momentum and

$$\psi_D(\mathbf{r}_\perp, z < z_{\mathrm{n}}\, ; p) = \frac{1}{(2\pi\hbar)^{3/2}} \int\!\!\int dp_x\, dp_y\, \psi_{FD}(\mathbf{r}_\perp, z; \mathbf{p}) , \qquad |\mathbf{p}_\perp| \ll p , \tag{4.2}$$

with $\psi_{FD}(\mathbf{r}_\perp, z; p)$ obtained from (2.13) by replacing the constants (s_+, s_-) by the functions $(s_+(\mathbf{p}), s_-(\mathbf{p}))$. Now, the z-evolution of each Fourier component $(\psi_D(\mathbf{r}; p))$ of $\Psi_D(\mathbf{r}, t)$ will have to be traced according the above formalism for monochromatic beam and the results will have to be integrated to get the z-evolution of the time dependent $\Psi_D(\mathbf{r}, t)$; generalization is straightforward in the case of description using density matrices. Using such a procedure it should be possible to account for the chromatic effects of static optical elements. First, one should be able to derive in this way the well known classical results on chromatic effects (see, *e.g.*,[1] and references therein) in the lowest order approximation. Note that in the monoenergetic case, with $\Delta p = 0$, the phase factor $\exp\left(-\,\mathrm{i}\, E(p_0)t/\hbar\right)$ drops out of the formalism making time simply a spectator.

To take into account the curvature of the system axis one should work with the Dirac equation written in the suitable curvilinear coordinate system adapted to the geometry of the design orbit. Some preliminary work in this direction is available in [22].

Analysis of global systems, like storage rings, should be possible by learning to patch together the quantum transfer maps for individual, or local, optical blocks to produce the quantum one-turn map (see [33] and references therein for help from classical beam dynamics).

Finally, the question of time-dependent fields: The present formalism can lead only to a relationship among the wavefunctions at transverse planes situated along the design orbit guided by static fields. To take into account time-dependent effects, radiation, etc., one will have to use only the traditional quantum dynamical time evolution equation. The present formalism is mainly intended to study effectively the static optical characteristics of the system. We believe that a hybrid approach to beam dynamics obtained by integrating the present formalism, suited for static characteristics of beam optics, with the traditional methods of quantum dynamics for studying the time-dependent aspects should be profitable.

We hope to return to these various problems elsewhere.

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