QUANTUM MECHANICS OF DIRAC PARTICLE BEAM TRANSPORT THROUGH OPTICAL ELEMENTS WITH STRAIGHT AND CURVED AXES†

R. JAGANATHAN‡

The Institute of Mathematical Sciences,
4th Cross Road, Central Institutes of Technology Campus, Tharamani
Chennai, TN 600113, INDIA

Abstract

Classical mechanical treatment of charged particle beam optics is so far very satisfactory from a practical point of view in applications ranging from electron microscopy to accelerator technology. However, it is desirable to understand the underlying quantum mechanics since the classical treatment is only an approximation. Quantum mechanical treatment of spin-\(\frac{1}{2}\) particle beam transport through optical elements with straight optic axes, based on the proper equation, namely, the Dirac equation, has been developed already to some extent. In such a theory the orbital and spin motions are treated within a unified framework. Here, after a brief review of the Dirac spinor beam optics for systems with straight optic axes it is outlined how the application of the formalism of general relativity leads to the use of the Dirac equation for getting a quantum theory of spin-\(\frac{1}{2}\) beam transport through optical elements with curved axes.

1. Introduction

It is surprising that the development of a quantum theory of electron beam optics based on the proper equation, namely, the Dirac equation, has only a recent origin [1 2 3]. The theory of charged particle beam optics, currently used in the design and operation of various beam devices, in electron

†To appear in the Proceedings of the Joint 28th ICFA Advanced Beam Dynamics and Advanced & Novel Accelerators Workshop on QUANTUM ASPECTS OF BEAM PHYSICS and Other Critical Issues of Beams in Physics and Astrophysics, January 7-11, 2003, Hiroshima University, Higashi-Hiroshima, Japan, Ed. Pisin Chen (World Scientific, Singapore)

‡E-mail: jagan@imsc.res.in
microscopes or accelerators, is largely based on classical mechanics and classical electrodynamics. Such a treatment has indeed been very successful in practice. Of course, whenever it is essential, quantum mechanics is used in accelerator physics to understand those quantum effects which are prominent perturbations to the leading classical beam dynamics [4]. The well-known examples are quantum excitations induced by synchrotron radiation in storage rings, the Sokolov-Ternov effect of spin polarization induced by synchrotron radiation, etc. Recently, attention has been drawn to the limits placed by quantum mechanics on achievable beam spot sizes in particle accelerators, and the need for the formulation of quantum beam optics relevant to such issues [5]. In the context of electron microscopy scalar wave mechanics based on the nonrelativistic Schrödinger equation has been the main tool to analyze the image formation and its characteristics, and the spin aspects are not considered at all [3].

In the context of accelerator physics it should be certainly desirable to have a unified framework based entirely on quantum mechanics to treat the orbital, spin, radiation, and every aspect of beam dynamics, since the constituents of the beams concerned are quantum particles. First, this should help us understand better the classical theory of beam dynamics. Secondly, there is already an indication that this is necessary too: it has been found that quantum corrections can substantially affect the classical results of tracking for trajectories close to the separatrix, leading to the suggestion that quantum maps can be useful in finding quickly the boundaries of nonlinear resonances [6]. Thus, a systematic formalism for obtaining the relevant quantum maps is required.

The aim of this article is present a brief summary of the formalism quantum beam optics of particles, in particular, Dirac particles, for treating problems of propagation through optical elements with straight and curved axes.

2. Quantum Beam Optics of Particles: An Outline

One may consider obtaining the relevant quantum maps for any particle optical system by quantizing the corresponding classical treatment directly. The best way to do this is to use the Lie algebraic formalism of classical beam dynamics developed particularly in the context of accelerator physics [7]. The question that arises is how to go beyond and obtain the quantum maps more completely starting \textit{ab initio} with the quantum mechanics of the concerned system since such a process should lead to other quantum corrections not
derivable simply from the quantization of the classical optical Hamiltonian. Essentially, one should obtain a quantum beam optical Hamiltonian $\hat{H}$ directly from the original time-dependent Schrödinger equation of the system such that the quantum beam optical Schrödinger equation

$$i\hbar \frac{\partial}{\partial z} \psi(r_{\perp}; z) = \hat{H} \psi(r_{\perp}; z)$$

(1)

describes the $z$-evolution of the beam wave function $\psi(r_{\perp}; z)$ where $z$ stands for the coordinate along the optics axis and $r_{\perp}$ refers to $(x, y)$ coordinates in the plane perpendicular to the beam at $z$. Since $|\psi(r_{\perp}; z)|^2$ represents the probability density in the transverse plane at $z$, with

$$\int \int dx dy |\psi(r_{\perp}; z)|^2 = 1,$$

(2)

the average of any observable $\hat{O}$ at $z$ is

$$\langle \hat{O}(z) \rangle = \langle \psi(z)|\hat{O}|\psi(z)\rangle = \int \int dx dy \psi^*(z)\hat{O}\psi(z).$$

(3)

We can write the formal solution of Eq. (1) as

$$|\psi(z_f)\rangle = \hat{U}_{fi}|\psi(z_i)\rangle,$$

$$\hat{U}_{fi} = \varphi \left\{ \exp \left( -\frac{i}{\hbar} \int_{z_i}^{z_f} dz \hat{H}(z) \right) \right\},$$

(4)

where $i$ and $f$ refer to some initial and final transverse planes situated at $z_i$ and $z_f$, respectively, along the beam axis and $\varphi$ indicates the path (or $z$) ordering of the exponential. Then, the required quantum maps are given by

$$\langle \hat{O}\rangle_f = \langle \psi(z_f)|\hat{O}|\psi(z_f)\rangle = \langle \psi(z_i)|\hat{U}_{fi}^\dagger\hat{O}\hat{U}_{fi}|\psi(z_i)\rangle = \langle \hat{U}_{fi}^\dagger\hat{O}\hat{U}_{fi}\rangle_i.$$ (5)

As an example of the above formalism let us consider a kick in the $xz$-plane by a thin sextupole represented by the classical phase-space map

$$x_f = x_i,$$

$$p_f = p_i + ax_i^2.$$ (6)
This would correspond to $\hat{U}_{fi} = \exp(\frac{2\pi i}{\hbar} \hat{x}^3)$ and following Eq. (5) the quantum maps for the averages become

$$
\langle \hat{x} \rangle_f = \langle \hat{x} \rangle_i, \\
\langle \hat{p} \rangle_f = \langle \hat{p} \rangle_i + a\langle \hat{x}^2 \rangle_i \\
= \langle \hat{p} \rangle_i + a\langle \hat{x} \rangle_i^2 + a\langle (\hat{x} - \langle \hat{x} \rangle)^2 \rangle_i.
$$

(7)

Now, we can consider the expectation values, such as $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$, as corresponding to their classical values à la Ehrenfest. Then, as the above simple example shows, generally, the leading quantum effects on the classical beam optics can be expected to be due to the uncertainties in the initial conditions like the term $a\langle (\hat{x} - \langle \hat{x} \rangle)^2 \rangle_i$ in Eq. (7). Such leading quantum corrections involve the Planck constant $\hbar$ not explicitly but only through the uncertainty principle which controls the minimum limits for the initial conditions as has been already pointed out [6]. This has been realized earlier also, particularly in the context of electron microscopy [8].

The above theory is only a single-particle theory. To include the multiparticle effects, it might be profitable to be guided by models such as the thermal wave model and the stochastic collective dynamical model developed for treating the beam phenomenologically as a quasiclassical many-body system [9, 10].

3. Quantum Beam Optics of Dirac Particles: Optical Elements with Straight Axes

The proper study of spin-$\frac{1}{2}$ particle beam transport should be based on the Dirac equation if one wants to treat all the aspects of beam optics including spin evolution and spin-orbit interaction. Let us consider the particle to have mass $m$, electric charge $q$ and an anomalous magnetic moment $\mu_a$. It should be noted that the electromagnetic fields of the optical systems are time-independent. In this case one can start with the time-independent equation for the 4-component Dirac spinor $\psi(r_\perp; z)$

$$
\hat{H} \psi(r_\perp; z) = E \psi(r_\perp; z), \\
\hat{H} = \beta mc^2 + q\phi + c\alpha_\perp \cdot \vec{\pi}_\perp + c\alpha_z \left(-i\hbar \frac{\partial}{\partial z} - q\hat{A}_z \right) - \mu_a \beta \Sigma \cdot B.
$$

(8)
including the Pauli term to take into account the anomalous magnetic moment. Here, we are using the standard notations as is clear from the context.

Let us assume that we are interested in studying the transport of a monoenergetic quasiparaxial particle beam through an optical element which has a straight optic axis along the cartesian $z$-direction. If $p$ is the design momentum of the beam the energy of a single particle of the beam is given by $E = \sqrt{m^2c^4 + c^2p^2}$. Further, the quasiparaxial beam propagating along the $z$-direction should have $|p_\perp| \ll |p| = p$ and $p_z > 0$. Then, actually Eq. (8) has the ideal structure (compare Eq. (1)) for our purpose since it is already linear in $\frac{d}{dz}$. So, one can readily rearrange the terms in it to get the desired form of Eq. (1). However, it is difficult to work directly with such an equation since there are problems associated with the interpretation of the results using the traditional Schrödinger position operator. In the standard theory of relativistic quantum mechanics the Foldy-Wouthuysen (FW) transformation technique is used to reduce the Dirac Hamiltonian to a form suitable for direct interpretation in terms of the nonrelativistic part and a series of relativistic corrections. The FW technique was used originally by Derbenev and Kondratenko to get their Hamiltonian for radiation calculations. This theory has been reviewed and used to suggest a quantum formulation of Dirac particle beam physics, particularly for polarized beams, in terms of machine coordinates, observables, and the Wigner function [11].

In an independent and different approach an FW-like technique has been used to develop a systematic formalism of Dirac particle beam optics in which the aim has been to expand the Dirac Hamiltonian as a series of paraxial and nonparaxial approximations [1, 2, 8, 12]. This leads to the reduction of the original 4-component Dirac spinor to an effective 2-component spinor

$$
\psi^a (r_\perp; z) = \begin{pmatrix}
\psi_1^a (r_\perp; z) \\
\psi_2^a (r_\perp; z)
\end{pmatrix}
$$

which satisfies an accelerator optical Schrödinger equation

$$
i\hbar \frac{\partial}{\partial z} \psi^a (r_\perp; z) = \hat{H} \psi^a (r_\perp; z).
$$

It should be noted that the 2-component $\psi^a$ is an accelerator optical approximation of the original 4-component Dirac spinor, valid for any value of the design momentum $p$ from nonrelativistic to extreme relativistic region.
As an example, consider the ideal normal magnetic quadrupole lens comprising of the magnetic field

\[ \mathbf{B} = (-Gy, -Gx, 0), \]  

(11)

associated with the vector potential

\[ \mathbf{A} = (0, 0, \frac{1}{2}G(x^2 - y^2)), \]  

(12)

where \( G \) is assumed to be a constant in the lens region and zero outside. The corresponding quantum accelerator optical Hamiltonian reads

\[
\hat{\mathcal{H}} \approx \frac{1}{2p} \left( \hat{p}_x^2 + \hat{p}_y^2 \right) - \frac{1}{2}qG\left( \hat{x}^2 - \hat{y}^2 \right) + \frac{1}{8p^3} \left( \hat{p}_x^2 + \hat{p}_y^2 \right)^2 \\
+ \frac{q^2G^2\hbar^2}{8p^3} (x^2 + y^2) + \frac{(q + \gamma\epsilon)G}{p} (\hat{x}\hat{S}_y + \hat{y}\hat{S}_x),
\]  

(13)

where \( \gamma = E/mc^2 \), \( \epsilon = 2m\mu_a/\hbar \) and \( \hat{S} = \frac{\hbar}{2}\sigma \) represents the spin of the particle defined with reference to its instantaneous rest frame. It is to be noted that this quantum accelerator optical Hamiltonian \( \hat{\mathcal{H}} \) contains all the terms corresponding to the classical theory plus the \( \hbar \)-dependent quantum correction terms. Using the formalism outlined in the previous section it can be shown that the first two ‘classical’ paraxial terms of the above \( \hat{\mathcal{H}} \) account for the linear phase-space transfer map corresponding to the focusing (defocusing) action in the \( yz \)-plane and defocusing (focusing) action in the \( xz \)-plane when \( G > 0 \) (\( G < 0 \)). The last spin-dependent term accounts for the Stern-Gerlach kicks in the transverse phase-space and the Thomas-Bargmann-Michel-Telegdi spin evolution \([12]\).

The following interesting aspect of quantum beam optics should be mentioned. In the case of a spin-0 particle also one can derive the quantum beam optical Hamiltonian \( \hat{\mathcal{H}} \) starting from the Schrödinger-Klein-Gordon equation \([8]\). It would also contain all the terms corresponding to the classical theory plus the quantum correction terms. But, these quantum correction terms are not identical to the quantum correction terms in the Dirac case. Thus, besides in the \( \hbar \)-dependent effects of spin on the orbital quantum map (e.g., the last term in Eq. (13)), even in the spin-independent quantum corrections the Dirac particle has its own signature different from that of a spin-0 particle \([13]\).
4. Quantum Beam Optics of Dirac Particles: Optical Elements with Curved Axes

For studying the propagation of spin-$\frac{1}{2}$ particle beams through optical elements with curved axes it is natural to start with the Dirac equation written in curvilinear coordinates adapted to the geometry of the system. Let us make the $z$-axis coincide with the space curve representing the optic axis of the system, or the ideal design orbit. Let the transverse, or off-axis, coordinates $(x,y)$ at each $z$ be defined in such a way that the spatial arc element $ds$ is given by

$$ds^2 = dx^2 + dy^2 + \zeta^2 dz^2,$$

$$\zeta = (1 + K_L \cdot \kappa_L), \quad (14)$$

where $K_x(z)$ and $K_y(z)$ are the curvature components at $z$.

Now, we have to start with the Dirac equation written in a generally covariant form. To this end, let us use the formalism of general relativity \cite{2,14,15}. Here, for the sake of simplicity let us drop the anomalous magnetic moment term. Then the generally covariant form of the time-dependent Dirac equation becomes

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi,$$

$$\hat{H} = \beta mc^2 + q\phi + c\alpha_L \cdot \hat{A}_L + \frac{c}{\zeta} \alpha_z \left(-i\hbar \frac{\partial}{\partial z} - \zeta q\hat{A}_z - \Gamma_z \right), \quad (15)$$

$$\Gamma_z = K_x S_y - K_y S_x.$$ 

Further, it should be noted that

$$B_x = \frac{1}{\zeta} \left(\frac{\partial(\zeta A_z)}{\partial y} - \frac{\partial A_y}{\partial z}\right),$$

$$B_y = \frac{1}{\zeta} \left(\frac{\partial A_x}{\partial z} - \frac{\partial(\zeta A_z)}{\partial x}\right),$$

$$B_z = \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right). \quad (16)$$

For a monoenergetic beam with particle energy $E$

$$\Psi(x,t) = \psi(x; t; z) \exp(-iEt/\hbar) \quad (17)$$
and $\psi (\mathbf{r}_\perp ; z)$ satisfies the time-independent equation

$$\hat{H} \psi (\mathbf{r}_\perp ; z) = E \psi (\mathbf{r}_\perp ; z)$$

(18)

where $\hat{H}$ is the same as in Eq. (15). We should now cast Eq. (18) in the form of Eq. (1) so that the corresponding beam optical Hamiltonian $\hat{\mathcal{H}}$ can be derived and the formalism of Sec. 2 can be applied for obtaining the transfer maps for the quantum averages. It should be noted that the quantum operators for the transverse position ($\hat{\mathbf{r}}_\perp$) and momentum ($\hat{\mathbf{p}}_\perp$), and spin ($\hat{\mathbf{S}}$), are unaltered.

The method of deriving $\hat{\mathcal{H}}$ proceeds in the same way as for systems with straight optic axes: a series of FW-like transformations are to be applied to Eq. (18) up to any desired order of accuracy so that finally a 2-component equation like Eq. (10) is obtained [2]. In general, for a magnetic system we get, up to the first order, or paraxial, approximation,

$$\hat{\mathcal{H}} = -\zeta p - q \zeta \hat{A}_z + \frac{\zeta}{2p} \hat{\pi}^2_\perp.$$  

(19)

For a closed orbit in the $xz$-plane, with no torsion, writing $\zeta = 1 + \frac{2}{\rho}$, it is clear that $\hat{\mathcal{H}}$ of Eq. (19) corresponds to the well known Hamiltonian of classical accelerator optics [16]. To get a more complete form of $\hat{\mathcal{H}}$ including the spin terms and other $\hbar$-dependent quantum corrections one has to carry out the FW-like transformations to higher orders.

5. Concluding Remarks

In summary, it is seen that the quantum theory of transport of particle beams through optical elements is very simple. Starting from a beam optical Schrödinger equation the transfer maps for quantum averages of phase-space and spin variables across an optical element can be computed by a straightforward procedure. To this end, one has to obtain the appropriate quantum beam optical Hamiltonian starting from the corresponding time-dependent Schrödinger equation of the system. As example, quantum theory of propagation of Dirac particle beams through optical elements with straight and curved optic axes was considered briefly. So far, the development of such a theory has not taken into account multiparticle effects. Also, such a theory has been developed only for optical systems. Taking into account the multiparticle effects and treating accelerating elements are issues of the theory to
be tackled in future.

Acknowledgments

I am very much thankful to Prof. Pisin Chen and Prof. Atsushi Ogata for the warm hospitality. I would also like to thank our Institute, and the director Prof. R. Balasubramanian, for the financial support for travel which made my participation in this workshop possible.

References

[1] R. Jagannathan, R. Simon, E. C. G. Sudarshan and N. Mukunda, Phys. Lett. A134, 457 (1989);

[2] R. Jagannathan, Phys. Rev. A42, 6674 (1990).

[3] For an excellent survey of electron wave optics, including historical notes on the use of the Dirac equation in electron optics, see P. W. Hawkes and E. Kasper, Principles of Electron Optics - 3: Wave Optics (Academic Press, San Diego, 1994).

[4] See, e.g., the following and references therein: Handbook of Accelerator Physics and Engineering, eds. A. W. Chao and M. Tigner (World Scientific, Singapore, 1999) (Hereafter referred to as HAPE); Quantum Aspects of Beam Physics, ed. P. Chen (World Scientific, Singapore, 1999) (Hereafter referred to as QABP-I); Quantum Aspects of Beam Physics, ed. P. Chen (World Scientific, Singapore, 2002) (Hereafter referred to as QABP-II).

[5] C. T. Hill, arXiv:hep-ph/0002230, and in QABP-II; M. Venturini and R. D. Ruth, in QABP-II.

[6] S. Heifets and Y. T. Yan in QABP-I.

[7] See, e.g., the following and references therein: A. J. Dragt, in QABP-II; E. Forest, Beam Dynamics: A New Attitude and Framework (Harwood Academic, 1998); A. J. Dragt, F. Neri, G. Rangarajan, D. R. Douglas, L. M. Healy and R. D. Ryne, Ann. Rev. Nucl. Part. Sci. 38, 455 (1988); E. Forest and K. Hirata, A Contemporary Guide to Beam Dynamics,
Technical Report No. 92-12, KEK; Articles of J. Irwin and A. J. Dragt, A. J. Dragt, M. Berz, H. Yoshida and Y. T. Yan in HAPE; K. Yokoya in HAPE.

[8] S. A. Khan and R. Jagannathan, Phys. Rev. E51, 2510 (1995); R. Jagannathan and S. A. Khan, in Advances in Imaging and Electron Physics 97 ed. P. W. Hawkes (Academic Press, San Diego, 1996) pp. 257-358; S. A. Khan, Quantum Theory of Charged Particle Beam Optics, Ph.D. Thesis, University of Madras, 1997; R. Jagannathan and S. A. Khan, ICFA Beam Dynamics Newsletter 13, 21 (1997).

[9] R. Fedele and G. Miele, Nuovo Cim. D13, 1527 (1991); R. Fedele and V. I. Man’ko, in QABP-I; M. A. Man’ko, in QABP-II and references therein; S. A. Khan and M. Pusterla, Eur. Phys. J. A7, 583 (2000); M. Pusterla, in QABP-II, this Proceedings and references therein.

[10] N. Cufaro Petroni, S. De Martino, S. De Siena, and F. Illuminati, in QABP-I, QABP-II, this Proceedings and references therein.

[11] See K. Heinemann and D. P. Barber, in QABP-I.

[12] M. Conte, R. Jagannathan, S. A. Khan, and M. Pusterla, Part. Accel. 56, 99 (1996); Articles of R. Jagannathan, M. Pusterla, and S. A. Khan in QABP-I; S. A. Khan, in QABP-II.

[13] R. Jagannathan, in QABP-II.

[14] This has been done also in the context of crystalline beams. See, J. Wei and A. M. Sessler, in QABP-II and references therein. I thank Prof. Pisin Chen for bringing this to my attention.

[15] For details of the formalism see, e.g., D. R. Brill and J. A. Wheeler, Rev. Mod. Phys. 29, 465 (1957); E. A. Lord, Tensors, Relativity and Cosmology (Tata-McGraw Hill, New Delhi, 1976).

[16] See, e.g., S. Y. Lee, Accelerator Physics (World Scientific, Singapore, 1999).