Quantum Mechanical Formalism of Particle Beam Optics

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Abstract: A general procedure for construction of the formalism of quantum beam optics for any particle is reviewed. The quantum formalism of spin-$\frac{1}{2}$ particle beam optics is presented starting ab initio with the Dirac equation. As an example of application the case of normal magnetic quadrupole lens is discussed. In the classical limit the quantum formalism leads to the well-known Lie algebraic formalism of classical particle beam optics.

I. INTRODUCTION

Whenever the possibility of a quantum formalism of particle beam optics is mentioned the immediate response, invariably, in the accelerator physics community is to ask what is the need to use quantum mechanics when classical mechanics has been so successful in the design and operation of numerous accelerators? Of course, this is a natural question and, though the system is quantum mechanical at the fundamental level, in most situations classical mechanics is quite adequate [1] since the de Broglie wavelength of the (high energy) beam particle is very small compared to the typical apertures of the cavities in accelerators as has been pointed out clearly by Chen. [2] But, the recent attention to the sensitivity of tracking of particle trajectories to quantum granularities in the stochastic regions of phase space [3] and the limits placed by quantum mechanics on the achievable beam spot sizes in accelerators [4] clearly indicates the need for a formalism of quantum beam optics relevant to such issues. [5] Besides this, with ever increasing demand for higher energies and luminosity and lower emittance beams, and the need for polarized beams, the interest in the studies on the various quantum aspects of beam physics is growing. [6] So, it is time that a quantum formalism of particle beam dynamics is developed in which all aspects (optical, spin, radiation, ... , etc.) are considered in a unified framework.

The grand success of the classical theories accounts for the very few quantum approaches to the charged-particle beam optics in the past. Notable among these are:

- 1986 Ferwerda et al.: Justified the use of scalar (Klein-Gordon) equation for image formation in practical electron microscopes operating even at relativistic energies. [7]

The formalism of quantum theory of charged-particle beam optics developed by Jagannathan et al., based on the Klein-Gordon and Dirac equations, provides a recipe to work out the quantum maps for any particle optical system up to any desired order. [8]− [11]. The classical limit (de Broglie wavelength → 0) of this quantum formalism reproduces the well-known Lie algebraic approach of Dragt et al. [12] for handling the classical beam optics. Spin evolution, independent of orbital motion, can also be treated classically using the Lie algebraic approach. [13] This brief note is to present the essential features of the quantum formalism of spin-$\frac{1}{2}$ particle beam optics based on the Dirac equation.

In many accelerator optical elements the electromagnetic fields are static or can be reasonably assumed to be static. In such devices one can further ignore the times of flights which may be negligible, or of no direct relevance, as the emphasis is more on the profiles of the trajectories. The idea is to analyze the evolution of the beam parameters of the various individual charged-particle beam optical elements (quadrupoles, bending magnets, · · ·) along the optic axis of the system. Let us consider a charged-particle at the point \( (r, s) \) where \( r \) is the transverse coordinate and \( s \) refers to the coordinate along the optic axis. After passing through the system this particle arrives at the point \( (r', s') \). Note that \( (r, s) \) constitute a curvilinear coordinate system, adapted to the geometry of the system. Given the initial quantities at an \( s \), the problem is to determine the final quantities at an \( s' \), and to design an optical device in such a way that the relations between the initial and final quantities have the desired properties. Since we want to know the evolution of the beam parameters along the optic axis of the system the starting equation of the quantum formalism should be desirably of the form

\[
i\hbar \frac{\partial}{\partial s} \psi(r; s) = \hat{H} \psi(r; s),
\]

linear in \( \partial/\partial s \), irrespective of the basic time-dependent equation (Schrödinger, Klein-Gordon, Dirac, · · ·) governing the system. So the step-I of building the quantum formalism is to cast the basic equation of quantum mechanics, relevant for the system under study, in the form (1). Once this is done the step-II would be to obtain the relationship for the quantities at any point \( s \) to the quantities at the point \( s' \). This in the language of the quantum formalism would require to obtain the relationship for an observable \( \{O(s)\} \) at the transverse plane at \( s \) to the observable \( \{O(s')\} \) at the transverse plane at \( s' \). This can be achieved by integrating (1). Formally,

\[
\psi(r; s) = \hat{U}(s, s') \psi(r; s'),
\]

which leads to the required transfer maps

\[
\langle O(s') \rangle \rightarrow \langle O(s) \rangle = \langle \psi(s) | O | \psi(s) \rangle = \left\langle \psi(s) \right| \hat{U}^{\dagger} \hat{U} \left| \psi(s') \right\rangle.
\]

Equation (1) is the basic equation of the quantum formalism of charged-particle beam optics and we call it as the beam optical equation, \( \hat{H} \) as the beam optical Hamiltonian and \( \psi \) as the beam optical wavefunction.

To summarize, we have a two-step algorithm to build a quantum formalism of charged-particle beam optics. On may question the applicability of the two-step algorithm: Does it always work? From experience we know that it works for the Schrödinger, Klein-Gordon and Dirac equations. The above description gives an oversimplified picture of the formalism than, it actually is. There are several crucial points to be noted to understand the success of the two-step algorithm. The first step in the algorithm to obtain the beam optical equation is much more than a mere mathematical transformation which eliminates ‘t’ in preference to a variable ‘s’ along the optic axis. There has to be a clever set of transformations ensuring that the resultant \( s \)-dependent equation has a very close physical and mathematical analogy with the original \( t \)-dependent equation of the standard quantum mechanics. Without this guiding requirement it would not be possible to execute the second step of the algorithm which ensures that we can use all the rich machinery of the quantum mechanics to compute the transfer maps characterizing the optical system. This summarizes the recipe of obtaining the quantum prescriptions for the optical transfer maps. Rest is mostly a computational affair which is inbuilt in the powerful algebraic machinery of the algorithm. As in any computation, there are some reasonable assumptions and some possible approximations coming from physical considerations. It is important to note that in the case of the Schrödinger, Klein-Gordon and Dirac equations the beam optical forms obtained are exact. Approximations necessarily enter only in the step-II of the algorithm, i.e., while integrating the beam optical equation and computing the transfer maps for the quantum averages of the beam observables. As in the classical theory, the approximations arise due to the fact that only the first few terms are retained in the infinite series expansion of the beam optical Hamiltonian. The beam optical Hamiltonian is obtained as a power series in \( \frac{\hat{p}_0}{p_0} \) where \( p_0 \) is the design (or average) momentum of the beam particles moving predominantly along the optic axis of the system and \( \hat{p}_0 \) is the small transverse kinetic momentum. The leading order contribution gives rise to the paraxial or the ideal behavior and higher order contributions give rise to the nonlinear or aberrating behavior. Both the paraxial and the aberrating behaviors deviate from their classical nature by quantum contributions which are in powers of the de Broglie wavelength of the beam particle (\( \lambda_0 = 2\pi\hbar/p_0 \)). The classical formalism is obtained from the quantum formalism by taking the limit \( \lambda_0 \rightarrow 0 \).
Now we shall see how the above algorithm works for the Dirac particle. Let us consider a monoenergetic beam of Dirac particles of mass $m$, charge $q$ and anomalous magnetic moment $\mu_a$, transported through a magnetic optical element with a straight optic axis characterized by the static potentials $(\phi(r), A(r))$. The beam propagation is governed by the stationary Dirac equation

\[ \hat{H}_D |\psi_D\rangle = E |\psi_D\rangle , \]  

where $|\psi_D\rangle$ is the time-independent 4-component Dirac spinor, $E$ is the total energy of the beam particle and the Hamiltonian $\hat{H}_D$, including the Pauli term, is given by

\[ \hat{H}_D = \beta mc^2 + c\alpha \cdot (-i\hbar \nabla - qA) - \mu_a \beta \Sigma \cdot B , \]  

where the symbols have their usual meanings. [14] To cast (4) in the required beam optical form (1) we multiply $\hat{H}_D$ (on the left) by $\alpha_z/c$ and rearrange the terms to get

\[ i\hbar \frac{\partial}{\partial z} |\psi_D\rangle = \hat{H}_D |\psi_D\rangle , \]

\[ \hat{H}_D = -p_0 \beta \chi \alpha_z - q A_z I + \alpha_z \alpha_\perp \cdot \hat{\pi} + (\mu_a/c) \beta \alpha_\perp \Sigma \cdot B , \]

where $\chi$ is a diagonal matrix with elements $(\xi, \xi, -1/\xi, -1/\xi)$ and $\xi = \sqrt{(E + mc^2)/(E - mc^2)}$. Equation (6) is still not in a completely desirable form. So we resort to a further transformation:

\[ |\psi_D\rangle \rightarrow |\psi'\rangle = M |\psi_D\rangle , \quad M = \frac{1}{\sqrt{2}} (I + \chi \alpha_z) . \]

Then we obtain

\[ i\hbar \frac{\partial}{\partial z} |\psi'\rangle = \hat{H}' |\psi'\rangle , \quad \hat{H}' = M \hat{H} D M^{-1} = -p_0 \beta + \hat{E} + \hat{O} , \]

where the nonvanishing matrix elements of the even term $\hat{E}$ and the odd term $\hat{O}$ are given by

\[ \hat{E}_{11} = -q A_z I - (\mu_a/2c) \{ (\xi + \xi^{-1}) \sigma_\perp \cdot B_{\perp} + (\xi - \xi^{-1}) \sigma_z B_z \} , \]

\[ \hat{E}_{22} = -q A_z I - (\mu_a/2c) \{ (\xi + \xi^{-1}) \sigma_\perp \cdot B_{\perp} - (\xi - \xi^{-1}) \sigma_z B_z \} , \]

\[ \hat{O}_{12} = \xi \left[ \sigma_\perp \cdot \hat{\pi}_{\perp} - (\mu_a/2c) \{ i (\xi - \xi^{-1}) (B_x \sigma_y - B_y \sigma_x) \right. \]

\[ \left. - (\xi + \xi^{-1}) B_z \Sigma \} \right] , \]

\[ \hat{O}_{21} = -\xi^{-1} \left[ \sigma_\perp \cdot \hat{\pi}_{\perp} + (\mu_a/2c) \{ i (\xi - \xi^{-1}) (B_x \sigma_y - B_y \sigma_x) \right. \]

\[ \left. + (\xi + \xi^{-1}) B_z \Sigma \} \right] . \]

The effect of the transformation (7) is to make the lower components of a Dirac spinor corresponding to a quasi-paraxial beam moving in the positive $z$-direction negligible compared to the upper components and thus effectively making the 4-component spinor as a 2-component spinor. Now one may observe the close analogy:

<table>
<thead>
<tr>
<th>Standard Dirac equation</th>
<th>Beam optical form</th>
</tr>
</thead>
<tbody>
<tr>
<td>$mc^2 \beta + \hat{E}_D + \hat{O}_D$</td>
<td>$-p_0 \beta + \hat{E} + \hat{O}$</td>
</tr>
<tr>
<td>Positive energy</td>
<td>Forward propagation</td>
</tr>
<tr>
<td>Nonrelativistic, $c</td>
<td>\pi</td>
</tr>
<tr>
<td>$mc^2$: Note $i\hbar \frac{\partial \phi}{\partial z} \approx mc^2 \psi$</td>
<td>$-p_0$: Note $i\hbar \frac{\partial \phi}{\partial z} \approx -p_0 \psi$</td>
</tr>
<tr>
<td>Nonrelativistic motion</td>
<td>Paraxial behavior</td>
</tr>
<tr>
<td>+ Relativistic corrections</td>
<td>+ Aberration corrections</td>
</tr>
</tbody>
</table>

This completes the step-I of the algorithm. To execute the step-II we proceed as follows.

The above analogy suggests that, as the most systematic way to understand the Dirac Hamiltonian as a nonrelativistic part plus relativistic correction terms is to use the Foldy-Wouthuysen (FW) transformation technique, [14] we should adopt a similar FW-like approach in the beam optical case to understand the beam optical Hamiltonian as a paraxial part plus nonparaxial correction terms. This leads to a procedure to obtain the paraxial behavior...
accompanied by a systematic method to compute the aberrations to all orders in powers of the expansion parameter $1/p_0$. To leading order, the first FW-like transformation is

$$\left| \psi^{(1)} \right\rangle = \exp \left( -\beta \hat{O}/2p_0 \right) |\psi\rangle.$$  \hspace{1cm} (10)

Then

$$i\hbar \frac{\partial}{\partial z} \left| \psi^{(1)} \right\rangle = \hat{H}^{(1)} \left| \psi^{(1)} \right\rangle, \quad \hat{H}^{(1)} = -p_0 \beta + \hat{E}^{(1)} + \hat{O}^{(1)},$$

$$\hat{E}^{(1)} = \hat{E} - \frac{1}{2p_0} \beta \hat{O}^2 + \cdots, \quad \hat{O}^{(1)} = -\frac{1}{2p_0} \beta \left\{ \left[ \hat{O}, \hat{E} \right] + i\hbar \frac{\partial}{\partial z} \hat{O} \right\} + \cdots$$ \hspace{1cm} (11)

It is to be noted that the transformation (10) keeps the upper components of the beam optical wavefunction large compared to its lower components. One can proceed with further FW-like transformations and stop at any desired stage. Let us denote the 2-component spinor comprising the upper components of the final 4-component spinor obtained in the above process as $|\psi\rangle$.

Up to now, all the observables, the field components, time etc., have been defined in the laboratory frame. The covariant description of the spin of the Dirac particle has the simplest operator representation in the rest frame of the particle. Thus, in accelerator physics the spin is defined in the rest frame of the particle. So we make a further transformation which takes us from the beam optical form to the accelerator optical form

$$\left| \psi^{(A)} \right\rangle = \exp \left\{ \frac{i}{2p_0} \left( \bar{\pi}_x \sigma_y - \bar{\pi}_y \sigma_x \right) \right\} |\psi\rangle.$$ \hspace{1cm} (12)

Thus, up to the paraxial approximation the accelerator optical Hamiltonian [10,11] is

$$i\hbar \frac{\partial}{\partial z} \left| \psi^{(A)} \right\rangle = \hat{H}^{(A)} \left| \psi^{(A)} \right\rangle, \quad \hat{H}^{(A)} \approx \left( -p_0 - qA_z + \frac{1}{2p_0} \pi \cdot \hat{\sigma} \right) \gamma \frac{m}{p_0} \mathbf{Q} \cdot \mathbf{S},$$ \hspace{1cm} (13)

where $\mathbf{Q} = -\frac{1}{\gamma \hbar} \{-q \mathbf{B} + \epsilon (\mathbf{B}_\parallel + \gamma \mathbf{B}_\perp)\}$. $\gamma = E/mc^2$ and $\epsilon = 2m \mu_a / \hbar$.

### IV. AN EXAMPLE OF APPLICATION: MAGNETIC QUADRUPOLE LENS

Let an ideal normal magnetic quadrupole of length $\ell$, characterized by the field $\mathbf{B} = (-Gy, -Gx, 0)$, be situated between the transverse planes at $z = z_{in}$ and $z = z_{out} = z_{in} + \ell$. The associated vector potential can be taken to be $\mathbf{A} = (0, 0, \frac{1}{2} G (x^2 - y^2))$ with $G$ as constant inside the lens and zero outside. The accelerator optical Hamiltonian [10] is

$$\hat{H}(z) = \begin{cases} 
\hat{H}_F = -p_0 + \frac{x^2}{2p_0} \hat{\pi}_x^2, & \text{for } z < z_{in} \text{ and } z > z_{out}, \\
\hat{H}_L(z) = -p_0 - \frac{\gamma}{\gamma \hbar} \hat{\pi}_y^2 - \frac{1}{2} q G (x^2 - y^2) + \frac{\gamma \mu_a}{\gamma \hbar} (y \sigma_x + x \sigma_y), & \text{for } z_{in} \leq z \leq z_{out}, \text{ with } \eta = (q + \gamma e) G \mathbf{F} \hbar / 2p_0.
\end{cases} \hspace{1cm} (14)$$

The subscripts $F$ and $L$ indicate the field-free and the lens regions respectively.

Best way to compute the $z$-evolution operator $\hat{U}$ is via the interaction picture, used in the Lie algebraic formulation [12] of classical beam optics. Using the transfer operator thus derived [10] we get the transfer maps for the averages of the transverse phase-space components: with the subscripts in and out standing for $(z_{in})$ and $(z_{out})$, respectively,

$$\begin{pmatrix} 
\langle x \rangle \\
\langle \hat{p}_x \rangle/p_0 \\
\langle y \rangle \\
\langle \hat{p}_y \rangle/p_0 
\end{pmatrix}_{\text{out}} \approx T_Q \begin{pmatrix} 
\langle x \rangle \\
\langle \hat{p}_x \rangle/p_0 \\
\langle y \rangle \\
\langle \hat{p}_y \rangle/p_0 
\end{pmatrix}_{\text{in}} + \eta \begin{pmatrix} 
\cosh (\sqrt{K} \ell) - 1 \\
- \sinh (\sqrt{K} \ell) \\
\cos (\sqrt{K} \ell) - 1 \\
- \sin (\sqrt{K} \ell) 
\end{pmatrix} \begin{pmatrix} 
\langle \sigma_y \rangle \\
\langle \sigma_y \rangle \\
\langle \sigma_x \rangle \\
\langle \sigma_x \rangle 
\end{pmatrix}_{\text{in}}.$$
\[ T_Q = M_\geq M_Q M_<, \quad M_\geq = \begin{pmatrix} 1 & \Delta z_\geq & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \Delta z_< \\ 0 & 0 & 0 & 1 \end{pmatrix}, \] 

\[ M_Q = \begin{pmatrix} \cosh(\sqrt{K}\ell) & \frac{1}{\sqrt{K}} \sinh(\sqrt{K}\ell) & 0 & 0 \\ \sqrt{K} \sinh(\sqrt{K}\ell) & \cosh(\sqrt{K}\ell) & 0 & 0 \\ 0 & 0 & \cos(\sqrt{K}\ell) & \frac{1}{\sqrt{K}} \sin(\sqrt{K}\ell) \\ 0 & 0 & -\sqrt{K} \sin(\sqrt{K}\ell) & \cos(\sqrt{K}\ell) \end{pmatrix}. \]

Thus we have got a fully quantum mechanical derivation of the combined effect of the focusing action of the quadrupole lens (note the traditional transfer matrices) and the Stern-Gerlach force. It may be noted that the quantum formalism of spinor beam optics supports, in principle, the idea of a Stern-Gerlach spin-splitter device to produce polarized beams. [15] The transfer map across the quadrupole lens for the spin components computed using the above accelerator optical Hamiltonian describes the well known Thomas-Bargmann-Michel-Telegdi spin evolution. [10]

V. CONCLUDING REMARKS

In fine, we have seen how one can obtain the formalism of quantum beam optics for any particle, starting ab initio from the relevant basic quantum equation, at the single-particle level. A two-step algorithm for this purpose has been suggested. Using the general principle, the construction of a spinor theory of accelerator optics, starting from the Dirac equation and taking into account the anomalous magnetic moment, has been demonstrated. As an example of application of the resulting formalism the normal magnetic quadrupole lens has been discussed. In the classical limit the quantum formalism leads to the Lie algebraic formalism of charged-particle beam optics.

To get a formalism taking into account the multiparticle effects, particularly for the intense beams, it should be worthwhile to be guided by the quantum-like approaches to the particle beam transport: Thermal Wave Model [16] and Stochastic Collective Dynamical Model [17]. Recently the quantum-like approach has been applied to construct a Diffraction Model for the beam halo. [18] This model provides numerical estimates for the beam losses. In this context, another useful approach could be to use the Wigner phase-space distribution functions. Heinemann and Barber [19] have initiated the derivation of such a formalism for the Dirac particle beam physics starting from the original work of Derbenev and Kondratenko [20] who used the FW technique to get their Hamiltonian for radiation calculations.

The present study is confined to systems with straight optic axis. An extension to the curved optic axis systems should be done. This would involve the subtleties of quantization in curvilinear coordinates. Then there are the well known questions related to the position operator in the relativistic quantum theory. Also, there are doubts about the exact form of the Stern-Gerlach force for a relativistic particle. [21] To address such questions from the point of view of experiments using particle beams the right platform would be the formalism of quantum beam optics.

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P. Chen (World Scientific, Singapore, 1999) (Hereafter referred to as QABP-I); Proceedings of this Workshop (Hereafter referred to as QABP-II).


[5] See also M. Venturini, in QABP-II.


[10] See also M. Venturini, in QABP-II.


[17] See the following and references therein: N. Cufaro Petroni, S. De Martino, S. De Siena, and F. Illuminati, in QABP-I; N. Cufaro Petroni, S. De Martino, S. De Siena, and F. Illuminati, in QABP-II; M. A. Man’ko, in QABP-II.