Quantum mechanics of charged-particle beam transport through magnetic lenses

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The quantum theory of charged-particle beam transport through a magnetic lens system with a straight optic axis, at the level of single-particle dynamics and disregarding spin (or, when nonzero, assuming it to be an independent spectator degree of freedom), is presented, based on the Schrödinger and Klein-Gordon equations in a form suitable for analyzing the paraxial and aberration aspects in a systematic way using a Lie algebraic approach. In the classical limit, the well known Lie algebraic treatment of the corresponding classical theory is obtained. As examples, quadrupole and axially symmetric magnetic lenses are considered. An extension of the theory to the cases of electrostatic and other electromagnetic lens systems is outlined. This work is complementary to an already known similar approach to the spinor electron optics based on the Dirac equation and provides the corresponding framework when the optics of charged particles, with or without spin, is described with scalar wave functions in the nonrelativistic and relativistic situations.

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I. INTRODUCTION

Optics of charged-particle beams, or the theory of transport of charged-particle beams through electromagnetic systems, is traditionally dealt with using classical mechanics; this is so in electron microscopy, ion optics, accelerator physics, etc. (see, e.g., [1–4]). Of course, in Glaser's theory of electron optical imaging process nonrelativistic quantum mechanics forms the basis [5] (see [6] for a recent, detailed account of the quantum mechanics of electron optics). The Dirac equation, the proper equation for the electron, was used in the study of diffraction of "electron waves" by Rubinowicz [7] and Van Loc [8]. Conditions under which the application of the Dirac equation can be approximated by the use of the Klein-Gordon equation, treating spin as a spectator degree of freedom, in an extension of Glaser's formalism to the relativistic electron microscopy, have been studied in detail by Ferwerda, Hoenders, and Slump [9]. Quantum theory of electron optics entirely based on the Dirac equation, at the level of single-particle dynamics, has been under development recently [10–12]. A path integral approach to the spinor electron optics has also been proposed [13]. The approach initiated in [10] and [11] for treating the optics of Dirac electrons is essentially algebraic and is suitable for adopting the Lie algebraic techniques pioneered by Dragt *et al.* for the classical theory of charged-particle beam optics (see, e.g., [14] and [15]). The purpose of this article is to present a similar algebraic approach for the quantum theory of charged-particle beam optics based on the Schrödinger and Klein-Gordon equations, at the level of single-particle dynamics, for the case when the spin is disregarded (or, in other words, assumed, if nonzero, to be an independent spectator degree of freedom). Here we are dealing mainly, in detail, with magnetic lens systems having straight optic axis and, as examples, quadrupole and axially symmetric magnetic lenses are considered. Corresponding aspects of the spinor electron optics [10–12] are also recalled at the end by way of comparison. An extension of the theory to electrostatic and other electromagnetic lenses is outlined briefly. The work presented in this paper is essentially complementary to the spinor electron optics [10–12], dealing with relativistic electron optics using an algebraic framework, and corresponds to a similar algebraic treatment of the quantum mechanics of the optics of charged-particles, with or without spin, described with scalar wave functions in the nonrelativistic and relativistic situations.

Recently a formal quantum theory of charged-particle beam optics has been developed with a Schrödinger-like basic equation in which the beam emittance plays the role of $\hbar$ (see [16] and references therein). The formalism we are developing is the canonical quantum theory of a charged-particle in an electromagnetic field suitably adapted to deal with beam propagation problems at the single-particle level.

II. OPTICAL FORM OF THE NONRELATIVISTIC SCHRÖDINGER EQUATION

The nonrelativistic Schrödinger equation for a particle of charge q and mass m moving in a static electromagnetic field with potentials $(\phi(\boldsymbol{r}),\ \boldsymbol{A}(\boldsymbol{r}))$ is

$$\left(i\hbar\frac{\partial}{\partial t} - q\phi\right)\Psi(\boldsymbol{r},t) = \frac{1}{2m}\left\{\hat{\pi}_\perp^2 + \left(-i\hbar\frac{\partial}{\partial z} - \frac{q}{c}A_z\right)^2\right\}\Psi(\boldsymbol{r},t), \quad (2.1)$$

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where $\hat{\boldsymbol{\pi}}_\perp = \hat{\boldsymbol{p}}_\perp - (q/c)\boldsymbol{A}_\perp$ and $\hat{\pi}_\perp^2 = \hat{\pi}_x^2 + \hat{\pi}_y^2$ with $\hat{\boldsymbol{p}}_\perp = -i\hbar\boldsymbol{\nabla}_\perp$. Let the optical element (i.e., the stationary electromagnetic field) through which the charged-particle beam propagates have a straight optic axis along the z direction and be situated, for all practical purposes, in the region $z_{\rm in} \le z \le z_{\rm out}$. Then we are interested in the evolution of the beam parameters along the z direction. Further, we are dealing with the scattering states of the system comprising of a time-independent field. The relevant wave function Ψ obeying Eq. (2.1) and representing an almost paraxial quasimonoenergetic beam of particles moving through the system along the $+z$ axis, with constant positive energy $[\approx E\,(p_0)]$, should be such that

$$\Psi(\boldsymbol{r}_\perp, z < z_{\rm in}, t) = \int_{p_0-\Delta p}^{p_0+\Delta p} dp \exp\left[-\frac{i}{\hbar}E(p)t\right] \times\psi(\boldsymbol{r}_\perp, z<z_{\rm in}; p), \quad \Delta p \ll p_0$$

$$\psi\left(\boldsymbol{r}_\perp, z < z_{\rm in}; p\right) = \int d^2p_\perp\, c(\boldsymbol{p}) \exp\left(\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}\right),$$

$$\boldsymbol{p} = \left(\boldsymbol{p}_\perp, +\sqrt{p^2 - p_\perp^2}\right),$$

$$p = |\boldsymbol{p}|, \quad |\boldsymbol{p}_\perp| \ll p, \quad E(p) = \frac{p^2}{2m}, \tag{2.2}$$

where $z < z_{\rm in}$ corresponds to the field-free input region. We have to relate $\Psi(\boldsymbol{r}_\perp, z > z_{\rm out}; t)$, the wave function in the output (field-free) region of the system, to the input wave function $\Psi(\boldsymbol{r}_\perp, z < z_{\rm in}; t)$. If we have a relation of the type

$$\psi(\boldsymbol{r}_\perp, z''; p) = \hat{G}(z'', z'; p)\psi(\boldsymbol{r}_\perp, z'; p) \tag{2.3}$$

for the time-Fourier component $\psi(\boldsymbol{r}_\perp, z; p)$ of $\Psi(\boldsymbol{r}_\perp, z, t)$, then we can write

$$\Psi(\boldsymbol{r}_\perp, z'' > z_{\rm out}, t) = \int_{p_0-\Delta p}^{p_0+\Delta p} dp\, \hat{G}(z'', z'; p)\psi(\boldsymbol{r}_\perp, z' < z_{\rm in}; p) \times \exp\left[-\frac{i}{\hbar}E(p)t\right]. \tag{2.4}$$

In the practically monoenergetic case ($\Delta p \approx 0$) we would have

$$\Psi(\boldsymbol{r}_\perp, z'' > z_{\rm out}, t) \approx \hat{G}(z'', z'; p_0)\Psi(\boldsymbol{r}_\perp, z' < z_{\rm in}, t). \tag{2.5}$$

To obtain the z propagator $\hat{G}(z'', z'; p)$ for $\psi(z; p)$ defined by Eq. (2.3) we have to integrate for the z evolution the time-independent nonrelativistic Schrödinger equation

$$\left\{\hat{\pi}_\perp^2 + \left(-i\hbar\frac{\partial}{\partial z} - \frac{q}{c}A_z\right)^2 - p^2\right\}\psi(\boldsymbol{r}_\perp, z; p) = 0, \tag{2.6}$$

where $p^2 = 2m(E - q\phi)$. We shall consider magnetic systems for which, with $\phi = 0$ in the lens region, $p = \sqrt{2mE}$ is a z-independent constant. Then, taking

$$\psi_+ = \frac{1}{2}\left\{\psi - \frac{1}{p}\left(i\hbar\frac{\partial}{\partial z} + \frac{q}{c}A_z\right)\psi\right\},$$

$$\psi_- = \frac{1}{2}\left\{\psi + \frac{1}{p}\left(i\hbar\frac{\partial}{\partial z} + \frac{q}{c}A_z\right)\psi\right\}, \tag{2.7}$$

Eq. (2.6) is seen to be equivalent to

$$i\hbar\frac{\partial}{\partial z}\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix} = H\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix},$$

$$H = -p\sigma_z - \frac{q}{c}A_z\mathbb{1} + \frac{\hat{\pi}_\perp^2}{2p}\left(\sigma_z + i\sigma_y\right), \tag{2.8}$$

where σ's are the Pauli matrices and $\mathbb{1}$ is the identity matrix. It may be noted that Eq. (2.8) is analogous to the Feshbach-Villars form [17] of the Klein-Gordon equation, namely, $(i\hbar\frac{\partial}{\partial t} - \mathrm{H})\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = 0$.

Let us now write

$$H = -p\sigma_z + \hat{\mathcal{E}} + \hat{\mathcal{O}},$$

$$\hat{\mathcal{E}} = -\frac{q}{c}A_z\mathbb{1} + \frac{\hat{\pi}_\perp^2}{2p}\sigma_z,$$

$$\hat{\mathcal{O}} = i\frac{\hat{\pi}_\perp^2}{2p}\sigma_y, \tag{2.9}$$

where $\hat{\mathcal{E}}$ and $\hat{\mathcal{O}}$ are, respectively, the "even" and "odd"parts of H in analogy with the Dirac electron theory. Now, employing a Foldy-Wouthuysen-type transformation technique [18] one can successively eliminate the odd part from the expression for H in Eq. (2.8). Carrying out these transformations up to the third step (see [11] for details) and collecting the terms of order up to $1/p^4$ we get

$$i\hbar\frac{\partial}{\partial z}\begin{pmatrix}\tilde{\psi}_+\\ \tilde{\psi}_-\end{pmatrix} = \mathcal{H}\begin{pmatrix}\tilde{\psi}_+\\ \tilde{\psi}_-\end{pmatrix},$$

$$\mathcal{H} \approx -\frac{q}{c}A_z\mathbb{1} - \left(p - \frac{\hat{\pi}_\perp^2}{2p} - \frac{\hat{\pi}_\perp^4}{8p^3}\right)\sigma_z - \frac{q}{32cp^4}\left[\hat{\pi}_\perp^2, \left[\hat{\pi}_\perp^2, A_z\right]\right] - \frac{i\hbar q}{32cp^4}\left[\hat{\pi}_\perp^2, \hat{\boldsymbol{p}}_\perp\cdot\frac{\partial \boldsymbol{A}_\perp}{\partial z} + \frac{\partial \boldsymbol{A}_\perp}{\partial z}\cdot\hat{\boldsymbol{p}}_\perp - \frac{q}{c}\frac{\partial\left(A_\perp^2\right)}{\partial z}\right]. \tag{2.10}$$

It is obvious that $\tilde{\psi}_+$ and $\tilde{\psi}_-$ correspond, respectively, to the wave functions associated with momenta $\pm p$ in the z direction; to see this, consider the free particle limit, i.e., $\boldsymbol{A} = (0,0,0)$. Since we are dealing with a beam moving in the $+z$ direction, the scalar equation relevant for us is given by, with $\psi_0 = \tilde{\psi}_+$,

$$i\hbar\frac{\partial\psi_0}{\partial z} = \mathcal{H}_0\psi_0\,,$$
$$\begin{aligned}\mathcal{H}_0 \approx & -\frac{q}{c}A_z - p + \frac{\hat{\pi}_\perp^2}{2p} + \frac{\hat{\pi}_\perp^4}{8p^3} \\ & -\frac{q}{32cp^4}[\hat{\pi}_\perp^2\,,\,[\hat{\pi}_\perp^2\,,\,A_z]] \\ & -\frac{i\hbar q}{32cp^4}\left[\hat{\pi}_\perp^2\,,\,\hat{\boldsymbol{p}}_\perp\cdot\frac{\partial \boldsymbol{A}_\perp}{\partial z} + \frac{\partial \boldsymbol{A}_\perp}{\partial z}\cdot\hat{\boldsymbol{p}}_\perp \right. \\ & \left. -\frac{q}{c}\frac{\partial\left(A_\perp^2\right)}{\partial z}\right]. \end{aligned} \tag{2.11}$$

It is interesting to see that the above "optical quantum Hamiltonian" $\mathcal{H}_0$ contains correction terms apart from the terms obtained directly by "quantizing" (or "wavizing" as is sometimes called) the classical optical Hamiltonian $-\sqrt{p^2-\pi_\perp^2}-(q/c)A_z$. Actually $\psi_0 \approx \psi$ of Eq. (2.6), for a quasiparaxial beam moving in the $+z$ direction, and what we have done is rewrite Eq. (2.6) as an equation for the z evolution linear in $\partial/\partial z$, with the corresponding optical Hamiltonian expressed as a power series in the parameter $1/p$, so that successive approximations should lead to the study of paraxial and aberration aspects in a systematic way. It is clear that in the paraxial case, when the terms beyond $\hat{\pi}_\perp^2/2p$ in Eq. (2.11) can be neglected, the optical form of the nonrelativistic Schrödinger equation, namely, Eq. (2.11), becomes the corresponding Glaser equation [5].

III. THE LIE ALGEBRAIC APPROACH

Let us now consider a monoenergetic beam associated with a wave function $\Psi_0 = \psi_0 \exp\left(-iEt/\hbar\right)$ in the optical representation obtained in Eq. (2.11). Formally integrating Eq. (2.11), we have

$$\Psi_0\left(\boldsymbol{r}_\perp, z'' > z_{\rm out}, t\right) = \hat{\mathcal{G}}_0\left(z'', z'; p\right)\Psi_0\left(\boldsymbol{r}_\perp, z' < z_{\rm in}, t\right)\,, \tag{3.1}$$

with

$$\begin{aligned}\hat{\mathcal{G}}_0\left(z'', z'; p\right) &= \mathcal{P}\left\{\exp\left(\frac{1}{i\hbar}\int_{z'}^{z''} dz\,\mathcal{H}_0(z;p)\right)\right\} \\ &= \exp\left\{\hat{\mathcal{L}}\left(z'', z'; p\right)\right\}\,,\end{aligned} \tag{3.2}$$

where $\mathcal{P}$ stands for z ordering of the exponential and $\hat{\mathcal{L}}$ can be obtained using the Magnus formula (see, e.g., [19]). The optical Hamiltonian $\mathcal{H}_0$ is seen to be manifestly Hermitian. Hence the propagator $\hat{\mathcal{G}}_0$ is unitary. The normalization $\int\int dxdy\,\Psi_0^*\left(\boldsymbol{r}_\perp, z\right)\Psi_0\left(\boldsymbol{r}_\perp, z\right) = 1$ will be preserved in the z evolution and we can take

$$\begin{aligned}\left\langle\hat{Q}\right\rangle(z) &= \left\langle\Psi_0(z)\left|\hat{Q}\right|\Psi_0(z)\right\rangle \\ &= \int\int dxdy\,\Psi_0^*\left(\boldsymbol{r}_\perp, z\right)\hat{Q}\Psi_0\left(\boldsymbol{r}_\perp, z\right)\end{aligned} \tag{3.3}$$

as the average value of any observable Q, represented by the operator $\hat{Q}$, in any chosen z plane; we are concerned only with z planes in the field-free regions outside the lens. Hereafter, we shall generally omit p in the notations of $\mathcal{H}_0$, $\hat{\mathcal{G}}_0$, $\hat{\mathcal{L}}$, etc., with the understanding that it usually corresponds to the mean (or design) momentum of the quasiparaxial beam under consideration.

For any observable Q we have, with $z'' > z_{\rm out}$ and $z' < z_{\rm in}$,

$$\begin{aligned}\left\langle\hat{Q}\right\rangle(z'') &= \left\langle\hat{\mathcal{G}}_0\left(z'', z'\right)^\dagger\,\hat{Q}\,\hat{\mathcal{G}}_0\left(z'', z'\right)\right\rangle(z') \\ &= \left\langle\exp\left\{-\hat{\mathcal{L}}\left(z'', z'\right)\right\}\hat{Q}\exp\left\{\hat{\mathcal{L}}\left(z'', z'\right)\right\}\right\rangle(z') \\ &= \left\langle\exp\left\{:-\hat{\mathcal{L}}\left(z'', z'\right):\right\}\hat{Q}\right\rangle(z') \\ &= \left\langle\sum_{k=0}^{\infty}\frac{:-\hat{\mathcal{L}}\left(z'', z'\right):^k}{k!}\hat{Q}\right\rangle(z')\,,\end{aligned} \tag{3.4}$$

where, for any operator $\hat{F}$,

$$\begin{aligned}&:\hat{F}:^0\hat{Q} = \hat{Q}\,, \qquad :\hat{F}:\hat{Q} = \left[\hat{F}\,,\,\hat{Q}\right]\,, \\ &:\hat{F}:^k\hat{Q} = \left[\hat{F}\,,\,:\hat{F}:^{k-1}\hat{Q}\right] \quad \text{for } k > 1\,.\end{aligned} \tag{3.5}$$

It is seen that the maps defined by Eq. (3.4), $\langle\hat{Q}\rangle(z') \longrightarrow \langle\hat{Q}\rangle(z'')$, for the transverse position and momentum operators $(\boldsymbol{r}_\perp, \hat{\boldsymbol{p}}_\perp)$ represent the quantization of the corresponding classical Lie maps (see [14] and [15]) and entail the canonical rule of replacement of the Poisson brackets by the commutator bracket $\{A, B\} \to (1/i\hbar)\,[\hat{A}, \hat{B}]$ and identifying the classical (ray optical) variables with their quantum averages $(\boldsymbol{r}_\perp, \partial\boldsymbol{r}_\perp/\partial z \longrightarrow \langle\boldsymbol{r}_\perp\rangle, \langle\hat{\boldsymbol{p}}_\perp\rangle/p)$ in the manner of Ehrenfest. One can easily recognize Eq. (3.4) to be the optical representation of the Heisenberg picture.

IV. QUANTUM MECHANICS OF THE OPTICS OF RELATIVISTIC CHARGED PARTICLES WITH SCALAR WAVE FUNCTIONS

In the relativistic situation, when $E - q\phi = +\sqrt{(m^2c^4 + c^2p^2)}$, one can easily verify that the corresponding Klein-Gordon equation has the same form as Eq. (2.6), except for the interpretation of p as the relativistic momentum. To this end, one just has to substitute $p^2 = \left(1/c^2\right)(E - q\phi)^2 - m^2c^2$ in Eq. (2.6) and observe that it is transformed into the time-independent Klein-Gordon equation corresponding to energy E. Hence it is obvious that the above formalism comprising Eqs. (2.7)–(2.11) is also valid in the relativistic case exactly in the same form. In other words, if one disregards spin (if nonzero), the quantum theory of the optics of charged-particles, described with scalar wave functions, can be based on Eqs. (2.7)–(2.11) with the appropriate expression for p, i.e., with the relevant approximation in the range from $p \approx \sqrt{2m(E - q\phi)}$ to $p = 1/c\sqrt{(E - q\phi)^2 - m^2c^2}$. This explains the straightforward extension of Glaser's semiclassical treatment of the nonrelativistic quantum mechanics of electron optics to the relativistic case based on the Klein-Gordon equation (of course, as an approximation to a treatment based on the Dirac equation) obtained by Ferwerda, Hoenders, and Slump [9].

V. EXAMPLES OF APPLICATIONS

Let us now consider the application of the above theory to the examples of quadrupole and axially symmetric magnetic lenses. For the ideal magnetic quadrupole lens, with $\boldsymbol{A} = (0, 0, (g/2)\left(x^2 - y^2\right))$ in the lens region ($z_{\rm in} \le z \le z_{\rm out}$) and $\boldsymbol{A} = (0, 0, 0)$ outside,

$$\mathcal{H}_0 \approx \begin{cases} -p + \frac{\hat{p}_\perp^2}{2p} - \frac{qg}{2c}\left(x^2 - y^2\right) + \frac{qg\hbar^2}{8cp^4}\left(\hat{p}_x^2 - \hat{p}_y^2\right) & \text{for } z_{\rm in} \le z \le z_{\rm out} \\ -p + \frac{\hat{p}_\perp^2}{2p} & \text{for } z < z_{\rm in}, z > z_{\rm out} \end{cases} \quad (5.1)$$

in the paraxial approximation (retaining only terms up to second order in $\boldsymbol{r}_\perp$ and $\hat{\boldsymbol{p}}_\perp$). Then the above map for the lens action on the transverse position and momentum components becomes

$$\begin{pmatrix} \langle x \rangle \\ \langle y \rangle \\ \frac{1}{p}\langle \hat{p}_x \rangle \\ \frac{1}{p}\langle \hat{p}_y \rangle \end{pmatrix}_{z_{\rm out}} = T_{QL} \begin{pmatrix} \langle x \rangle \\ \langle y \rangle \\ \frac{1}{p}\langle \hat{p}_x \rangle \\ \frac{1}{p}\langle \hat{p}_y \rangle \end{pmatrix}_{z_{\rm in}}, \quad (5.2)$$

$$T_{QL} = \begin{pmatrix} 1 - \frac{w}{2f} - \frac{\lambda^2}{32\pi^2 f^2} & 0 & w\left(1 - \frac{w}{6f}\right) + \frac{\lambda^2}{16\pi^2 f} & 0 \\ 0 & 1 - \frac{w}{2f} + \frac{\lambda^2}{32\pi^2 f^2} & 0 & w\left(1 - \frac{w}{6f}\right) - \frac{\lambda^2}{16\pi^2 f} \\ -\frac{1}{f}\left(1 - \frac{w}{6f} - \frac{\lambda^2}{96\pi^2 f^2}\right) & 0 & 1 - \frac{w}{2f} - \frac{\lambda^2}{32\pi^2 f^2} & 0 \\ 0 & \frac{1}{f}\left(1 + \frac{w}{6f} - \frac{\lambda^2}{96\pi^2 f^2}\right) & 0 & 1 + \frac{w}{2f} - \frac{\lambda^2}{32\pi^2 f^2} \end{pmatrix}, \quad (5.3)$$

with $w = z_{\rm out} - z_{\rm in}$, $1/f = -qgw/cp$, and $\lambda = h/p$, in the thin lens approximation (retaining only terms up to first order in w/f, assuming $w \ll f$), reproducing the familiar transfer matrix for the quadrupole lens, except for the presence of the quantum correction terms depending on the de Broglie wavelength λ. These quantum correction terms precisely indicate how the classical (ray optics) picture breaks down in the extreme nonrelativistic limit of very low energy beams when $\lambda \gg f$.

For the axially symmetric magnetic lens, one has, under the paraxial approximation,

$$\mathcal{H}_0 \approx \begin{cases} -p + \frac{\hat{p}_\perp^2}{2p} + \left(\frac{q^2 B(z)^2}{8c^2 p} r_\perp^2 - \frac{q}{2cp} B(z) \hat{L}_z\right) \\ \quad + \frac{\hbar^2 q^2 B(z) B'(z)}{32 c^2 p^4}\left(\boldsymbol{r}_\perp \cdot \hat{\boldsymbol{p}}_\perp + \hat{\boldsymbol{p}}_\perp \cdot \boldsymbol{r}_\perp\right) & \text{for } z_{\rm in} \le z \le z_{\rm out} \\ -p + \frac{\hat{p}_\perp^2}{2p} & \text{for } z < z_{\rm in}, \ z > z_{\rm out}, \end{cases} \quad (5.4)$$

where $B'(z) = dB(z)/dz$, $\hat{L}_z$ is the usual z component of the angular momentum operator, and the last term in $\mathcal{H}_0$ for the lens region is the quantum correction term. Correspondingly, for the lens region the $\hat{\mathcal{L}}$ operator becomes

$$\hat{\mathcal{L}} \approx \frac{1}{i\hbar}\left\{ -wp + \frac{w}{2p}\hat{p}_\perp^2 + \frac{p}{2f} r_\perp^2 - \theta \hat{L}_z + \epsilon\left(\boldsymbol{r}_\perp \cdot \hat{\boldsymbol{p}}_\perp + \hat{\boldsymbol{p}}_\perp \cdot \boldsymbol{r}_\perp\right) \right\}, \quad (5.5)$$

with

$$\frac{1}{f} = \int_{z_{\rm in}}^{z_{\rm out}} dz\, \frac{q^2 B(z)^2}{4c^2 p^2}, \qquad \theta = \int_{z_{\rm in}}^{z_{\rm out}} dz\, \frac{qB(z)}{2cp}, \quad (5.6)$$

and

$$\epsilon = \frac{\hbar^2 q^2}{64 c^2 p^4}\left[B\left(z_{\rm out}\right)^2 - B\left(z_{\rm in}\right)^2\right] \quad (5.7)$$

in the thin lens approximation which now entails, in addition to the assumption that $w/f \ll 1$, also approximating the z-ordered exponential in Eq. (3.2) by the ordinary exponential. It is straightforward to see that, under this approximation, the transfer matrix T_{RL} has all the familiar aspects of the classical transfer matrix; the quantum correction term $\epsilon()$ in Eq. (5.5) is seen to vanish under this approximation and only for a thick lens can the quantum correction term in $\mathcal{H}_0$ [see Eq. (5.4)] be expected to contribute to $\hat{\mathcal{L}}$ when the z-ordered exponential in Eq. (3.2) cannot be approximated by the ordinary exponential.

It is to be noted that we have used the thin lens approximation in the above examples only for the purpose of illustrating the way the formalism works. It is clear that the basic formulas (3.2)–(3.5) are quite general and valid in any context (i.e., for any lens field configuration that supports a beam propagation). The only point to be noted is that in the practical computations involving thick lenses, the approximation of the expression for $\hat{\mathcal{L}}$

and the extent of aberrations being taken into account must be consistent. We hope to deal with this topic further, with detailed examples, elsewhere.

VI. QUANTUM MECHANICS OF THE OPTICS OF RELATIVISTIC ELECTRON BEAMS: SPINOR ELECTRON OPTICS

For the electron ($q = -e$), the above formalism is valid in the nonrelativistic case, with the spin ignored. In the relativistic case, if the spin can be regarded as a spectator degree of freedom or the electron wave function can be considered to be a scalar (of course, approximately), the above formalism based on the Klein-Gordon equation (i.e., with the appropriate relativistically correct expression for p) is adequate, as has been noted by Ferwerda, Hoenders, and Slump [9]. If the spin is not disregarded, then one has to treat the quantum mechanics of the optics of relativistic electron beams on the basis of the Dirac equation, the proper equation for the electron. Such a theory based on the Dirac equation, taking into account the four-component spinor character of the wave function and using an algebraic framework as above, already exists (see [10–12] for details). In this theory one can show that in the optical representation the spinor wave function of the quasimonoenergetic quasiparaxial electron beam moving in the $+z$ direction can be represented with two components exactly like for the positive energy electron in the Foldy-Wouthuysen representation of the Dirac theory. Then the corresponding relations for $\left(\langle \boldsymbol{r}_\perp \rangle , \langle \hat{\boldsymbol{p}}_\perp \rangle /p\right)_{\rm in} \longrightarrow \left(\langle \boldsymbol{r}_\perp \rangle , \langle \hat{\boldsymbol{p}}_\perp \rangle /p\right)_{\rm out}$ in the case of the magnetic quadrupole lens are

$$\begin{aligned}
\langle x \rangle_{\rm out} &= \langle x \rangle_{\rm in} - \frac{\lambda}{4\pi f} \langle \sigma_z y \rangle_{\rm in} + \frac{w}{p} \langle \hat{p}_x \rangle_{\rm in} \,, \\
\langle y \rangle_{\rm out} &= -\frac{\lambda}{4\pi f} \langle \sigma_z x \rangle_{\rm in} + \langle y \rangle_{\rm in} + \frac{w}{p} \langle \hat{p}_y \rangle_{\rm in} \,, \\
\frac{1}{p} \langle \hat{p}_x \rangle_{\rm out} &= -\frac{1}{f} \langle x \rangle_{\rm in} - \frac{\lambda}{4\pi f^2} \langle \sigma_z y \rangle_{\rm in} \\
&\quad + \frac{1}{p} \langle \hat{p}_x \rangle_{\rm in} + \frac{\lambda}{4\pi f p} \langle \sigma_z \hat{p}_y \rangle_{\rm in} \,, \\
\frac{1}{p} \langle \hat{p}_y \rangle_{\rm out} &= -\frac{\lambda}{4\pi f^2} \langle \sigma_z x \rangle_{\rm in} + \frac{1}{f} \langle y \rangle_{\rm in} \\
&\quad + \frac{\lambda}{4\pi f p} \langle \sigma_z \hat{p}_x \rangle_{\rm in} + \frac{1}{p} \langle \hat{p}_y \rangle_{\rm in} \,,
\end{aligned} \qquad (6.1)$$

wherein we have omitted the w/f terms of the type occurring in Eq. (5.3). The effect of spin is manifest in the above relations; these spin-dependent terms are also seen to be dominating only when λ becomes comparable to f, as for very low energy electron beams. Similar results can be derived also for the axially symmetric magnetic lens, based on the spinor electron optics. It should be interesting to study the polarization aspects of the electron beam dynamics using such an optical formalism of the Dirac theory.

We have mentioned here the case of the spinor electron optics (see [10–12] for details) only by way of comparison [see Eqs. (5.3) and (6.1)]. If the spin terms are neglected in Eq. (6.1), then it becomes identical to Eq. (5.3) [with the ω/f terms neglected, as in Eq. (6.1)] as is to be expected since the formalism leading to Eq. (5.3) is independent of whether p is relativistic, or nonrelativistic, as already noted. Thus it is seen that the scalar theory developed above on the basis of the nonrelativistic Schrödinger equation (or the Klein-Gordon equation for the relativistic case) is complementary to the spinor electron optics and can be used for understanding the quantum mechanics of the optics of nonrelativistic or relativistic charged particles with scalar wave functions corresponding to the cases of spin being zero or treated only as a spectator degree of freedom. We have developed above the theory for only the case of magnetic electron lenses and to make it complete we have to extend it also to the cases of electrostatic and other electromagnetic lenses. We shall indicate briefly how this can be done in the following, concluding, section.

VII. CONCLUSION: EXTENSION OF THE THEORY TO ELECTROSTATIC AND OTHER ELECTROMAGNETIC LENSES

So far, we have developed an optical formalism of the quantum theory of charged-particle beam transport through magnetic lens systems, at the single-particle level and disregarding spin (or, when nonzero, treating it as an independent, spectator, degree of freedom, thus permitting the wave function to be taken essentially as a scalar), based on the Schrödinger and Klein-Gordon equations, and shown how the quantum theory becomes the conventional ray optical theory in the classical limit. This treatment follows closely a similar theory available for the spinor electron optics based on the Dirac equation, relevant for understanding the quantum mechanics of the optics of relativistic electron (or charged spin-1/2 particle) beams, and hence complements it.

It may be noted that, as already mentioned, the above formalism would be complete only when it is extended also to the cases of electrostatic and other electromagnetic lenses. To this end, we outline in the following how the above formalism can be generalized in a straightforward manner when the electric field is nonzero in the lens region, i.e., $\phi(\boldsymbol{r})$ in Eq. (2.1) cannot be taken to be zero, unlike for a magnetic lens.

Let us rewrite the Schrödinger and Klein-Gordon equation (2.6) for the motion of the charged particle in an electromagnetic field, in general with $p^2 = (1/c^2)\left[(E - q\phi)^2 - m^2c^4\right]$, as

$$\begin{aligned}
&-\frac{1}{\bar{p}} \left(i\hbar \frac{\partial}{\partial z} + \frac{q}{c} A_z \right) \begin{pmatrix} \psi \\ -\frac{1}{\bar{p}} \left(i\hbar \frac{\partial}{\partial z} + \frac{q}{c} A_z \right) \psi \end{pmatrix} \\
&\quad = \begin{pmatrix} 0 & 1 \\ \frac{1}{\bar{p}^2} \left(p^2 - \hat{\pi}_\perp^2 \right) & 0 \end{pmatrix} \begin{pmatrix} \psi \\ -\frac{1}{\bar{p}} \left(i\hbar \frac{\partial}{\partial z} + \frac{q}{c} A_z \right) \psi \end{pmatrix} ,
\end{aligned} \qquad (7.1)$$

where $\bar{p} = +(1/c)\sqrt{E^2 - m^2c^4}$ is the magnitude of the momentum of the beam particle in the field-free input region ($z < z_{\rm in}$) corresponding to the constant energy E. It is clear that the constant $1/\bar{p}$ is the expansion parameter we need for the development of the theory in the general case along the same lines as in the case of the magnetic lens; in the field-free output region also $\bar{p}$ would be the magnitude of the momentum, since the energy E is constant, though its components would have been altered by the lens field. For a lens system supporting beam propagation one should expect that $\bar{p}^2 - p^2 \ll \bar{p}^2$. Now define

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \psi \\ -\frac{1}{\bar{p}}\left(i\hbar\frac{\partial}{\partial z} + \frac{q}{c}A_z\right)\psi \end{pmatrix} . \quad (7.2)$$

This transformation turns Eq. (7.1) into

$$-\frac{1}{\bar{p}}\left(i\hbar\frac{\partial}{\partial z} + \frac{q}{c}A_z\right)\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 + \frac{1}{\bar{p}^2}\left(p^2 - \hat{\pi}_\perp^2\right) & -1 + \frac{1}{\bar{p}^2}\left(p^2 - \hat{\pi}_\perp^2\right) \\ 1 - \frac{1}{\bar{p}^2}\left(p^2 - \hat{\pi}_\perp^2\right) & -1 - \frac{1}{\bar{p}^2}\left(p^2 - \hat{\pi}_\perp^2\right) \end{pmatrix} \times \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} , \quad (7.3)$$

which can be rearranged to give the desired optical representation

$$i\hbar\frac{\partial}{\partial z}\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = H\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} , \qquad H = -\bar{p}\sigma_z + \hat{\mathcal{E}} + \hat{\mathcal{O}} ,$$

$$\hat{\mathcal{E}} = -\frac{q}{c}A_z 1\!\!1 + \frac{1}{2\bar{p}}\left(\hat{\pi}_\perp^2 + \tilde{p}^2\right)\sigma_z , \quad \hat{\mathcal{O}} = \frac{1}{2\bar{p}}\left(\hat{\pi}_\perp^2 + \tilde{p}^2\right)i\sigma_y ,$$

$$\text{with} \quad \tilde{p}^2 = \bar{p}^2 - p^2 = \frac{1}{c^2}q\phi(2E - q\phi). \quad (7.4)$$

The expressions for p and $\bar{p}$ can be approximated depending on how far relativistic the situation is; in the nonrelativistic limit one can take $p^2 \approx 2m(E - q\phi)$, $\bar{p} \approx +\sqrt{2mE}$, and $\tilde{p}^2 \approx 2mq\phi$. Again, one should note the generality of the formalism.

It is clear that in the case of the magnetic lens, with $\phi = 0$, $\tilde{p} = 0$ and Eq. (7.4) coincides with Eq. (2.8). Now Eq. (7.4), corresponding to any general electromagnetic lens configuration, is of the same form as Eq. (2.8) and hence a theory of the same type as above, with $1/\bar{p}$ as the expansion parameter, can be developed for dealing with it. The quantum transfer map of a large system can be constructed from the knowledge of the propagators of the "local" blocks comprising it, as in the classical case following the Lie methods (see, e.g., [15] for details).

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