Quantum Theory of Charged-Particle Beam Optics

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- References

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Motivation for a Quantum Theory of Charged-Particle Beam Optics

Charged particle beam optics, or the theory of transport of charged particle beams through electromagnetic systems, is traditionally dealt with using classical mechanics. This is the case in ion optics, electron microscopy, accelerator physics etc. Though the classical treatment has been very successful, in the designing and working of numerous optical components, it is natural to look for a prescription based on quantum theory, since any physical system is quantum at the fundamental level!. Such a prescription can be believed to lead surely to a deeper understanding of the working of charged particle beam devices.

- 1930 Glaser
  Quantum theory of Image Formation in Electron Microscopy
  Nonrelativistic Schrödinger equation, Semiclassical

  Paraxial   exact

  Aberrations   put by hand

- 1934 Rubinovicz, 1953 Durand, 1953 Phan-Van-Loc
  Electron Diffraction based on the Dirac Equation

- 1986, Ferwerda *et al*
  Justified the use of scalar (Klein-Gordon) equation for image formation, in practical microscopes

- 1989-90, Jagannathan *et al*
  For the first time focusing theory of electron lenses was derived using Dirac equation

  1. R. Jagannathan, R. Simon, E. C. G. Sudarshan and N. Mukunda,
     Quantum theory of magnetic electron lenses based on the Dirac equation
     Phys. Lett. A **134** (1989) 457-464.
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  3. R. Jagannathan,
     Quantum theory of electron lenses based on the Dirac equation
     Phys. Rev. A **42** (1990) 6674-6689.

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- 1992
  Phase-space Wigner distribution functions

  In paraxial approximation

- 1995
  Quantum theory of aberrations to all orders

  Klein-Gordon Theory

  Dirac Theory

- 1996
  Spin dynamics of the Dirac-particle beam

Quantum Methodology

In designing and evaluating the performance of optical elements in a charged-particle beam device we are interested in studying the evolution of the device parameters along the optic axis of the system. Thus, if quantum methodology is used one would like to know the evolution of the wavefunction of the beam particle as a function of s, the coordinate along the optic axis. Hence, the appropriate equation for study is

$$i\hbar \frac{\partial}{\partial s} \psi(x, y; s) = H(x, y; s) \psi(x, y; s) \,, \tag{1}$$

where x, y and s constitute a curvilinear coordinate system adapted to the symmetry of the system. Whether one is dealing with the system using the nonrelativistic Schrödinger equation, or Klein-Gordon equation, Dirac equation, or any other relativistic wave equations (higher spin ones for example), the first step would be to cast the time-independent basic equation, relevant for treating the static or optical properties (not the dynamic or time-dependent elements), in the above form (1). Then, one must find a way to expand the optical Hamiltonian H as a series in $|\hat{\pi}_\perp / p_0|$ where p_0 is the design (or average) momentum of the beam particles moving predominantly along the direction of the optic axis and $\hat{\pi}_\perp$ represents the small transverse kinetic momentum. The value of $|\pi_\perp / p_0|$ is a measure of the divergence of the beam and when it is very small $\ll 1$ the beam is paraxial or ideal. Deviation from this ideal paraxial situation leads to all the problems of nonlinearity or aberrations. Once the optical Hamiltonian is expanded in such a series one can use approximations to suit the situation by truncating the H appropriately. When H is suitably modeled (approximated to be hermitian, ignoring the dissipating terms) straightforward integration of (1) gives

$$\psi(x, y; s) = U \left(s, s_0\right) \psi \left(x, y; s_0\right) \,. \tag{2}$$

Then, the transfer maps

$$\left\langle \psi \left(s_0\right) \left| \hat{O} \right| \psi \left(s_0\right) \right\rangle \longrightarrow \left\langle \psi \left(s\right) \left| \hat{O} \right| \psi \left(s\right) \right\rangle = \left\langle \psi \left(s_0\right) \left| U^\dagger \hat{O} U \right| \psi \left(s_0\right) \right\rangle \tag{3}$$

for all the relevant observables $\{\hat{O}\}$ are what are wanted for obtaining a picture of the behaviour of the system; in the case of imaging systems the relevant observables are the transverse phase-space coordinates and in the case of polarized beam storage rings the spin components are also relevant. That is all for the general framework of quantum methodology in beam physics - the rest are the technical details of how to implement this programme in particular cases. In the case of electron beam storage rings approximation of H by a hermitian expression would not be appropriate since radiation losses (synchrotron radiation), occuring when the beam passes through bending magnets, will not be ignorable; in this case H will have contain also the nonhermitian dissipating terms.

Dirac Equation

$$\hat{\mathrm{H}}_D \left|\psi_D\right\rangle = E \left|\psi_D\right\rangle \,, \tag{4}$$

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 $\hat{\mathrm{H}}_D$, including the Pauli term is given by

$$\begin{aligned}
\hat{\mathrm{H}}_D &= \beta m_0 c^2 + c\boldsymbol{\alpha} \cdot (-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}) - \mu_a \beta \boldsymbol{\Sigma} \cdot \boldsymbol{B}\,, \\
\beta &= \begin{pmatrix} 1\!\!1 & \boldsymbol{0} \\ \boldsymbol{0} & -1\!\!1 \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \boldsymbol{0} \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\sigma} \end{pmatrix}, \\
1\!\!1 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad I = \begin{pmatrix} 1\!\!1 & \boldsymbol{0} \\ \boldsymbol{0} & 1\!\!1 \end{pmatrix}, \\
\sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{aligned} \tag{5}$$

Note that we are dealing with the scattering states of the time-independent Hamiltonian $\hat{\mathrm{H}}_D$ with conserved positive energy

$$E = +\sqrt{m_0^2 c^4 + c^2 p_0^2}\,, \quad p_0 = |\boldsymbol{p}_0|\,, \tag{6}$$

where $\boldsymbol{p}_0$ is the momentum of the beam particle entering the system from the field-free input region.

Paraxial Condition

$$|p_x| \ll p_0\,, \quad |p_y| \ll p_0\,.p_z \approx p_0 = |\boldsymbol{p}_0| = \sqrt{p_x^2 + p_y^2 + p_z^2} \tag{7}$$

The Desired Form

We are interested in the evolution of the beam parameters along the optic axis of the system, the desired form of the Dirac equation is:

$$
\mathrm{i}\hbar \frac{\partial}{\partial z} \left|\psi_D\right\rangle = \hat{\mathcal{H}}_D \left|\psi_D\right\rangle \,, \tag{8}
$$

So we multiply $\hat{\mathcal{H}}_D$ (on the left) by α_z/c and rearrange the terms to get the desired form : The result is that

$$
\begin{aligned}
\hat{\mathcal{H}}_D &= -p_0 \beta \chi \alpha_z - q A_z I + \alpha_z \boldsymbol{\alpha}_\perp \cdot \hat{\boldsymbol{\pi}}_\perp + (\mu_a/c) \beta \alpha_z \boldsymbol{\Sigma} \cdot \boldsymbol{B} \,, \\
\chi &= \begin{pmatrix} \xi \mathbb{1} & \mathbf{0} \\ \mathbf{0} & -\xi^{-1} \mathbb{1} \end{pmatrix} , \quad \xi = \sqrt{\frac{E + m_0 c^2}{E - m_0 c^2}} \,, \\
\hat{\boldsymbol{\pi}}_\perp &= \left(-\mathrm{i}\hbar \boldsymbol{\nabla}_\perp - q \boldsymbol{A}_\perp\right) = \left(\hat{\boldsymbol{p}}_\perp - q \boldsymbol{A}_\perp\right) .
\end{aligned} \tag{9}
$$

To Obtain the Standard Form

Define,

$$M = \frac{1}{\sqrt{2}}(I + \chi\alpha_z)\,, \qquad M^{-1} = \frac{1}{\sqrt{2}}(I - \chi\alpha_z)\,. \tag{10}$$

and

$$|\psi_D\rangle \longrightarrow |\psi'\rangle = M\,|\psi_D\rangle\ . \tag{11}$$

Then

$$\mathrm{i}\hbar\frac{\partial}{\partial z}\,|\psi'\rangle = \hat{\mathcal{H}}'\,|\psi'\rangle\ , \quad \hat{\mathcal{H}}' = M\hat{\mathcal{H}}_D M^{-1} = -p_0\beta + \hat{\mathcal{E}} + \hat{\mathcal{O}}\,, \tag{12}$$

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

$$\begin{aligned}
\hat{\mathcal{E}}_{11} &= -qA_z1\!\!1 - (\mu_a/2c)\left\{\left(\xi + \xi^{-1}\right)\boldsymbol{\sigma}_\perp\cdot\boldsymbol{B}_\perp + \left(\xi - \xi^{-1}\right)\sigma_z B_z\right\}\,, \\
\hat{\mathcal{E}}_{12} &= \hat{\mathcal{E}}_{21} = \mathbf{0}\,, \\
\hat{\mathcal{E}}_{22} &= -qA_z1\!\!1 - (\mu_a/2c)\left\{\left(\xi + \xi^{-1}\right)\boldsymbol{\sigma}_\perp\cdot\boldsymbol{B}_\perp - \left(\xi - \xi^{-1}\right)\sigma_z B_z\right\}\,,
\end{aligned} \tag{13}$$

and

$$\begin{aligned}
\hat{\mathcal{O}}_{11} &= \hat{\mathcal{O}}_{22} = \mathbf{0}\,, \\
\hat{\mathcal{O}}_{12} &= \xi\,\Big[\boldsymbol{\sigma}_\perp\cdot\hat{\boldsymbol{\pi}}_\perp - (\mu_a/2c)\Big\{\mathrm{i}\left(\xi - \xi^{-1}\right)(B_x\sigma_y - B_y\sigma_x) \\
&\qquad\qquad - \left(\xi + \xi^{-1}\right)B_z1\!\!1\Big\}\Big]\,, \\
\hat{\mathcal{O}}_{21} &= -\xi^{-1}\,\Big[\boldsymbol{\sigma}_\perp\cdot\hat{\boldsymbol{\pi}}_\perp + (\mu_a/2c)\Big\{\mathrm{i}\left(\xi - \xi^{-1}\right)(B_x\sigma_y - B_y\sigma_x) \\
&\qquad\qquad + \left(\xi + \xi^{-1}\right)B_z1\!\!1\Big\}\Big]\,.
\end{aligned} \tag{14}$$

The Significance of the above transformation:
Example of the standard free Dirac plane-wave:

$$
\begin{aligned}
\left(\begin{array}{c}
\psi_{FD1}(\boldsymbol{r}_\perp, z) \\
\psi_{FD2}(\boldsymbol{r}_\perp, z) \\
\psi_{FD3}(\boldsymbol{r}_\perp, z) \\
\psi_{FD4}(\boldsymbol{r}_\perp, z)
\end{array}\right)
& = & \frac{1}{4}\sqrt{\frac{\xi c p}{\pi^3 \hbar^3 E}}
\left(\begin{array}{c}
s_+ \\
s_- \\
\{s_- p_- + s_+ p_z\}/\xi p \\
\{s_+ p_+ - s_- p_z\}/\xi p
\end{array}\right) \\
& & \times\ \exp\left\{\frac{\mathrm{i}}{\hbar}\left(\boldsymbol{p}_\perp \cdot \boldsymbol{r}_\perp + p_z z\right)\right\}\,, \\
\boldsymbol{r}_\perp & = & (x, y)\,, \quad |s_+|^2 + |s_-|^2 = 1\,, \\
p_+ & = & p_x + \mathrm{i} p_y\,, \quad p_- = p_x - \mathrm{i} p_y\,. \qquad (15)
\end{aligned}
$$

Correspondingly,

$$
\begin{aligned}
\left(\begin{array}{c}
\psi'_{F1}(\boldsymbol{r}_\perp, z) \\
\psi'_{F2}(\boldsymbol{r}_\perp, z) \\
\psi'_{F3}(\boldsymbol{r}_\perp, z) \\
\psi'_{F4}(\boldsymbol{r}_\perp, z)
\end{array}\right)
& = & \frac{1}{4}\sqrt{\frac{\xi c p}{2\pi^3 \hbar^3 E}}
\left(\begin{array}{c}
\{s_+(p + p_z) + s_- p_-\}/p \\
\{s_-(p + p_z) - s_+ p_+\}/p \\
-\{s_+(p - p_z) - s_- p_-\}/\xi p \\
\{s_-(p - p_z) + s_+ p_+\}/\xi p
\end{array}\right) \\
& & \times\ \exp\left\{\frac{\mathrm{i}}{\hbar}\left(\boldsymbol{p}_\perp \cdot \boldsymbol{r}_\perp + p_z z\right)\right\}\,, \qquad (16)
\end{aligned}
$$

Lower spinor components are very small compared to the upper spinor components!

The Anology

Standard Dirac Equation	**Beam Optical Form**
$m_0 c^2 \beta + \hat{\mathcal{E}}_D + \hat{\mathcal{O}}_D$	$-p_0 \beta + \hat{\mathcal{E}} + \hat{\mathcal{O}}$
$\mathrm{i}\hbar\frac{\partial}{\partial t}$	$\mathrm{i}\hbar\frac{\partial}{\partial z}$
Positive Energy	Forward Propagation
Nonrelativistic, $\lvert\boldsymbol{\pi}\rvert \ll m_0 c$	Paraxial Beam, $\lvert\boldsymbol{\pi}_\perp\rvert \ll p_0$
Non relativistic Motion	Paraxial Behavior
+ Relativistic Corrections	+ Aberration Corrections

The Beam Optical Form $\equiv$ The Standard Dirac Equation

The Foldy-Wouthuysen-like Transformation Technique

It reduces the strength of the odd operator which couples the upper pair and lower pair components of the Dirac spinor.

$$\left|\psi'\right\rangle = \exp\left(\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right)\left|\psi^{(1)}\right\rangle \,. \tag{17}$$

Then

$$\begin{aligned}
{\rm i}\hbar\frac{\partial}{\partial z}\left|\psi^{(1)}\right\rangle &= \hat{\mathcal{H}}^{(1)}\left|\psi^{(1)}\right\rangle \,, \\
\hat{\mathcal{H}}^{(1)} &= \exp\left(-\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right)\hat{\mathcal{H}}' \, \exp\left(\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right) \\
&\qquad -{\rm i}\hbar\exp\left(-\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right)\frac{\partial}{\partial z}\left\{\exp\left(\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right)\right\} \\
&= -p_0\beta + \hat{\mathcal{E}}^{(1)} + \hat{\mathcal{O}}^{(1)} \,, \\
\hat{\mathcal{E}}^{(1)} &= \hat{\mathcal{E}} - \frac{1}{2p_0}\beta\hat{\mathcal{O}}^2 + \cdots \,, \\
\hat{\mathcal{O}}^{(1)} &= -\frac{1}{2p_0}\beta\left\{\left[\hat{\mathcal{O}},\hat{\mathcal{E}}\right] + {\rm i}\hbar\frac{\partial}{\partial z}\hat{\mathcal{O}}\right\} + \cdots \,.
\end{aligned} \tag{18}$$

The 11-block element of $\hat{\mathcal{H}}^{(1)}$:

$$\begin{aligned}
\hat{\mathcal{H}}_{11}^{(1)} &= -p_0 1\!\!1 + \hat{\mathcal{E}}_{11}^{(1)} \\
&= \left\{-p_0 - qA_z + \frac{1}{2p_0}\hat{\pi}_\perp^{\,2} - \frac{\epsilon\hbar^2}{4p_0^2}({\rm curl}\,\boldsymbol{B})_z + \frac{\epsilon^2\hbar^2}{8p_0^3}\left(B_\perp^2 + \gamma^2 B_z^2\right)\right\} 1\!\!1 \\
&\quad -\frac{1}{p_0}\left\{(q+\epsilon)B_z S_z + \gamma\epsilon\boldsymbol{B}_\perp\cdot\boldsymbol{S}_\perp\right\} \\
&\quad +\frac{\epsilon}{2p_0^2}\left\{\gamma\left(B_z\boldsymbol{S}_\perp\cdot\hat{\boldsymbol{\pi}}_\perp + \boldsymbol{S}_\perp\cdot\hat{\boldsymbol{\pi}}_\perp B_z\right) - \left(\boldsymbol{B}_\perp\cdot\hat{\boldsymbol{\pi}}_\perp + \hat{\boldsymbol{\pi}}_\perp\cdot\boldsymbol{B}_\perp\right)S_z\right\} \,,
\end{aligned}$$

$$\hat{\pi}_\perp^{\,2} = \hat{\pi}_x^2 + \hat{\pi}_y^2 \,, \quad \epsilon = 2m_0\mu_a/\hbar \,, \quad \gamma = E/m_0c^2 \,, \quad \boldsymbol{S} = \frac{1}{2}\hbar\boldsymbol{\sigma} \;\;. \tag{19}$$

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\partial\psi^{(3)}}{\partial z} &\approx \hat{H}^{(3)}\psi^{(3)} && (20)\\
\hat{H}^{(3)} &= -p_0\beta + \hat{\mathcal{E}} - \frac{1}{2p_0}\beta\hat{\mathcal{O}}^2 - \frac{1}{8p_0^2}\left[\hat{\mathcal{O}}, \left(\left[\hat{\mathcal{O}}, \hat{\mathcal{E}}\right] + \mathrm{i}\hbar\left(\frac{\partial\hat{\mathcal{O}}}{\partial z}\right)\right)\right] \\
&\qquad + \frac{1}{8p_0^3}\beta\left\{\hat{\mathcal{O}}^4 + \left(\left[\hat{\mathcal{O}}, \hat{\mathcal{E}}\right] + \frac{\mathrm{i}\lambda_0}{2\pi}\left(\frac{\partial\hat{\mathcal{O}}}{\partial z}\right)\right)^2\right\}. && (21)
\end{aligned}
$$

$$
\mathrm{i}\hbar\frac{\partial}{\partial z}\hat{\mathcal{T}}\left(z, z^{(1)}\right) = \hat{\mathcal{H}}_o\hat{\mathcal{T}}\left(z, z^{(1)}\right), \quad \hat{\mathcal{T}}\left(z^{(1)}, z^{(1)}\right) = \hat{\mathcal{I}}
$$

$$
\begin{aligned}
&\hat{\mathcal{T}}\left(z^{(2)}, z^{(1)}\right) = \wp\left\{\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{z^{(1)}}^{z^{(2)}} dz\,\hat{\mathcal{H}}_o(z)\right)\right\} \\
&\quad = \hat{\mathcal{I}} - \frac{\mathrm{i}}{\hbar}\int_{z^{(1)}}^{z^{(2)}} dz\,\hat{\mathcal{H}}_o(z) \\
&\qquad + \left(-\frac{\mathrm{i}}{\hbar}\right)^2\int_{z^{(1)}}^{z^{(2)}} dz\int_{z^{(1)}}^{z} dz'\,\hat{\mathcal{H}}_o(z)\hat{\mathcal{H}}_o(z') \\
&\qquad + \left(-\frac{\mathrm{i}}{\hbar}\right)^3\int_{z^{(1)}}^{z^{(2)}} dz\int_{z^{(1)}}^{z} dz'\int_{z^{(1)}}^{z'} dz''\,\hat{\mathcal{H}}_o(z)\hat{\mathcal{H}}_o(z')\hat{\mathcal{H}}_o(z'') \\
&\qquad + \ldots, && (22)
\end{aligned}
$$

$$
\begin{aligned}
\langle\boldsymbol{r}_\perp\rangle(z) &= \left\langle\hat{\mathcal{T}}^{I\,\dagger}\hat{U}_p^\dagger\boldsymbol{r}_\perp\hat{U}_p\hat{\mathcal{T}}^I\right\rangle(z_{\mathrm{o}}) && (23)\\
\langle\boldsymbol{p}_\perp\rangle(z) &= \left\langle\hat{\mathcal{T}}^{I\,\dagger}\hat{U}_p^\dagger\hat{\boldsymbol{p}}_\perp\hat{U}_p\hat{\mathcal{T}}^I\right\rangle(z_{\mathrm{o}}). && (24)
\end{aligned}
$$

Beam-Optical Form $\longrightarrow$ Accelerator Optical Form

Laboratory frame $\longrightarrow$ Instantaneous Rest frame

$$\left|\tilde{\psi}\right\rangle = \exp\left\{\frac{\mathrm{i}}{2p_0}\left(\hat{\pi}_x\sigma_y - \hat{\pi}_y\sigma_x\right)\right\}\left|\psi^{(A)}\right\rangle \, . \tag{25}$$

Then

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial z}\left|\psi^{(A)}\right\rangle &= \hat{H}^{(A)}\left|\psi^{(A)}\right\rangle \, , \\
\hat{H}^{(A)} &\approx \left(-p_0 - qA_z + \frac{1}{2p_0}\hat{\pi}_\perp^{\,2}\right) + \frac{\gamma m_0}{p_0}\underline{\boldsymbol{\Omega}}_s\cdot\boldsymbol{S} \, , \\
\text{with } \ \underline{\boldsymbol{\Omega}}_s &= -\frac{1}{\gamma m_0}\left\{q\boldsymbol{B} + \epsilon\left(\boldsymbol{B}_\parallel + \gamma\boldsymbol{B}_\perp\right)\right\} \, ,
\end{aligned} \tag{26}$$

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

$$\begin{aligned}
\hat{O}^{(A)} = \ & \text{the hermitian part of the } 11 - \text{block element of} \\
& \Bigg(\exp\left\{-\frac{\mathrm{i}}{2p_0}\left(\hat{\pi}_x\Sigma_y - \hat{\pi}_y\Sigma_x\right)\right\} \\
& \times\exp\left(-\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right)M\hat{O}_D M^{-1}\exp\left(\frac{1}{2p_0}\beta\hat{\mathcal{O}}\right) \\
& \times\exp\left\{\frac{\mathrm{i}}{2p_0}\left(\hat{\pi}_x\Sigma_y - \hat{\pi}_y\Sigma_x\right)\right\}\Bigg) \, .
\end{aligned} \tag{27}$$

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

$$\boldsymbol{S}_R = \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} - \frac{c^2(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\cdot\boldsymbol{\sigma})}{2E(E+m_0c^2)} & \frac{c\hat{\boldsymbol{\pi}}}{E} \\ \frac{c\hat{\boldsymbol{\pi}}}{E} & -\boldsymbol{\sigma} + \frac{c^2(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\cdot\boldsymbol{\sigma})}{2E(E+m_0c^2)} \end{pmatrix} . \tag{28}$$

$$\boldsymbol{S}_R^{(A)} \approx \frac{\hbar}{2}\boldsymbol{\sigma} \tag{29}$$

Normal Magnetic Quadrupole

$$\boldsymbol{B} = (-Gy, -Gx, 0), \tag{30}$$

$$\boldsymbol{A} = \left(0, 0, \frac{1}{2}G\left(x^2 - y^2\right)\right)\,, \tag{31}$$

Accelerator optical Hamiltonian

$$\hat{H}(z) = \begin{cases} \hat{H}_F = -p_0 + \frac{1}{2p_0}\hat{p}_\perp^{\,2}\,, \quad \text{for} \ \ z < z_{\rm n} \ \ \text{and} \ \ z > z_{\rm x}\,, \\ \\ \hat{H}_L(z) = -p_0 + \frac{1}{2p_0}\hat{p}_\perp^{\,2} - \frac{1}{2}qG\left(x^2 - y^2\right) + \frac{\eta p_0}{\ell}\left(y\sigma_x + x\sigma_y\right)\,, \\ \\ \qquad\qquad \text{for} \ \ z_{\rm n} \le z \le z_{\rm x}\,, \quad \text{with} \ \ \eta = (q + \gamma\epsilon)G\ell\hbar/2p_0^2\,. \end{cases} \tag{32}$$

$$\begin{aligned} \hat{H}(z) &= \hat{\bar{\bar{H}}}(z) + \hat{\tilde{\bar{H}}}(z)\,, \\ \\ \hat{\bar{\bar{H}}}(z) &= \begin{cases} \hat{\bar{\bar{H}}}_F \equiv \hat{\hat{H}}_F\,, \quad \text{for} \ \ z < z_{\rm n} \ \ \text{and} \ \ z > z_{\rm x}\,, \\ \\ \hat{\bar{\bar{H}}}_L(z) = -p_0 + \frac{1}{2p_0}\hat{p}_\perp^{\,2} - \frac{1}{2}qG\left(x^2 - y^2\right)\,, \quad \text{for} \ \ z_{\rm n} \le z \le z_{\rm x}\,. \end{cases} \\ \hat{\tilde{\bar{H}}}(z) &= \begin{cases} \tilde{H}_F = 0\,, \quad \text{for} \ \ z < z_{\rm n} \ \ \text{and} \ \ z > z_{\rm x}\,, \\ \\ \hat{\tilde{\bar{H}}}_L(z) = \frac{\eta p_0}{\ell}\left(y\sigma_x + x\sigma_y\right)\,, \quad \text{for} \ \ z_{\rm n} \le z \le z_{\rm x}\,. \end{cases} \end{aligned} \tag{33}$$

Let us take $z_{\rm o}$ and z to be respectively in the field-free input and output regions of the quadrupole magnet : $z_{\rm o} < z_{\rm n}$, $z > z_{\rm x}$.

$$\hat{\hat{U}}\,(z, z_{\rm o}) = \hat{\hat{U}}_F(z, z_{\rm x})\hat{\hat{U}}_L(z_{\rm x}, z_{\rm n})\hat{\hat{U}}_F(z_{\rm n}, z_{\rm o})\,,$$

$$\hat{\hat{U}}_i\,(z, z_{\rm o}) = \hat{\hat{U}}_{i,F}(z, z_{\rm x})\hat{\hat{U}}_{i,L}(z_{\rm x}, z_{\rm n})\hat{\hat{U}}_{i,F}(z_{\rm n}, z_{\rm o}) \equiv \hat{\hat{U}}_{i,L}(z_{\rm x}, z_{\rm n})\,,$$

$$\hat{\hat{U}}_F(z, z_{\rm x}) = \exp\left\{\frac{\rm i}{\hbar}\Delta z_> \left(p_0 - \frac{1}{2p_0}\hat{p}_\perp^{\,2}\right)\right\}\,, \quad \text{with} \;\; \Delta z_> = z - z_{\rm x}\,,$$

$$\hat{\hat{U}}_L(z_{\rm x}, z_{\rm n}) = \exp\left\{\frac{\rm i}{\hbar}\ell\left[\left(p_0 - \frac{1}{2p_0}\hat{p}_\perp^{\,2}\right) + \frac{1}{2}p_0K(x^2 - y^2)\right]\right\}\,,$$

$$\text{with} \;\; K = qG/p_0\,,$$

$$\hat{\hat{U}}_F(z_{\rm n}, z_{\rm o}) = \exp\left\{\frac{\rm i}{\hbar}\Delta z_< \left(p_0 - \frac{1}{2p_0}\hat{p}_\perp^{\,2}\right)\right\}\,, \quad \text{with} \;\; \Delta z_< = z_{\rm n} - z_{\rm o}\,,$$

$$\begin{aligned}
&\hat{\hat{U}}_{i,L}(z_{\rm x}, z_{\rm n}) \\
&\quad = \exp\left\{-\frac{\rm i}{\hbar}\eta\left[\left(\left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell}\right)p_0x + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K\ell}\right)\hat{p}_x\right)\sigma_y\right.\right. \\
&\qquad\quad \left.\left. + \left(\left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell}\right)p_0y - \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K\ell}\right)\hat{p}_y\right)\sigma_x\right]\right\}\,. \quad (34)
\end{aligned}$$

The Transfer Maps

$$\begin{pmatrix} \langle x\rangle(z) \\ \langle \hat{p}_x\rangle(z)/p_0 \\ \langle y\rangle(z) \\ \langle \hat{p}_y\rangle(z)/p_0 \end{pmatrix} \approx \begin{pmatrix} T^x_{11} & T^x_{12} & 0 & 0 \\ T^x_{21} & T^x_{22} & 0 & 0 \\ 0 & 0 & T^y_{11} & T^y_{12} \\ 0 & 0 & T^y_{21} & T^y_{22} \end{pmatrix} \left(\begin{pmatrix} \langle x\rangle(z_{\rm o}) \\ \langle \hat{p}_x\rangle(z_{\rm o})/p_0 \\ \langle y\rangle(z_{\rm o}) \\ \langle \hat{p}_y\rangle(z_{\rm o})/p_0 \end{pmatrix} + \eta \begin{pmatrix} \left(\frac{\cosh\left(\sqrt{K}\,\ell\right)-1}{K\ell}\right)\langle \sigma_y\rangle(z_{\rm o}) \\ -\left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell}\right)\langle \sigma_y\rangle(z_{\rm o}) \\ -\left(\frac{\cos\left(\sqrt{K}\,\ell\right)-1}{K\ell}\right)\langle \sigma_x\rangle(z_{\rm o}) \\ -\left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell}\right)\langle \sigma_x\rangle(z_{\rm o}) \end{pmatrix} \right),$$

$$\begin{pmatrix} T^x_{11} & T^x_{12} \\ T^x_{21} & T^x_{22} \end{pmatrix} = \begin{pmatrix} 1 & \Delta z_> \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cosh\left(\sqrt{K}\,\ell\right) & \frac{1}{\sqrt{K}}\sinh\left(\sqrt{K}\,\ell\right) \\ \sqrt{K}\,\sinh\left(\sqrt{K}\,\ell\right) & \cosh\left(\sqrt{K}\,\ell\right), \end{pmatrix} \begin{pmatrix} 1 & \Delta z_< \\ 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} T^y_{11} & T^y_{12} \\ T^y_{21} & T^y_{22} \end{pmatrix} = \begin{pmatrix} 1 & \Delta z_> \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\left(\sqrt{K}\,\ell\right) & \frac{1}{\sqrt{K}}\sin\left(\sqrt{K}\,\ell\right) \\ -\sqrt{K}\,\sin\left(\sqrt{K}\,\ell\right) & \cos\left(\sqrt{K}\,\ell\right) \end{pmatrix} \begin{pmatrix} 1 & \Delta z_< \\ 0 & 1 \end{pmatrix},$$

$$
\begin{aligned}
\langle S_x \rangle (z) \approx{}& \langle S_x \rangle (z_{\rm o}) + \\
& \frac{4\pi\eta}{\lambda_0} \left(\left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle x S_z \rangle (z_{\rm o}) \right. \\
& \left. + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K \ell p_0} \right) \langle \hat{p}_x S_z \rangle (z_{\rm o}) \right) \,, \\
\langle S_y \rangle (z) \approx{}& \langle S_y \rangle (z_{\rm o}) - \\
& \frac{4\pi\eta}{\lambda_0} \left(\left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle y S_z \rangle (z_{\rm o}) \right. \\
& \left. - \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K \ell p_0} \right) \langle \hat{p}_y S_z \rangle (z_{\rm o}) \right) \,, \\
\langle S_z \rangle (z) \approx{}& \langle S_z \rangle (z_{\rm o}) - \\
& \frac{4\pi\eta}{\lambda_0} \left\{ \left(\frac{\sinh\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle x S_x \rangle (z_{\rm o}) \right. \\
& - \left(\frac{\sin\left(\sqrt{K}\,\ell\right)}{\sqrt{K}\,\ell} \right) \langle y S_y \rangle (z_{\rm o}) \\
& + \left(\frac{\cosh\left(\sqrt{K}\,\ell\right) - 1}{K \ell p_0} \right) \langle \hat{p}_x S_x \rangle (z_{\rm o}) \\
& \left. + \left(\frac{\cos\left(\sqrt{K}\,\ell\right) - 1}{K \ell p_0} \right) \langle \hat{p}_y S_y \rangle (z_{\rm o}) \right\} \,. \qquad (35)
\end{aligned}
$$

The above transfer maps are consistent with the Thomas-BMT Equation.

(to be Generalized!)

Axially symmetric magnetic lens

$$
\begin{aligned}
\phi(\boldsymbol{r}) &= 0 \qquad (36)\\
\boldsymbol{A} &= \left(-\frac{y}{2}\Pi(\boldsymbol{r}_\perp, z)\,,\,\frac{x}{2}\Pi(\boldsymbol{r}_\perp, z)\,,\,0\right)\,, \qquad (37)
\end{aligned}
$$

with

$$
\begin{aligned}
\Pi(\boldsymbol{r}_\perp, z) &= \sum_{n=0}^{\infty} \frac{1}{n!(n+1)!}\left(-\frac{r_\perp^2}{4}\right)^n B^{(2n)}(z)\\
&= B(z) - \frac{1}{8}r_\perp^2 B''(z) + \frac{1}{192}r_\perp^4 B''''(z) - \ldots\,,
\end{aligned}
\qquad (38)
$$

The corresponding magnetic field is

$$
\begin{aligned}
\boldsymbol{B}_\perp &= -\frac{1}{2}\left(B'(z) - \frac{1}{8}r_\perp^2 B'''(z) + \ldots\right)\boldsymbol{r}_\perp\\
B_z &= B(z) - \frac{1}{4}r_\perp^2 B''(z) + \frac{1}{64}r_\perp^4 B''''(z) - \ldots\,, \qquad (39)
\end{aligned}
$$

$$
\begin{aligned}
\phi(\boldsymbol{r}) &= 0 \qquad (40)\\
\boldsymbol{A} &= \left(-\frac{1}{2}y\Pi(\boldsymbol{r}_\perp, z)\,,\,\frac{1}{2}x\Pi(\boldsymbol{r}_\perp, z)\,,\,0\right)\,,\\
&\quad \text{with}\ \ \Pi(\boldsymbol{r}_\perp, z) = B(z) - \frac{1}{8}r_\perp^2 B''(z)\,. \qquad (41)
\end{aligned}
$$

Then, the beam-optical Hamiltonian becomes

$$
\begin{aligned}
\hat{\mathcal{H}}_o &= \hat{\mathbb{H}}_{o,p} + \hat{\mathbb{H}}_{o,(4)} + \hat{\mathcal{H}}_o^{(\lambda_0)} && (42)\\
\hat{\mathbb{H}}_{o,p} &= = -p_0 + \frac{1}{2p_0}\left(\hat{p}_\perp^{\,2} + \frac{1}{4}q^2 B^2(z) r_\perp^{\,2} - qB(z)\hat{L}_z\right)\,, && (43)\\
\hat{\mathbb{H}}_{o,(4)} &= \frac{1}{8p_0^3}\hat{p}_\perp^{\,4} - \frac{1}{2p_0^2}\alpha \hat{p}_\perp^{\,2}\hat{L}_z - \frac{1}{8p_0}\alpha^2\left(\hat{\boldsymbol{p}}_\perp\cdot\boldsymbol{r}_\perp + \boldsymbol{r}_\perp\cdot\hat{\boldsymbol{p}}_\perp\right)^2 \\
&\quad + \frac{3}{8p_0}\alpha^2\left(\hat{p}_\perp^{\,2} r_\perp^{\,2} + r_\perp^{\,2}\hat{p}_\perp^{\,2}\right) + \frac{1}{8}\left(\alpha'' - 4\alpha^3\right)\hat{L}_z r_\perp^{\,2} \\
&\quad + \frac{p_0}{8}\left(\alpha^4 - \alpha\alpha''\right) r_\perp^{\,4}\,, \\
&\qquad \text{with} \ \ \alpha = \frac{qB(z)}{2p_0}\,, \quad \hat{L}_z = x\hat{p}_y - y\hat{p}_x && (44)\\
\hat{\mathcal{H}}_o^{(\lambda_0)} &= \lambda_0 - \text{dependent constant } + \hat{\mathbb{H}}_{o,p}^{(\lambda_0)} + \hat{\mathbb{H}}_{o,(4)}^{(\lambda_0)} + \mathcal{A}_{o,p}^{(\lambda_0)} && (45)\\
\hat{\mathbb{H}}_{o,p}^{(\lambda_0)} &= \frac{\lambda_0^2 q^2}{64\pi^2 p_0^2} B(z)B'(z)\left(\boldsymbol{r}_\perp\cdot\hat{\boldsymbol{p}}_\perp + \hat{\boldsymbol{p}}_\perp\cdot\boldsymbol{r}_\perp\right) && (46)\\
\hat{\mathbb{H}}_{o,(4)}^{(\lambda_0)} &= \frac{\lambda_0^2 q}{256\pi^2 p_0^2} B'''(z)\hat{L}_z\left(\boldsymbol{r}_\perp\cdot\hat{\boldsymbol{p}}_\perp + \hat{\boldsymbol{p}}_\perp\cdot\boldsymbol{r}_\perp\right) && (47)\\
&\quad - \frac{\lambda_0^2 q^2}{512\pi^2 p_0^2}\left(B(z)B''(z)\right)'\left\{r_\perp^{\,2}, \boldsymbol{r}_\perp\cdot\hat{\boldsymbol{p}}_\perp + \hat{\boldsymbol{p}}_\perp\cdot\boldsymbol{r}_\perp\right\}\,, \\
\mathcal{A}_{o,p}^{(\lambda_0)} &= \frac{\mathrm{i}\lambda_0}{8\pi p_0}\left(\frac{1}{2}q^2 B(z)B'(z) r_\perp^{\,2} - qB'(z)\hat{L}_z\right)\,. && (48)
\end{aligned}
$$

$$
\begin{aligned}
\begin{pmatrix}
\langle x\rangle_{(3)}(z_{\mathrm{i}}) \\
\langle y\rangle_{(3)}(z_{\mathrm{i}}) \\
\langle p_x\rangle_{(3)}(z_{\mathrm{i}})/p_0 \\
\langle p_y\rangle_{(3)}(z_{\mathrm{i}})/p_0
\end{pmatrix}
&\approx \left(\begin{pmatrix} M & 0 \\ -1/f & 1/M \end{pmatrix} \otimes R(\vartheta)\right) \\
&\quad \times \left(\begin{pmatrix}
\langle x\rangle(z_{\mathrm{o}}) \\
\langle y\rangle(z_{\mathrm{o}}) \\
\langle p_x\rangle(z_{\mathrm{o}})/p_0 \\
\langle p_y\rangle(z_{\mathrm{o}})/p_0
\end{pmatrix} + \begin{pmatrix}
(\delta x)_{(3)}(z_{\mathrm{o}}) \\
(\delta y)_{(3)}(z_{\mathrm{o}}) \\
(\delta p_x)_{(3)}(z_{\mathrm{o}})/p_0 \\
(\delta p_y)_{(3)}(z_{\mathrm{o}})/p_0
\end{pmatrix}\right) && (49)
\end{aligned}
$$

where

$$
\begin{aligned}
(\delta x)_{(3)}(z_{\rm o}) \;=\; & C_s \left\langle \hat{p}_x \hat{p}_\perp^{\,2} \right\rangle (z_{\rm o})/p_0^3 \\
& +K \left\langle \frac{1}{2} \left\{ \hat{p}_x \,,\, \hat{\boldsymbol{p}}_\perp \cdot \boldsymbol{r}_\perp + \boldsymbol{r}_\perp \cdot \hat{\boldsymbol{p}}_\perp \right\} \right. \\
& \qquad \left. + \frac{1}{2} \left\{ x \,,\, \hat{p}_\perp^{\,2} \right\} \right\rangle (z_{\rm o})/p_0^2 \\
& +k \left\langle \left\{ \hat{p}_x \,,\, \hat{L}_z \right\} - \frac{1}{2} \left\{ y \,,\, \hat{p}_\perp^{\,2} \right\} \right\rangle (z_{\rm o})/p_0^2 \\
& +A \left\langle \frac{1}{2} \left\{ x \,,\, \hat{\boldsymbol{p}}_\perp \cdot \boldsymbol{r}_\perp + \boldsymbol{r}_\perp \cdot \hat{\boldsymbol{p}}_\perp \right\} \right\rangle (z_{\rm o})/p_0 \\
& +a \left\langle \frac{1}{2} \left\{ x \,,\, \hat{L}_z \right\} \right. \\
& \qquad \left. - \frac{1}{2} \left\{ y \,,\, \hat{\boldsymbol{p}}_\perp \cdot \boldsymbol{r}_\perp + \boldsymbol{r}_\perp \cdot \hat{\boldsymbol{p}}_\perp \right\} \right\rangle (z_{\rm o})/p_0 \\
& +F \left\langle \frac{1}{2} \left\{ \hat{p}_x \,,\, r_\perp^2 \right\} \right\rangle (z_{\rm o})/p_0 \\
& +D \left\langle x r_\perp^2 \right\rangle (z_{\rm o}) \\
& -d \left\langle y r_\perp^2 \right\rangle (z_{\rm o})
\end{aligned}
\qquad (50)
$$

The corresponding aberration coefficients are:

$$
\begin{aligned}
C(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)h^4+2\alpha^2h^2h'^2+h'^4\right\}\\
K(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)gh^3+\alpha^2(gh)'hh'+g'h'^3\right\}\\
k(z,z_{\rm o}) &= \int_{z_{\rm o}}^{z} dz\,\left\{\left(\frac{1}{8}\alpha''-\frac{1}{2}\alpha^3\right)h^2-\frac{1}{2}\alpha h'^2\right\}\\
A(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)g^2h^2+2\alpha^2gg'hh'+g'^2h'^2-\alpha^2\right\}\\
a(z,z_{\rm o}) &= \int_{z_{\rm o}}^{z} dz\,\left\{\left(\frac{1}{4}\alpha''-\alpha^3\right)gh-\alpha g'h'\right\}\\
F(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)g^2h^2+\alpha^2\left(g^2h'^2+g'^2h^2\right)+g'^2h'^2+2\alpha^2\right\}\\
D(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)g^3h+\alpha^2gg'(gh)'+g'^3h'\right\}\\
d(z,z_{\rm o}) &= \int_{z_{\rm o}}^{z} dz\,\left\{\left(\frac{1}{8}\alpha''-\frac{1}{2}\alpha^3\right)g^2-\frac{1}{2}\alpha g'^2\right\}\\
E(z,z_{\rm o}) &= \frac{1}{2}\int_{z_{\rm o}}^{z} dz\,\left\{\left(\alpha^4-\alpha\alpha''\right)g^4+2\alpha g^2g'^2+g'^4\right\}\,. \qquad (51)
\end{aligned}
$$

$$\boldsymbol{r}''_\perp(z)+\alpha^2\boldsymbol{r}_\perp(z)=0\,, \qquad (52)$$

Symmetry property of the aberration coefficients

It is interesting to note the following symmetry of the nine aberration coefficients : under the exchange $g \longleftrightarrow h$, the coefficients transform as $C_s \longleftrightarrow E$, $K \longleftrightarrow D$, $k \longleftrightarrow d$, $A \longleftrightarrow F$, and a remains invariant. To see the connection $A \longleftrightarrow F$ we have to use the relation $gh' - hg' = 1$.

- Firstly, there are the explicit λ_0-dependent contributions to the paraxial behaviour and aberration coefficients (of all order aberrations), which have no analogues in the classical treatment. For instance, we worked out the explicit λ_0-dependent corrections to the spherical aberration. It is seen that the effects of such quantum corrections can be of any significance only at low energies.

- Secondly, we find that *the aberrations depend not only on the quantum mechanical averages of* $\boldsymbol{r}_\perp$ *and* $\boldsymbol{p}_\perp$ *but also on their higher order central moments corresponding to the wave packets.* An immediate consequence of this fact is that contrary to the classical wisdom, coma, astigmatism, etc., *cannot* vanish for the object point situated on the optic axis.

Scherzer's Theorem

An important result to be recalled in this connection is the Scherzer's theorem which shows that the spherical aberration coefficient C_s is always positive and cannot be reduced below some minimum value governed by practical limitations.

$$\tilde{C}_s = \frac{1}{2} \int_{z_{\mathrm{o}}}^{z_{\mathrm{i}}} dz \left\{ \left(\alpha^4 - \alpha \alpha'' \right) h^4 + \frac{\lambda_0^4}{8 \pi^2} \left(\alpha \alpha'' \right)' h^3 h' + 2 \alpha^2 h^2 h'^2 + h'^4 \right\} . \quad (53)$$

Some Directions for Further Research

- Systems with curved optic axis
- Systems with non-monoenergetic beams
- Extending the phase-space formalism to study:

  Coherence Theory for charged-particle beams

  Image reconstruction etc.
- Generalization of the beam-optical form of the Thomas-BMT equation
- Applications to spin-splitter devices
- Analysis of global systems
- Long term stability of particle motion is storage rings
  Quantum suppression of classical chaos
- An Experiment! The Choice of the Position Operator ?

Further ideas are available in:

1. R. Jagannathan and S. A. Khan,
   Quantum mechanics of accelerator optics,
   in: International Committee for Future Accelerators (ICFA) Newsletter
   No. 13, pp. 21-27 (April 1997).

2. M. Conte, R. Jagannathan, S. A. Khan and M. Pusterla,
   A quantum mechanical formalism for studying the transport of Dirac-particle beams through magnetic optical elements in accelerators
   In preparation

The Generalized Accelerator Optical Transformation
$$\downarrow$$
Generalized beam-optcal form of the Thomas-BMT equation

Section IV of Ref. 2 above

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