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ELECTRON OPTICS WITH DIRAC EQUATION

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ABSTRACT

Basic theory of the quantum mechanics of electron optics is outlined, using an algebraic framework built on the Dirac equation, with particular reference to the propagation of an almost paraxial quasi monoenergetic electron beam through an axially symmetric thin magnetic lens system. The theory is easily generalizable to other electron optical systems with straight optic axes.

KEY WORDS: Dirac equation, space-time, Quantum optics, klein Gordon,quadrupole

1. INTRODUCTION:-

It is surprising to find that nonelativistic Schordinger equation has become the traditional basis for understanding the quantum mechanics of electron optics: while dealing with instruments employing electron beams with relativistic energies the non-relativistic formulae are used with "relativistic corrections" for the mass and de Broglie wavelength. It is only recently that there has been a serious attempt to analyze the central problem, namely the propagation of the electron beam through the system, on the proper basis: the Dirac equation. But, even this treatment falls short of one's expectations for it leads ultimately to the suggestion that the spin of

the electron can be regarded as a spectator degree of freedom and the space-time dependence can be handled through the Klein-Grodon propagator for the evolution of the wave function along the system axis, obtained from a straight forward generalization of the semi-classical approach of Glaser's nonrelativistic theory.²

2. LITERATURE:

The Dirac equation joins the amplitudes of the components of the 4-spinor to their space-time variation. The conventional description of the electron optic corresponds to a scalar theory wherein one component of spinor is taken as the scalar wave-function, thus ignoring the subtle way in which the Dirac equation couples the four components of the spinor. This is clearly an inconsistency and native generalizations of the non-relativistic scalar theory cannot, in principle, account for all aspects of the quantum mechanics of electron optics in a relativistic situation. Such theory has been recently developed by us^3 , and here I shall give a brief account of this theory. We have developed our theory with particular reference to axially symmetric magnetic electron lenses. But, generalization of the following treatment to deal with other electron optical systems, such as quadrupole lenses and lenses comprising of both electric and magnetic fields, with straight optic axes, is straightforward.

Let us consider the propagation of an electron beam through a magnetic lens system formed by an axially symmetric (about z-axis) static field B; the field B is usually characterized by a vector potential A, with $A_z=0$. The beam wave function is governed by the Dirac equation,

$$
i\hbar \frac{\delta \Psi(X,t)}{\delta t} = (m c^2 \beta + c \underline{\alpha}.\hat{\pi}) \Psi(\underline{x}, t),
$$

$$
\hat{\pi} = \hat{p} + (e/c) \underline{A}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \underline{\alpha} = \begin{pmatrix} 0 & \underline{\sigma} \\ \underline{\sigma} & 0 \end{pmatrix}
$$
(1)

We are dealing with the scattering states of the system and are concerned only with quasimonoenergetic beams moving very close to the z-axis (optic axis). Hence, our interest is only in the solutions of (1) representing such almost paraxial quasi-monoenergetic beams for which the wave functions are of the form

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$$
\Psi(\underline{\mathbf{X}}, t) = \int_{P_0 \triangle P}^{P_{0+\triangle P}} d\mathbf{p} \exp(-i \mathbf{E}(\mathbf{p})t / \hbar) \Psi(\underline{\mathbf{X}}; P), \Delta \ll P_0,
$$

\n
$$
\mathbf{E}(\mathbf{P}) = + (\mathbf{m}^2 \mathbf{c}^4 + \mathbf{c}^2 \mathbf{P}^2)^{1/2}
$$
\n(2)

with

$$
\Psi(\underline{x}_{\perp}, Z_{in}; P) = \int d^2 \underline{p}_{\perp} \, \emptyset_{in} \, (\underline{p}) \, \exp \{ i / \hbar [p_{\perp} \cdot x_{l} + (p^2 - p_1^2)^{1/2} \, Z_{in}] \} \left| \underline{p}_{\perp} \right| \ll P
$$

$$
\emptyset_{in} \, (\underline{P}) = [a_{+} (\underline{P}) u_{+} (\underline{P}) + a_{-} (\underline{P}) u_{-} (\underline{P})]
$$

$$
\underline{P} = \left(\underline{p}_{\perp} + (P^2 - P_{\perp}^2)^{1/2} \right) \tag{3}
$$

Where $\{u_{\pm} (p) \exp i (p \cdot x / \hbar) \}$ are the standard positive energy plave-wave solutions of the free Dirac equation, p_0 is the mean momentum of the beam electrons, and z_{in} refers to the z-coordinate n the input (object) space. Similarly, the z-coordinate in the output (image) space will be denoted z_{out} . The input and output spaces are practically field-free regions lying outside the lens; though an electron lens does not have a sharp boundary, for all practical purpose it can be considered to lie within finite interval on the z-axis, say, between z_1 and z_r ; $(z_{in} < z_1 < z_{out})^4$.

Our aim is to study the evolution of the beam wave function $\Psi(x,t)$ along the optic axis of the system. Since the system is stationary, with time-independent Dirac Hamiltonian, it is clear from (1) and (2) that the time-Fourier coefficient $\Psi(x, p)$ of $\Psi(x, t)$ satisfies the time-independent equation,

$$
\left[\mathbf{E}(\mathbf{p})-\mathbf{m}\,\mathbf{c}^2\boldsymbol{\beta}-\mathbf{c}\,\underline{\alpha}_{\perp}\,\underline{\hat{\pi}}_{\perp}+\mathbf{c}\,\alpha_2\,\,\mathrm{i}\,\hbar\,\frac{\delta}{\delta_z}\right]\Psi(\mathbf{x}_1,\mathbf{z};\mathbf{p})=0.\qquad(4)
$$

Now, the integral of this equation for the z-development of **Ψ**, in the form

$$
\Psi(z',p)=\widehat{G}(z',z';p)\Psi z';p,
$$
\n(5)

Would yield the desired relation for the z-evolution of $\Psi(\mathbf{x}, t)$:

$$
\Psi(z^{"},t) = \int_{p_0-\Delta p}^{p_0+\Delta p} dp \exp[-i E(p) t/\hbar] \widehat{G}(z^{"},z';p) \Psi z';p
$$

\n
$$
\cong \widehat{G}(z^{"},z';p_0)(z^{'},t)
$$

\n(in the highly monometric situation) (6)

(in the highly monoenergetic situation)

Thus to solve th e problem on hand we should get the explicit expression for the z-propagator $\hat{\mathbf{G}}(\mathbf{z}^{\text{T}}, \mathbf{z}^{\prime}; \mathbf{p})$ defined by (4) and (5).

Multiplying throughout from left by α_z , rearranging the terms, and defining

$$
\Psi \qquad \Psi' \,=\, M \Psi
$$

$$
\mathbf{M} = \frac{1}{\sqrt{2}} (1 + \mathbf{x} \propto_z), \mathbf{x} \begin{pmatrix} \xi & 0 \\ 0 & -1/\xi \end{pmatrix}, \xi = (\mathbf{E} + \mathbf{m}c^2) / \mathbf{cp}
$$
(7)

One can rewrite (4) as

$$
i\hbar \frac{\delta \Psi'}{\delta z} = \hat{H}_0 \Psi'_1, \hat{H}_0 = (-p\beta + \hat{O}), \hat{O} = x\underline{\alpha}_\perp \cdot \hat{\pi}_\perp.
$$
\n(8)
\nNow, make a further transformation

$$
\Psi_o = \widehat{T}\Psi',
$$

$$
\widehat{T} = \exp\left[-\frac{1}{2}\tanh^{-1}(\beta\widehat{O}\ /\ p)\right]
$$

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 $= \exp(-\beta \hat{O} / 2p + \beta \hat{O}^3 / 6p^3 - \cdots),$ (9) This takes (8) to the form $i\hbar \frac{\partial \Psi_0}{\partial \theta}$ $\frac{\partial \Psi_0}{\partial z} \cong \beta \widehat{H}_0 \Psi_0$ $\hat{H}_o = \beta \hat{T} \hat{H}_0 \hat{T}^{-1} = -(p^2 + \hat{O}^2)$ $\frac{1}{2}$ $= -\{p^2 - [\hat{\pi}_\perp^2 + (2 \, e/c) B_z S_z] \}^{1/2}$ $= -p + (1/2p)[\hat{\pi}_{\perp}^2 + (2 e/c)B_zS_z],$ $+(1/8p^3)[\hat{\pi}_{\perp}^2 + (2 e/c)B_zS_z]^2$ $+ ...$ (10) B_z is the z-component of the lens field \underline{B} and S_z is the z-component of the spin operator $S = ($ $\overline{\mathbf{0}}$ 0 $\frac{1}{0}$ $\frac{\sigma}{2}$.

In deriving (10) from (8) by substituting (9) the approximation used entails neglecting terms relatively small in view of (i) the z-dependence of Ψ is largely due to the factor $\exp(i\pi / \hbar)$, and (ii) the relative changes in A[⊥] over distances of the order of ℏ **/** p are small compared to unity since the condition that the beam to contain Fourier components comparable to p / h so that no transitions between free-particle states with momentum difference of the order \sim p are possible.

One can easily recognize the transformation (9) to be the analogue of the well known Foldy-Wouthuysen transformation⁵ for the standard Dirac equation (1) . In fact, the analogy is complete; the transformation (9) eliminates from (8) the "odd" operators (coupling the upper and lower pairs of components of Ψ) systematically, leading to a series representation for the transformed equation (10) with $1/p$ as the expansion parameter. This would help to analyse the electron optical Dirac equation (8) as paraxial part + nonparaxial corrections just like the usual

Foldy –Wouthuysen transformation helps to analyze the Dirac equation (1) as non-relativistic part $+$ relativistic corrections.

It may be recalled that in the Hamiltonian treatment of geometrical (or classical) electron optics⁴ the transformation of the ray parameters $(\underline{x_1}, d\underline{x_1}/d\underline{z_1})$, or phase-space coordinates (note that $p^{\frac{dx_1}{dz}} \cong p_1$ in free space), across the system is governed by the Hamiltonian – $(p^2 - \pi_1^2)^{1/2}$. It is the power series expansion in terms of π^2 $\!/\rho^2$ that leads to the analysis of the system under successive approximations, the paraxial approximation followed by aberrations of various orders. Looking at (10) it is clear that the geometrical optics description should follow naturally from the classical limit of the Dirac theory. Also, comparing the first two terms of the r.h.s. of (10) with the Hamiltonian (optical) operator of Glaser's non-relativistic paraxial. Schrodinger equation it is evident that \hat{H}_0 minus the spin terms corresponds to the scalar theory Hamiltonian and it is Ψ_0 that goes in the non-relativistic limit into the Schrodinger-Pauli wave function; this is exactly analogous to the fact that it is the Foldy-Wouthuysen representation of the Dirac spinor that goes into the Schrödinger-Pauli wave function in the non-relativistic limit of (1).

Let us now note that in the absence of the lens field the equation (10) is exact and correspondingly for any free-space solution Ψ_0 representing a beam moving in the forward zdirection the lower pair of components become zero. Hence, for the input wave function in our problem,

Industrial Engineering Journal ISSN: 0970-2555 Volume : 52, Issue 8, No. 3, August : 2023 $\beta \Psi_0(z_{in}) = \Psi_0$ $(z_{in}),$ (11)

As can also verified direct by from (3) (7) and (9). Our primary aim is to obtain the relation between the beam wave-functions in the input space and the output space, or in other words we want to know \hat{G} (z_{out} , z_{in} ; p). To this end, we shall integrate (10) formally, dropping β in view (11) and the fact that β commutes with \hat{H}_0 , and go back to the Dirac representation $\Psi_0 \to \Psi$ through (7) and (9). The result can be expressed as follows:

$$
(\mathbf{z}_{out}, \mathbf{z}_{in}; \mathbf{p}) = \mathbf{p} \left\{ \exp \left[-\frac{i}{\hbar} \int_{z_{in}}^{z_{out}} d \mathbf{z} \, \hat{\mathbf{H}}(\mathbf{z} \, ; \mathbf{p}) \right] \right\}
$$

$$
= \left\{ \mathbf{l} + \left(\frac{i}{\hbar} \right) \int_{z_{in}}^{z_{out}} d \mathbf{z} \, \hat{\mathbf{H}}(\mathbf{z} \, ; \mathbf{p}) + \left(-\frac{i}{\hbar} \right)^2 \int_{z_{in}}^{z_{ut}} d \mathbf{z} \, \mathbf{1} \int_{z_{in}}^{z_1} d \mathbf{z} \, \hat{\mathbf{H}}(\mathbf{z}_1 \, ; \mathbf{p}) \hat{\mathbf{H}}(\mathbf{z} \, ; \mathbf{p}) + \dots \right\}, \qquad 12
$$

Where p stands for the z-ordering operation, and

$$
\widehat{H}(z;p) = \widehat{T}^l \widehat{H}_o(z;p) \widehat{T},
$$

$$
\widehat{T} = \widehat{T} \text{ (free) } M = \left[exp \left\{ -\frac{1}{2} \tanh^{-1} \left(\beta x \underline{\alpha}_{\perp} \cdot \underline{\widehat{p}}_{\perp} / p \right) \right\} \right] M
$$

$$
= \left[\exp\left\{ -\underline{\alpha}_{\perp}, \underline{\hat{p}}_{\perp}/2p + \cdots \right\} \right] M. \tag{13}
$$

Essentially, \hat{H} is obtained from the scalar Hamiltonian, namely $\hat{H} = -(p^2 - \hat{\pi}_{\perp}^2)^{1/2}$, by first replacing $\hat{\pi}_{\perp}^2 \rightarrow (\underline{\propto}_{\perp} \cdot \hat{\pi}_{\perp}^2) = [\hat{\pi}_{\perp}^2 + (2 \text{ e } / \text{ c}) B_z S_z] \Rightarrow \hat{H} \rightarrow \hat{H}_0,$ (14)

and then making substitutions for $\underline{x_1}$ and S_z in \widehat{H}_0 as

$$
\underline{\mathbf{x}}_{\perp} \rightarrow \underline{\widehat{\mathbf{Q}}}_{\perp} = \widehat{\mathbf{T}}^1 \underline{\mathbf{x}}_{\perp} \widehat{\mathbf{T}} = \underline{\mathbf{x}}_{\perp} - (\mathbf{i} \hbar / 2\mathbf{p}) \beta \mathbf{x} \underline{\alpha}_{\perp} + ..., \qquad (15)
$$

and

$$
\mathbf{S}_{\mathbf{z}} \rightarrow \hat{\mathbf{S}}_{\mathbf{z}} = \mathbf{\hat{T}}^1 \mathbf{S}_{\mathbf{z}} \mathbf{\hat{T}} = \mathbf{S}_{\mathbf{z}} - (1/p) \beta x \alpha_z \underline{\mathbf{S}}_{\perp} \cdot \underline{\hat{\mathbf{p}}}_{\perp} + \cdots; \tag{16}
$$

the similarity transformation with \hat{T} leaves \hat{p}_{\perp} invariant.

 One can show that in the scalar theory the z-propagator Ĝwould have the same expression as in (12) with Ĥreplaced by Ĥ. Thus the scalar theory can be readily transformed into the spinor theory by an algebraic rule contained in (14) — (16) . This is very much analogous to the process of passing from the scalar (Helmholtz) theory to the vector (Max well) theory in the light optics.⁶

Let us now see how the above spinor theory looks in the paraxial case. In general, from the multiplicative property of the formal integration of equations like (10), it follows that we can write $\hat{G}(Z_{\text{out}}, Z_{\text{in}}; p) = \hat{G}_{F}(Z_{\text{out}}'Z_{r}; p)\hat{G}_{L}(Z_{r}, Z_{l}; p)\hat{G}_{F}(Z_{l'} Z_{\text{in}}; p),$ (17) where the subscripts F and L denote respectively free propagation and propagation through the lens; with

$$
\hat{H}(\boldsymbol{z};\boldsymbol{p}) = -\left\{\boldsymbol{p}^2 - \left[\left(\hat{p}_1 + \frac{\mathrm{e}}{\mathrm{c}}\underline{A}_\perp\left(\widehat{\underline{Q}}_\perp,\boldsymbol{z}\right)\right)^2 + (2 \mathrm{e/c})B_z\left(\widehat{\underline{Q}}_\perp,\boldsymbol{z}\right)\widehat{S}_z\right]\right\}^{1/2}
$$

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$$
= -p + (1/2 p) \left[\left(\underline{\hat{p}}_{\perp} + e_{\ell} \underline{A}_{\perp} \left(\underline{\hat{Q}}_{\perp}, z \right) \right)^2 + (2e/c) B_z \left(\widehat{Q}_{\perp}, z \right) \widehat{S}_z \right] + \cdots, \tag{18}
$$

and

$$
\widehat{H}(\text{free};\,p) = -\left(p^2 - p_\perp^2\right)^{1/2} = -p + p_\perp^{2/2}p + \dots \tag{19}
$$

we have

$$
\widehat{G}_F(Z'', Z'; p) = \exp\left[-\frac{i}{h}(Z'' - Z')\widehat{H}(free; p)\right]
$$
 (20)

and

$$
\mathbf{G}_{\mathbf{L}}(\mathbf{z}_{\mathbf{r}}, \mathbf{z}_{\mathbf{l}}, \mathbf{p}) = \mathbf{p} \left\{ \exp \left(-\sum_{i=1}^{k} \int_{\mathbf{z}_{i}}^{\mathbf{z}_{\mathbf{r}}} d\mathbf{z} \, \widehat{\mathbf{H}}(\mathbf{z} \, ; \, \widehat{\mathbf{p}}) \right) \right\} \tag{21}
$$

In the paraxial situation $\pi_1^2 \ll p^2$ and the lens field is effective only in the paraxial region. The one can neglect terms of ordr $1/p³$ and higher in the series expension of (17) (using (18)–(21) and (15) – (16) and take

$$
\underline{\mathbf{A}}_{\perp}(\underline{\mathbf{x}}_{\perp},\mathbf{z}) \cong \left(-\frac{1}{2}\mathbf{B}(\mathbf{z})\mathbf{y}, \frac{1}{2}\mathbf{B}(\mathbf{z})\mathbf{x}\right),\tag{22}
$$

the lowest order (paraxial) expression in terms of the off-axis coordinates \underline{x}_\perp , where B(z) characterizes the field along the system axis \underline{B}_{\perp} (0, 0, z) = (0, 0), \underline{B}_{z} (0, 0, z) = B(z)). As a result, in the paraxial case we get, for a practically mono-energetic beam,

$$
\Psi(Z_{out}) \cong \widehat{G}^{1}(\mathbf{z}_{out} \ \mathbf{z}_{in}; \ \mathbf{p}_{0}) \Psi(z_{in}),
$$

\n
$$
\widehat{G}^{1}(\mathbf{z}_{out}, \mathbf{z}_{in}; \mathbf{p}_{0}) = [\mathbf{G}_{F}^{1}(\mathbf{z}_{out}, \mathbf{z}_{r}; \mathbf{p}_{0})] [\widehat{G}_{L}^{1}(\mathbf{z}_{r}, \mathbf{z}_{l}; \mathbf{p}_{0})] [\widehat{G}_{F}^{1}(\mathbf{z}_{l}, \mathbf{z}_{in}; \mathbf{p}_{0})]
$$

\n
$$
\cong_{\bigcap_{h=1}^{n} (\mathbf{z}_{out} - \mathbf{z}_{r}) (\mathbf{p}_{0} - \widehat{\mathbf{p}}_{L}^{2} / 2 \mathbf{p}_{0}) \bigg] \times
$$

$$
\begin{bmatrix}\n\exp\left\{\frac{i}{\hbar}(z_r - z_l)(p_0 - \hat{p}_\perp^2/2p_0) - i\left(\frac{\hat{p}_0}{2\hbar}f\right)x_\perp^2 - \beta x(p_0)\underline{\alpha}_\perp, \underline{x}_\perp/2f\right\}\right]X \\
\exp\left\{-\frac{i\theta}{\hbar}(\hat{L}_z + S_z)\right\}\exp\left(-\frac{i\theta}{\hbar}(s_z - \beta x(p_0)\alpha_\perp S_\perp \cdot \hat{p}_\perp/p_0)\right]\right\}X \\
\exp\left\{\frac{i}{\hbar}(z_l - z_{in})(p_0 - p_\perp^2/2p_0)\right\},\n\end{bmatrix},\n\qquad (23)
$$

where $\hat{\mathbf{L}}_z$ is the usual z-component of the angular momentum operator,

$$
\frac{1}{f} = \left(\frac{e^2}{4} p_0^2 c^2\right) \int_{z_1}^{z_r} dz B(z)^2 \cong \left(e^2 / 4 p_0^2 c^2\right) \int_{-\infty}^{\infty} dz B(z)^2,
$$
\nand\n
$$
\theta = (e / 2p_0 c) \int_{z_1}^{z_r} dz B(z).
$$
\n(25)

Now, if one takes the input wave function in (23) to be a plane wave of momentum p_0 corresponding to the Dirac current density $(c \Psi^* \propto \Psi)$ given by $v_0(o, o, 1)$, $(v_0 = c^2 p_0 / E)$, or in other words, a system of rays parallel to the z-axis, then it is fornd⁷ that the output wave function at the transverse plane at $z = z_r$, $(\Psi(z_{out} = z_r))$ corresponds to the Dirac current density \approx $v_0\left(-\frac{x}{f}\right)$ $(\frac{\lambda}{f}, -y/f, 1)$. Under the approximation $(z_r - z_l) \ll f$. Thus our system acts as a converging lens of focal length f for the Direct current and approximate $(z_r - z_l) \ll f$ is the this lens

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approximation. The presence of the term $\exp(-i \theta \hat{L}_z/\hbar)$ in (23) explains the quantum mechanics of the well-known. Electron optical image rotation through the angle .

Thus, for the first time, we are led to the quantum mechanical explanation of the well known, basic features of an axially symmetric thin magnetic electron lens and the classical formulae (24) – (25) of Busch⁸ as the lowest order approximation result in a formalism based on the Dirac equation. It should be noted that in the scalar theory the expression corresponding to (23) will be the same, but without the matrix terms in the exponential. Thus in the scalar theory the term $-(i p_0 x_\perp^2/2 \hbar f)$ contributes to the converging output current (Schrodinger) density whereas in the spinor theory it is the matrix part $(-\beta x \propto \frac{1}{2f})$ that plays the crucial role in the lens propagator. If noon relativistic scalar theory is extended naively into the relativistic domain of p_0 the use of Schrodinger current density formula (identical to the Klein-Gordon case) forces one to replace the rest mass by the "relativistic mass" so that current may be identified with velocity. This explains the substitution rules in practice and shows how the Dirac theory leads to the proper relativistic extension of the nonrelativistic quantum mechanics of electron optics.

Higher order corrections to the paraxial optics described by $(23) - (25)$ through a systematic inclusion of more terms in Ĥ will account for the aberrations suffered by Dirac electron beam propagation. It should be worthwhile to study the practical design aspects including the aberration calculations based on the above formalism. As already mentioned, the theory contained in $(1) - (2)$ is general for any lens system with a straight axis and can be applied for example to quadrupole lens systems. The extension of the above formalism to a lens system having electric field in addition to (or instead of) the magnetic field is also straight forward: in (4) E (p) will have to be replaced by $\left[mc^2 + e(V + \phi(x))\right]$ where V is the accelerating potential for the input beam and $\phi(x)$ is the electric potential of the lens field. Then using the same algebraic procedure as above, with some suitable modifications, the quantum theory of such electromagnetic lenses can be worked out⁹.

3. CONCLUSION:

In conclusion, let me point out the following. Our formulation of the quantum theory of electron lenses as above is not based abinitio on the solutions for the classical trajectories of the also system as is the case with semiclassical approaches: \cdot .² with the conventional treatment of light optics, is bypassed. Essentially our function (or point-spread function) would correspond to the matrix element $\langle x^{\prime} | \hat{G} | \underline{x_1}' \rangle$. In this, we have been guided by the recent significant theoretical developments in light optics and classical electron optics: group theoretic synthesis of paraxial systems derived direc1ly from the Maxwell equations by-passing the Fresnel-Kirchhoff formulation:" operator extension of matrix methods of Gaus sian optics leading to Lie algebraic techniques in the Hamiltonian treatment of geometrical optics:" extension of the Lie algebraic techniques of geometrical light optics to classical (geometrical) electron optics (including relativistic considerations. particularly problems of accelerator design).' Essentially these algebraic techniques stem from the application of the Baker-Campbell-Hausdorff (BCH) formulas related to exponential operators. Since we have the propagators G above expressed in the exponential form such algebraic techniques should get extended in a natural way in the Dirac theory of electron optics. We hope to return to the topic elsewhere.

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