Gouy Phase and Fractional Orbital Angular Momentum in Relativistic Electron Vortex Beams

R. Ducharme\textsuperscript{1}, I. G. da Paz\textsuperscript{2} and Armen G. Hayrapetyan\textsuperscript{3,4}

\textsuperscript{1} Departamento de Física, Universidade Federal do Piauí, Campus Ministro Petrônio Portela, CEP 64049-550, Teresina, PI, Brazil
\textsuperscript{2} 2112 Oakmeadow Pl., Bedford, TX 76021, USA
\textsuperscript{3} d-fine GmbH, Bavariafilmplatz 8, 82031 Grünwald, Germany and
\textsuperscript{4} Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

A Bateman-Hillion solution to the Dirac equation for a Gaussian electron beam taking explicit account of the 4-position of the beam waist is presented. This solution has a pure Gaussian form in the paraxial limit but beyond it contains higher order Laguerre-Gaussian components attributable to the tighter focusing. One implication of the mixed mode nature of strongly diffracting beams is that the expectation values for spin and orbital angular momentum are fractional. Our results for these properties aligns with earlier work on Bessel beams that also showed fractional angular momenta can be parameterized in terms of a Berry phase. Laguerre-Gaussian beams contain Gouy phase that Bessel beams do not. We show that Gouy phase shift from far field to far field in a Gaussian beam can also be parameterized in terms of Berry phase indicating that these two fundamental phases are unexpectedly related to each other.

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Introduction.— In the past decade, there has been considerable progress towards solving the Dirac equation (DE) for the purpose of calculating detailed properties of electron beams. The earliest of this work modeled Bessel beams \cite{1, 2} as a linear superposition of plane waves solutions to the DE. This led to an elucidation of the nature of fractional orbital angular momentum (FOAM) in Bessel beams including a clear understanding of FOAM in terms of Berry phase \cite{3}. More recently, the attention of some investigators \cite{4, 5} has turned to Laguerre-Gaussian beams as a means to better understand relativistic vortex formation. Our intention here is to build on this previous work to calculate FOAM for a tightly focused Gaussian beam that will contain higher order Laguerre-Gaussian beam modes as a result of the tight focusing. We will also calculate the total energy of the electron as well as a property called Gouy phase \cite{6, 7} that Bessel beams do not contain.

In a typical electron microscope assembly, a Gaussian beam passes from an electron gun to a magnetic lens that focuses it to a small waist diameter. Assuming a modest current of energetic (~ 100keV) electrons, the average separation between them will be large enough that electron repulsion can be ignored. Under these conditions the expected diameter of the beam waist will be about a hundred times the wavelength of the electrons unless corrective measures are taken to reduce the strong spherical and chromatic aberration that is a normal feature of magnetic lenses \cite{6}.

Orbital angular momentum (OAM) \cite{8, 9} is used in electron microscopy for measuring materials properties. Beams that carry OAM are also known as vortex beams since it is the OAM flowing around the axis of the beam that leads to the formation of the vortex. In optical beams, the vortex can be used to trap and move biological materials indicating a further possible application for electron beams to trap and move nanomaterials.

Gaussian solutions of relativistic wave equations are often called Bateman-Hillion \cite{11–13} solutions. Following Bialynicki-Birula \cite{4} we use a Bateman-Hillion ansatz to solve the Klein-Gordon equation (KGE) then convert it to a solution of the full DE. It is important to be clear though that Bialynicki-Birula ran into difficulties interpreting their solution owing to the presence of light cone coordinates that Barnett \cite{5} was only able to resolve in an approximate sense, thus, limiting the validity of his solution to the paraxial limit. Our resolution to the light cone issue following earlier work \cite{14, 15} is to recognize that the position of the beam waist in a relativistic beam must be a 4-vector and cannot be zeroed out as customarily done for non-relativistic beams. The presence of the additional 4-position coordinate in the solution then enables the time dependence of the troublesome light cone coordinates to be eliminated using a constraint dynamics \cite{16, 17} approach in a manner that is form preserving under Lorentz transformations.

Bliokh \textit{et al} \cite{1} showed using the Foldy-Wouthuysen (FW) transformation applied to Dirac operators that an electron can pick up a Berry phase as result of the presence of its angular momentum in a strongly diffracting beam but that the effect otherwise vanishes in the paraxial limit. These investigators also showed that the amount of FOAM in the beam is directly proportional to the Berry phase.

Gouy phase is accumulated along the direction of propagation of a wave beam as a result of the transverse localization of the beam \cite{8}. It has been measured experimentally in many different kinds of wave beam including
electron beams. We shall show that like FOAM the total Gouy phase shift in a Gaussian beam, from far field to far field, can also be completely parameterized in terms of Berry phase.

Exact Bateman-Hillion-Gaussian beams from Dirac equation.— Consider a beam of electrons each having a mass of \( m \), a 4-position \( x_\mu = (ct, \mathbf{r}) \) and a 4-momentum \( p_\mu = (E/c, -\mathbf{p}) \), where \( \mu = \{0, 1, 2, 3\} \) and \( c \) is the speed of light in vacuum. It follows the particle has an energy \( E \) and 3-momentum \( \mathbf{p} \) at world time \( t \) and world position \( \mathbf{r} \). Let us also assume that each electron passes through a beam waist with a 4-position \( X_\mu = (cT, \mathbf{R}) \) where \( \mathbf{R} \) is the world position of the beam waist at world time \( T \). Note, we introduce two different time coordinates since the equality \( T = t \) is not form preserving under Lorentz transformations. The Dirac DE describing the dynamics of each of the electrons in the beam can then be expressed as

\[
(\gamma^\mu \hat{p}_\mu - mc) \Psi_\pm (x_\mu, X_\mu) = 0 .
\]

(1)

Here, \( \hat{p}_\mu = \hbar \partial / \partial x^\mu \) is the canonical 4-momentum operator, \( \gamma^\mu \) are Dirac matrices, \( \hbar \) is the reduced Planck’s constant, while \( \Psi_\pm (x_\mu, X_\mu) \) represents a bi-spinor wave function of each individual electron, where “±” stand for (positive-energy) spin-up and spin-down states, respectively. Equation \( \Psi_\pm \) also has two negative-energy bi-spinor solutions that we will not consider since they describe anti-particles.

The DE \( \Psi_\pm \) can be simplified using the substitution

\[
\Psi_\pm (x_\mu, X_\mu) = \left[ \left( \hat{p}_0 + mc \right) \chi_\pm \right] \Psi (x_\mu, X_\mu)
\]

(2)

with

\[
\chi_+ = \left( \begin{array}{c} 1 \\ 0 \end{array} \right), \quad \chi_- = \left( \begin{array}{c} 0 \\ 1 \end{array} \right)
\]

(3)

being two-component spinors, \( \Psi \) a scalar function and \( \sigma_i \) the Pauli matrices \( \{i = \{1, 2, 3\}\} \) with the inner product \( \sigma_i \hat{p}_i \equiv \sigma_1 \hat{p}_1 + \sigma_2 \hat{p}_2 + \sigma_3 \hat{p}_3 \). Combining Eqs. \( \Psi_\pm \) and \( \Psi \) leads to the KGE for \( \Psi \)

\[
(\hat{p}_\mu \hat{p}^\mu - m^2 c^2) \Psi_\pm (x_\mu, X_\mu) = 0 .
\]

(4)

The clear understanding here is that the bi-spinor solution \( \Psi_\pm \) satisfies the DE provided that the scalar function \( \Psi \) acts as the solution of the KGE.

It is well known to mathematicians specializing in the theory of waves but less so in the vortex beam community that relativistic wave equations have exact Gaussian solutions called Bateman-Hillion solutions. A key feature of these solutions is that they are restricted to treat space and time coordinates on an equal footing, thus, ensuring the Lorentz invariance of physical formula constructed in this manner.

The solution to the KGE \( \Psi_\pm \) for the Gaussian beam mode has been developed in two earlier papers [14, 15]. It is helpful to start from the Bateman-Hillion based ansatz

\[
\Psi (x_\mu, X_\mu) = C \Phi(\xi_1, \xi_2, \xi_3 + \xi_0) \exp \left[ i (k_\mu + \kappa_\mu) x^\mu \right],
\]

(5)

where \( C \) is a constant number, \( \xi_0 = x_\mu - X_\mu \) is the 4-position of the electron relative to the beam waist, \( k_\mu \) is the wave vector, \( \kappa_\mu = (0, 0, \kappa_-) \) and \( \kappa = [w_0^2(k_3 + k_0)]^{-1} \) is a shift \( k_\mu \rightarrow k_\mu - \kappa_\mu \) in the wave vector introduced through the unitary transformation \( e^{i \kappa \mu x^\mu} \). The purpose of this shift is to take into account the affect of transverse localization on the dynamics of the electrons in the beam [15] such that the quantity \( \hbar k_\mu \) has a straightforward meaning as the expected mass current per electron.

Following Ref [15], we insert the Bateman-Hillion ansatz \( \Psi_\pm \) into the KGE \( \Psi \) and solving the resulting equation for \( \Phi(\xi_\rho, \xi_\phi, \xi_3 + \xi_0) \) in the cylindrical system of coordinates (with the ‘radial’ \( \xi_\rho = \sqrt{\xi_1^2 + \xi_2^2} \) and ‘azimuthal’ \( \xi_\phi = \tan(\xi_2/\xi_1) \) coordinates) leads to the Laguerre-Gaussian solution

\[
\Phi_{lp} = \sqrt{\frac{2p!}{\pi |w|^2 (p + |l|)!}} \frac{(\sqrt{2} \xi_\rho/|w|) |l|}{L_{lp}^{2|l|} (2 |\xi_\rho|^2/|w|^2)}
\times \exp \left[ - \frac{\xi_\rho^2}{w_0 w} + i l \xi_\phi - g_{lp} \right],
\]

(6)

alongside the dispersion relation

\[
k_\mu k^\mu - \frac{m^2 c^2}{h^2} + 2k^\mu \kappa_\mu.
\]

(7)

Furthermore, \( L_{lp}^{2|l|} \) are the generalized Laguerre polynomials and

\[
g_{lp} = (1 + |l| + 2p) \arctan \left[ 2 \kappa (\xi_3 + \xi_0) \right].
\]

(8)

is the Gouy phase in terms of the radial, \( p \geq 0 \), and the azimuthal, \(-\infty < l < \infty \), indices. The solution \( \Phi_{lp} \) also contains the complex parameter

\[
w = w_0 \left[ 1 + 2 \kappa (\xi_3 + \xi_0) \right],
\]

(9)

whose modulus, \( |w| \), characterizes the beam radius such that \( w_0 \) is the radius of the beam at the waist.

Eqs. \( \Phi_{lp} \) and \( \Phi_{00} \) constitute exact solution to the DE for a Laguerre-Gaussian electron beam modes. For brevity, we shall only focus attention on the Gaussian-beam so-}

solution leaving a treatment of more general Laguerre-Gaussian beam modes for future work. Putting \( \Psi = \Psi_{00} = C \Phi_{00} \exp \left[ i (k_\mu + \kappa_\mu) x^\mu \right] \) into Eq. \( \Psi \) leads to

\[
\Psi_\pm = \left( \begin{array}{c} b \chi_+ \\ \pm \hbar k_0 \chi_0 \end{array} \right) \Psi_{00} + \left( \begin{array}{c} h \kappa \chi_+ \\ \pm h \kappa \chi_0 \end{array} \right) \Psi_{01} \pm \left( \begin{array}{c} 0 \\ \frac{\sqrt{2} w_0}{w} \chi_+ \end{array} \right) \Psi_{\pm 10}
\]

(10)

where \( b = \hbar k_0 + mc \). This is the exact solution to the DE for the lowest order (Gaussian) bi-spinor electron beam mode.
The constant $C$ in Eq. [15] can be determined from the Dirac current $j^+_p = \Psi^+ \gamma_\mu \Psi^-$ using the normalizing condition

$$
\langle j^+_p \rangle = \int_{-\infty}^{+\infty} j^+_p (\xi_1, \xi_2, \xi_3 + \xi_0) \, d\xi_1 \, d\xi_2 = \frac{k_3}{k_0},
$$

(11)

to give

$$
C = \sqrt{\frac{1}{2(hk_0 b + h^2 k^2)}}.
$$

(12)

As $j_\mu (\xi_1, \xi_2, \xi_3 + \xi_0)$ is a conserved quantity we both expect and find that $\langle j_\mu \rangle$ is independent of $\xi_3$ and $\xi_0$ even though there is no averaging over these coordinates.

The Dirac current gives the expected velocity of the electron along the axis of the beam to be

$$
\langle j_3 \rangle = \frac{\xi_3}{\xi_0} = \frac{k_3}{k_0}
$$

(13)

Inserting this expressions into Eqs. [8] and [9] to eliminate the relative time coordinate $\xi_0$ thus recovers the standard Laguerre-Gaussian beam formula for Gouy phase and beam radius to be

$$
g_{\text{Ip}} = (1 + |l| + 2p) \arctan \left( \frac{\xi_1}{\xi_R} \right),
$$

(14)

$$
|w| = w_0 \sqrt{1 + \left( \frac{\xi_1}{\xi_R} \right)^2}
$$

(15)

where $\xi_R = \frac{1}{2} k_3 w_0^2$ is the Rayleigh range. The beam radius $|w|$ further implies

$$
\sin \theta_D = \lim_{\xi_3 \to \infty} \frac{|w|}{\xi_3} = \frac{2}{w_0 k_3}
$$

(16)

where $\theta_D$ is the divergence half angle of the beam.

To estimate the size of terms in the solution [11], we evaluate the averaged probability density as

$$
\langle |\Psi_\pm|^2 \rangle = (b^2 + h k_0^2)(|\Psi_{00}|^2) + 2h k_0^2 (|\Psi_{01}|^2) + 2h^2 k_0^2 (|\Psi_{10}|^2),
$$

(17)

where we can use $\langle |\Psi_\pm|^2 \rangle = C^2$ to confirm $\langle j_0 \rangle = \langle |\Psi_\pm|^2 \rangle = 1$. Thus, it follows from this argument that

$$
\frac{2h^2 k_0^2 (|\Psi_{10}|^2)}{|\langle |\Psi_\pm|^2 \rangle |} = 2h^2 k_0^2 C^2 < 10^{-8}
$$

(18)

owing to current imperfections in magnetic lenses that limit $w_0$ to values of about 50 pm or greater. For our further purposes, it is therefore reasonable to drop the negligible term in Eq. [10] giving $\Psi_\pm (x_\mu, \xi_\mu)$ to be

$$
\left( \begin{array}{c}
\frac{b x_{\pm}}{\pm h k_3 \chi_{\pm}} \\
\frac{b x_{\pm}}{\pm h k_3 \chi_{\pm}} + \left( \begin{array}{c}
0 \\
\frac{\sqrt{2\sigma_3}}{w_0 \chi_{\pm}}
\end{array} \right)
\end{array} \right) \Psi_{00} (x_\mu, \xi_\mu) \pm \left( \begin{array}{c}
0 \\
\frac{\sqrt{2\sigma_3}}{w_0 \chi_{\pm}}
\end{array} \right) \Psi_{+0} (x_\mu, \xi_\mu)
$$

(19)

and $C \cong \sqrt{1/(2\hbar k_0 b)}$, which holds to a very high accuracy. Equation [19] completes the solution of the DE for the Gaussian electron beam. Next, we shall calculate the linear and angular momentum in the beam.

**Momentum and energy of the beam.** — Many relativistic beam solutions, although reasonable in other respects, actually carry an infinite beam energy. Bateman-Hillion solutions do not have this problem. In particular, the expectation values for the 4-momentum in a beam may be determined from the integral expression

$$
\langle \Psi^+_p \tilde{p}_\mu \Psi^- \rangle = \int_{-\infty}^{+\infty} \langle \Psi^+_p \tilde{p}_\mu \Psi^- \rangle \, d\xi_1 \, d\xi_2
$$

(20)

to give $\langle \Psi^+_p \tilde{p}_\mu \Psi^- \rangle = h k_\mu$. Inserting this result into the dispersion relation [17] we obtain the averaged total energy of a single Dirac particle in a Gaussian beam

$$
\langle \Psi^+_x \tilde{E} \Psi_x \rangle = c \sqrt{h^2 k_3^2 + \frac{2h^2}{w_0^2} + m^2 c^2},
$$

(21)

where $\tilde{E} = \tilde{p}_0 c$ is the energy operator. The middle term in Eq. [21] represents the contribution to energy from the transverse components of the momentum of the electron as can be seen clearly from the expression

$$
\langle \Psi^+_x \tilde{p}_3^2 \Psi_x \rangle + \langle \Psi^+_x \tilde{p}_s^2 \Psi_x \rangle = \frac{2h^2}{w_0^2},
$$

(22)

Equation [21] has been obtained elsewhere [15] for a Klein-Gordon particle in a Gaussian beam. Ref. [15] also connects the stored kinetic energy in the beam to the Bohm potential [26].

**Gouy phase and fractional OAM** — Expected values for the spin and orbital angular momentum of an electron parallel to the axis of the beam can be determined from the expressions

$$
\langle \Psi^+_x \tilde{S}_3 \Psi_x \rangle = \frac{\hbar}{2} \int_{-\infty}^{+\infty} \langle \Psi^+_x \frac{\sigma_3}{0} \rangle \, \Psi_x \, d\xi_1 \, d\xi_2
$$

(23)

$$
\langle \Psi^+_x \tilde{L}_3 \Psi_x \rangle = \frac{\hbar}{i} \int_{-\infty}^{+\infty} \langle \Psi^+_x \frac{\partial \Psi_x}{\partial x_2} - \xi_2 \frac{\partial \Psi_x}{\partial x_1} \rangle \, d\xi_1 \, d\xi_2
$$

(24)

These results give

$$
\langle \Psi^+_x \tilde{S}_3 \Psi_x \rangle = (1 - \Delta) s \hbar, \quad \langle \Psi^+_x \tilde{L}_3 \Psi_x \rangle = \Delta s \hbar
$$

(25)

where $s = \pm \frac{1}{2}$,

$$
\Delta = \left( 1 - \frac{m c^2}{E} \right) \sin^2 \theta_D,
$$

(26)

and $\theta_D$ is the divergence angle of the beam. There is little need for us to dwell on these expressions since
they are clearly special case of the more general results \( \langle S_\parallel \rangle = (1 - \Delta) s h \) and \( \langle L_\parallel \rangle = (1 + \Delta s) h \) that Bliokh et al. \[1\] obtained using the FW transformation. In particular, it is clear that the operation of focusing a Gaussian beam will cause a quantity of angular momentum \( \Delta s \) to disappear from the expected SAM of the beam and reappear as FOAM. The total angular momentum of the beam \( \langle \Psi_\parallel^+ J_3 \Psi_\parallel^- \rangle = s h \) where \( J_3 = L_3 + \hat{S}_3 \) is conserved in this process. Bliokh et al. also calculate the Berry phase \( \gamma_B \) of a FOAM carrying beam to be \( \gamma_B = 2\pi \Delta s \).

For a tightly focused Gaussian electron beam, the expected Gouy phase

\[
\bar{g}_T = \sum_{LP} \langle \Psi_\parallel^+ g_{LP} \Psi_\parallel^- \rangle = \left[ 1 + \frac{1}{2} \Delta(\theta_D) \right] g_{00} \tag{27}
\]
is larger than would be the case for a pure Gaussian beam owing to the fractional presence of the OAM carrying \( \Psi_{10} \) mode that adds FOAM to the beam. The total Gouy phase shift from far field to far field in the beam is therefore given by

\[
\mu T = \lim_{\xi \to \infty} (g_T) - \lim_{\xi \to -\infty} (g_T) = \pi + \frac{1}{2} |\gamma_B| \tag{28}
\]
showing that Gouy phase as well as FOAM increases in direct proportion to the Berry phase that is itself a function of the beams divergence angle \( \theta_D \).

In Figure 1 we show the behavior of the angular momentum and Gouy phase as a function of the divergence angle for spin up electrons with a kinetic energy of 0.5 MeV. It can be seen that both the fractional orbital angular momentum and total Gouy phase shift increase in proportion to the Berry phase that is also plotted.

**Discussion.**—Dirac published his quantum theory of the electron in 1928. Some ninety years later it now being applied to understand the effects of transverse localization on electron beams. As previously stated, Bliokh et al. \[1\] made significant progress in this direction by obtaining the first exact solution to the Dirac equation for Bessel beams, calculating FOAM in the beams and showing its direct proportionality to the Berry phase. In just the past year, Bialynicki-Birula \[4\] and Barnett \[5\] have shown how the Dirac equation can be approximately solved for Laguerre-Gaussian beams. What we have presented is a more detailed solution of the Dirac equation for a Gaussian beam that takes account of the 4-position of the beam waist. This has enabled us to calculate the energy, FOAM and Gouy phase in the beam. Our most interesting result is that both FOAM and Gouy phase are directly proportional to the Berry phase. This both corroborates the earlier finding of Bliokh et al. for FOAM and takes it a step further with our inclusion of Gouy phase into the evolving understanding of the role geometric phase has to play in electron beams.
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