Analysis of Singularities and Internal Dynamics of Electron Beams

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Abstract. In this work we present an analysis of phase singularities in Laguerre-Gaussian beams. The cases to be analyzed are static and dynamic singularities. We consider the composition of canonical and kinetic currents around the singularities and velocities on each momentum state. We compare the behavior of time-dependent and stationary systems. We obtain the topological charge numbers that characterize the rotation of currents around the singularities. Finally, we present some analytical and numerical results to illustrate our model.

1. Introduction

An electron beam can be understood as a solution of the Shrödinger equation analogous to a solution to the Helmholtz equation [1]. Many of these beams can be generated by injecting electrons through a holographic mask in the transmission electron microscopy technique (TEM), imprinting the beam an orbital angular momentum (OAM) [2]. One of the well known beams possessing definite OAM are the Laguerre-Gaussian (LG) beams. The LG beams are characterized by a helicoidal wavefront leading to a singularity in the phase of the wave function.

The singularities are regions in the domain where the wave function vanishes and the phase cannot be determined [3]. In some cases it is easy to determine the topological charge of the beam, which is an integer number indicating the turns of the helicoidal wavefront in a distance equivalent to one wavelength [4]. Unlike plane waves having plane phases and null OAM [5], the beams possessing non-trivial OAM are partially coherent and exhibit isolated points where the phase has a singularity. In the neighborhood of these points we can find current vortices [6]. These electronic currents can be obtained by means of the definition of either the momentum or the velocity operators [7].

Nowadays, we can find some new methods to analyze materials through TEM enabling new researches about the electron beams. The results show that we can produce LG electron beams in free space, meaning that it is not necessary any field that confines the orbits. Thus, it is feasible to produce beams with high values of OAM opening the possibility to use them in the design of magnetic imaging techniques [1].

The LG beams can be also used as electronic tweezers, because they are able to hold atoms at the center of the vortex of diameters about the atomic radius leading to novel application in...
areas as, e.g., material science [8].

It is well known that the beams of electromagnetic radiation carrying definite OAM may transmit forces and torques to material objects [9]. In this paper we will focus on some effects produced by the dynamical singularities in electronic beams, a topic which is, so far, not exhaustively considered in the literature. We will study the relation between the currents produced by two fixed singularities and singularities moving along a definite path. We will obtain the topological charge of the singularity to determine the helicity of the currents. Through this analysis we will understand the behavior of the singularities to improve the transport of OAM in electron beams.

2. Singularities

Let us consider a system whose state is represented by a wave function with the following form: $\Psi = Ae^{i\phi}$ where $A$ and $\phi$ are real functions of $(x, y, t)$, the phase $\phi$ has only relevant values between two points of the same function [10, p. 54]. The phase singularities are regions in the wave function domain where the phase vanishes. All the singularities have a point called node which is defined as $\Psi(x, y) = 0$.

The singularities can be represented in the complex plane as bidimensional single points [11]. Around the neighborhood of each point, a singularity vortex are generated [7]. In this vortex the phase circulates around the point. This circulation is defined by the following relation:

$$S = \frac{1}{2\pi} \oint_{c} \nabla \phi \cdot dl = \frac{1}{2\pi} \int_{0}^{2\pi} \frac{d\phi}{d\theta} d\theta,$$

(1)

where $S$ is called topological charge and $c$ is a closed path around the singularity. A topological charge that is circulating counter-clockwise is positive and negative if it is circulating clockwise.

3. Laguerre-Gaussian Modes

Let us consider the Hamiltonian of an electron in a uniform magnetic field with the following form [7]:

$$\hat{H} = \frac{1}{2m} (\hat{p} + e\hat{A})^2,$$

(2)

where we can impose the symmetric norm $\hat{A} = -\frac{B}{2} \hat{y}i + \frac{B}{2} \hat{x}j$,

(3)

with $\hat{x} \hat{y} \hat{y} \hat{x}$ the position operators.

We solve the Shrödinger equation for the Hamiltonian (2) in polar coordinates [12]. The solutions can be expressed in the form the Fock-Darwin states [7] given by:

$$\Psi_{l,n}^{LG}(x, y) = \frac{1}{\sqrt{2\pi l!B}} \exp \left[ -\frac{zz^*}{4l^2B} \right] \times \left\{ \begin{array}{ll}
(-1)^l \sqrt{\frac{n!}{l!}} \left( \frac{z^*}{\sqrt{2l}B} \right)^{n-l} L_l^{n-l} \left( \frac{zz^*}{2l^2B} \right), & n \geq l, \\
(-1)^n \sqrt{\frac{n!}{l!}} \left( \frac{z}{\sqrt{2l}B} \right)^{l-n} L_l^{l-n} \left( \frac{zz^*}{2l^2B} \right), & l \geq n,
\end{array} \right. $$

(4)

where $z = x + iy$, $l$, $n$ are integer numbers, $l_B = \sqrt{\hbar/m\omega}$ is the magnetic length and $L_p^q(r)$ stands for the associated Laguerre polynomial of degree $p$ and order $q$. The equation (4) shows the expression for the $l, n$ LG modes.

We can represent any beam as a linear combination of these LG modes [7] as follows:

$$\Psi(x, y) = \sum_{l,n} A_{l,n} \Psi_{l,n}^{LG}(x, y)$$

(5)
where $A_{l,n}$ is the probability amplitude that the beam is projected onto the $l, n$ LG mode in a measurement.

4. Canonical and kinetic currents

The selection of the vector potential $A$ is fundamental to find the symmetry of the curl of the magnetic field. It is possible to define two different kinds of density currents. The kinetic current, which is related to the velocity operator $\hat{v}$, and the canonical current that is related to the canonical momentum $\hat{p} \propto -i\hbar \nabla$. We can calculate these currents from the wave equation [7].

The expressions for the kinetic and canonical currents in the $x$ and $y$ directions can be cast in the form [13]

$$J^K_x = \text{Re} \left[ \frac{i\omega B}{\sqrt{2}} \sum_{l',n,n'} A_{l',n'}^* A_{l,n} e^{i\omega(l'-l)t} \Psi_{l',n'}^{LG*} \left( \sqrt{1 + i\Psi_{l+1,n}^{LG}} - \sqrt{i\Psi_{l-1,n}^{LG}} \right) \right]$$

$$J^K_y = \text{Re} \left[ \frac{\omega B}{\sqrt{2}} \sum_{l',n,n'} A_{l',n'}^* A_{l,n} e^{i\omega(l'-l)t} \Psi_{l',n'}^{LG*} \left( \sqrt{1 + i\Psi_{l+1,n}^{LG}} + \sqrt{i\Psi_{l-1,n}^{LG}} \right) \right]$$

$$J^C_x = \text{Re} \left[ \frac{i\omega B}{2\sqrt{2}} \sum_{l',n,n'} A_{l',n'}^* A_{l,n} e^{i\omega(l'-l)t} \Psi_{l',n'}^{LG*} \left( \sqrt{1 + i\Psi_{l+1,n}^{LG}} - \sqrt{i\Psi_{l-1,n}^{LG}} \right) \right]$$

$$J^C_y = \text{Re} \left[ \frac{\omega B}{2\sqrt{2}} \sum_{l',n,n'} A_{l',n'}^* A_{l,n} e^{i\omega(l'-l)t} \Psi_{l',n'}^{LG*} \left( \sqrt{1 + i\Psi_{l+1,n}^{LG}} + \sqrt{i\Psi_{l-1,n}^{LG}} \right) \right]$$

5. Analysis of singularities

For the analysis of singularities we choose a function with two singularities and calculate the currents around them. Recalling the definition of a singularity, this function must contain nodes and points where the phase vanishes. The nodes are represented by particular shifts characterized by the parameters $\omega_T$ and $\omega'_T$. In this way, our model with two singularities reads as follows

$$\Psi(x,y,t) = A(z - e^{-i\omega_T t})(z^* - e^{-i\omega'_T t})e^{\exp \left(-\frac{zz^*}{4}\right)}.$$ (10)

Here, the normalization factor $A$ is dependent on the values of $\omega_T$ and $\omega'_T$, and the introduction of time in the equation (10) provide the dynamical nature to the singularities in an analogous way as that shown in [7].

The expression of the function (10) as a linear superposition of LG modes can be determined by using the orthogonality properties of these modes. Recalling the equation (4), the probability amplitudes corresponding to each mode can be readily obtained. In general, it turns out that the proposed wave function can be written as a superposition of LG modes such that the highest order one is the $\Psi_{11}^{LG}$ mode [13].
5.1. One static and one dynamical (time varying) singularity

Let $\omega_T = 0$ and $\omega'_T = -2\pi$, so that a static singularity can be associated to the parameter $\omega_T$ (white dot in Figure 1) and a dynamical one to $\omega'_T$ (orange dot in Figure 1). In our system of coordinates the magnitude $l_0 = \sqrt{\hbar/eB} = 1$.

In Figure 1 we present the probability amplitude in the complex plane for different values of $t \in [0, 1]$. We can see that the white dot remains static, consistently with the chosen value of $\omega_T$. The orange dot is following the dashed orange circular path of radius 1 (both singularities are shifted from the origin by one unit of length).

Next, in order to made an analysis in terms of the probability amplitudes, we calculated the temporal evolution of the currents through the equations (6)-(7), (8) and (9). As we can see in Figure 2 the singularities are located in opposite sides of the probability amplitude distribution. This was done by choosing $t = 0.5$ (compare to the central plot of Figure 1). We observe different behavior for canonical (left) and kinetic (right) currents associated to the wave function (10).

![Figure 1. Time evolution of a pair of singularities, the static (white dot) and the dynamical (orange dot).](image)

![Figure 2. Canonical (a) and kinetic (b) currents at time $t = 0.5$ for which the singularities are located at opposite sides in the distribution.](image)

5.2. Two dynamical singularities

For the study of the currents around the neighborhood of the singularities we have proposed a pair of singularities with similar paths moving in opposite directions. This is achieved by choosing $\omega_T = \omega'_T$. We can see from Figure 3 that the singularities start their motion at point $(1, 0)$ of the complex plane. The orange point is associated to $\omega'_T$ and its motion is counter-clockwise. On other hand the white point is associated to $\omega_T$ and its motion is clock-wise. The main feature of the motion of these singularities is that they perform circular paths of radius $r = l_0 = 1$ in the complex plane. We made an analysis with high and low velocities of the singularities.
Figure 3. Time evolution of a pair of singularities following circular path of opposite directions in a half period of motion.

5.2.1. High velocity singularities. We choose $\omega' T = \omega_T = 50\pi$. This high angular velocity produces that one period of motion is completed at time $t = 0.04$. In Figure 4 we present the behavior of these currents for $t = 0.01$ where the points are located in the opposite side and at time $t = 0.02$ where the singularities are colliding. In both plots the white vector fields correspond to the canonical current, while the orange ones to the kinetic one.

Figure 4. Canonical (white vector fields) and kinetic (orange vector fields) currents associated to a pair of singularities with high velocity that are located in opposite sides of the distribution at $(t = 0.01)$ (a),(b), and when the singularities are colliding $(t = 0.02)$ (c),(d).

5.2.2. Low velocity singularities. For the analysis of these singularities we choose $\omega' T = \omega_T = 2\pi$. Here the complete period of motion is completed at $t = 1$. Again, our cases of interest will be the moments at which the singularities are located in opposite sides ($t = 0.25$) and at which they are colliding ($t = 0.5$).

Figure 5. Canonical (white vector fields) and kinetic (orange vector fields) currents associated to a pair of singularities with low velocity that are located in opposite sides of the distribution at $(t = 0.25)$ (a),(b), and when the singularities are colliding $(t = 0.5)$ (c),(d).
6. Comparison between static and dynamical singularities

In this section we analyze the behavior of the dynamical currents. We made a comparison between the singularities moving in time and static singularities fixed at selected points.

6.1. One static and one dynamical singularity

In the first case proposed, one singularity is fixed ($\omega_T = 0$) and other is moving along the circular path of radius 1 ($\omega'_T = -2\pi$). We choose the time $t = 0.5$ for which the singularities are located at opposite sides of the distribution. We compare the results with the case of a wave function with $\omega_T = 0$ and $\omega'_T = \frac{\pi}{2}$.

Figure 6 shows the canonical and kinetic currents in the complex plane. In this case the orange vector field corresponds to the currents that are produced by static singularities while the white one represent the currents associated dynamical singularities. We can observe that the currents have a similar behavior. Also, we can see that both currents are shifted from the singularity located at $z^* + 1$ but they retain the additive behavior.

A numerical calculation of the norms of the dynamical current vectors and the static ones reveals that the difference between them is in the interval $[0, 1 \times 10^{-17}]$, this means that the currents have similar magnitudes. Also, it can be shown that the topological charge corresponding to the pole $z^* + 1$ is $S = -1$ as well as that related to the static singularity. The currents that form a vortex that rotate clockwise have a topological charge $S = 1$.

![Figure 6](image)

(a) (b)

Figure 6. Comparison between the canonical currents (a) and kinetic currents (b). The orange vectors are produced by the statical singularities ($\omega_T = 0$ and $\omega'_T = \frac{\pi}{2}$) and the white vectors are related with the dynamical singularities ($\omega_T = 0$ and $\omega'_T = -2\pi$). In both cases $t = 0.5$.

6.2. Two dynamical singularities: high velocity and low velocities

We made a comparison between a wave function with two fixed singularities at the points $(0, \pm i)$ ($\omega_T = \omega'_T = \frac{\pi}{2}$), and the wave functions mentioned in the sections 5.2.1 and 5.2.2. We choose the time $t = 0.01$ and $t = 0.25$ respectively. In all our analysis we could see that the white vectors are smaller than the orange ones. This is only a scheme to state the difference between the currents produced by the statical and the kinetic singularities.

From the Figures 7 and 8 we can conclude that there is no difference between the dynamical (white vectors) and static system (orange vectors) current behaviors. Both currents preserve the properties reported in the literature 7. Again, the canonical currents retain the constructive superposition along the negative imaginary axis. It can be also seen that the singularities generate vortices around them with a rotation direction that is associated to the helicity each singularity. The numerical defference between the magnitude of the currents vectors in the systems was in the interval $[0, 1 \times 10^{-18}]$. 
Figure 7. Comparison between the canonical currents (a) and kinetic currents (b) for a system with low velocity. The orange vectors are produced by the static singularities \((ω_T = ω'_T = \frac{π}{2})\) and the white vectors are related with the dynamical singularities \((ω_T = ω'_T = 2π)\). In both cases \(t = 0.25\).

Figure 8. Comparison between the canonical currents (a) and kinetic currents (b) for a system with high velocity. The orange vectors are produced by the statical singularities \((ω_T = ω'_T = \frac{π}{2})\) and the white vectors are related with the dynamical singularities \((ω_T = ω'_T = 50π)\). In both cases \(t = 0.01\).

6.3. Colliding singularities with high and low velocities

Figure 9 shows the canonical and kinetic currents for two colliding singularities. In this case we choose moving poles at the points \((±1, 0)\) in the complex plane corresponding to \(t = 0.01\) and \(t = 0.5\) respectively. We also consider a wave function that has two static singularities \((ω_T = ω'_T = 0)\). We can observe that there is no difference between the currents.

Figure 9. Comparison between the canonical and kinetic currents for a pair of static colliding singularities \((ω_T = ω'_T = 0)\) and two dynamical ones at the points \((±1, 0)\).
7. Conclusions

In this work we studied the behavior of the kinetic and canonical currents in the neighborhood of the phase singularities in electron beams. The statical singularities do not change in time and the dynamic singularities follow a definite path. We compare the values of the canonical and kinetic currents produced by dynamical singularities with currents produced by fixed singularities and we found that there is no difference between them in all the cases we have proposed. To confirm these results we have considered high and low angular velocities in the following cases: when the singularities are in the opposite sides of the distribution and when they are colliding. In both we obtain the same results.

This result is important in the study the time evolution of a beam, and in stating methods to control the OAM and currents around the singularities. In particular, a pair of singularities can be fixed at some points, or they can be traveling along definite paths and the results will be equivalent.

Acknowledgments

The financial support of CONACyT México (Master scholarship for GJT, grant 994641) is acknowledged. The authors are grateful to the anonymous referee for valuable comments and suggestions. GJT wants to thank his wife Diana Junco, to Dr. JL Cardoso and to the Quantum Fest 2019 Organizing Committee. He is also indebted to Dr. Sara Cruz y Cruz for invaluable help in reading and commenting this work.

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