General quantum-mechanical solution for twisted electrons in a uniform magnetic field

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Abstract

A theory of twisted (and other structured) paraxial electrons in a uniform magnetic field is developed. The obtained general quantum-mechanical solution of the relativistic paraxial equation contains the commonly accepted result as a specific case of unstructured electron waves. In the weak-field limit, our solution (unlike the existing theory) is consistent with the well-known equation for free twisted electron beams. The observable effect of a different behavior of relativistic Laguerre-Gauss beams with opposite directions of the orbital angular momentum penetrating from the free space into a magnetic field is predicted. Distinguishing features of the quantization of the velocity and the effective mass of structured electrons in the uniform magnetic field are analyzed.

Keywords: twisted electrons; relativistic quantum mechanics; paraxial electron beams; orbital angular momentum; uniform magnetic field
The discovery of twisted (vortex) electron states with a nonzero intrinsic orbital angular momentum (OAM) [2] has confirmed their theoretical prediction [1] and has created new applications of electron beams. Twisted electrons are successfully used in the electron microscopy and in investigations of magnetic phenomena (see Refs. [3–11] and references therein). Twisted electron beams with large intrinsic OAMs (up to 1000ℏ) have been recently obtained [12]. Due to large magnetic moments of twisted electrons, their above-mentioned applications are very natural. This situation makes a correct and full description of twisted electrons in a magnetic field to be very important.

In the present study, we use the system of units ℏ = 1, c = 1. We include ℏ and c explicitly when this inclusion clarifies the problem.

Let us direct the z axis of the cylindrical coordinates r, φ, z along the uniform magnetic field, \( B = Be_z \). It is now generally accepted [13–18] that twisted electron states in a uniform magnetic field are defined by the Landau wave function [19, 20] or its relativistic generalizations [16, 21–24]. This function being an eigenfunction of the nonrelativistic Hamiltonian

\[
H = \frac{\pi^2 - e\sigma \cdot B}{2m}, \quad \pi^2 = -\nabla^2 + ieB \frac{\partial}{\partial \phi} + \frac{e^2B^2r^2}{4}
\]

reads

\[
\psi = A \exp(i\ell\phi) \exp(ip_z z), \quad \int \psi^\dagger \psi rdrd\phi = 1, \quad A = C_n \ell \left( \frac{\sqrt{2}r}{w_m} \right)^{|\ell|} L_n^{(|\ell|)} \left( \frac{2r^2}{w_m^2} \right) \exp \left( -\frac{r^2}{w_m^2} \right) \eta,
\]

\[
C_n \ell = \sqrt{\frac{2n!}{\pi(n + |\ell|)!}}^{|\ell|}, \quad w_m = \frac{2}{\sqrt{|e|B}}.
\]

Here \( \pi = p - eA \) is the kinetic momentum, the real function \( A \) defines the beam amplitude, and \( L_n^{(|\ell|)} \) is the generalized Laguerre polynomial. When the cylindrical coordinates are used, \( A_\phi = Br/2, A_r = A_z = 0 \). For the electron, \( e = -|e| \). The spin function \( \eta \) is an eigenfunction of the Pauli operator \( \sigma_z \) (cf. Ref. [25]):

\[
\sigma_z \eta^\pm = \pm \eta^\pm, \quad \eta^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \eta^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]

The distinctive feature of the Landau solution is the trivial (exponential) dependence of the electron wave function on z. Values of \( p_z \) are fixed and \( \psi \) is an eigenfunction of the operator \( p_z \equiv -i\hbar \partial/(\partial z) \).
The twisted states of free photons and electrons are defined by the paraxial wave equation [3, 26, 27]:

\[
\left( \nabla^2 - 2ik \frac{\partial}{\partial z} \right) \Psi = 0,
\]

\[
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}.
\]  (4)

For electrons, it can be obtained from the Dirac equation in the Foldy-Wouthuysen (FW) representation provided that \( |p_\perp| \ll p \) [28]. The paraxial wave function of free electrons and photons characterizes the Laguerre-Gauss (LG) beams and reads [26, 29, 30]

\[
\Psi = A \exp(i\Phi),
\]

\[
\int \Psi^\dagger \Psi r dr d\phi = 1,
\]

\[
A = \frac{C_{n\ell}}{w(z)} \left( \frac{\sqrt{2}r}{w(z)} \right)^{|\ell|} L_n^{(\ell)} \left( \frac{2r^2}{w^2(z)} \right) \exp \left( -\frac{r^2}{w^2(z)} \right) \eta,
\]

\[
\Phi = l\phi + \frac{k r^2}{2R(z)} - \Phi_G(z),
\]  (5)

where

\[
w(z) = w_0 \sqrt{1 + \frac{z^2}{z_R^2}},
\]

\[
R(z) = z + \frac{z_R^2}{z},
\]

\[
z_R = \frac{k w_0^2}{2},
\]

\[
\Phi_G(z) = N \arctan \left( \frac{z}{z_R} \right),
\]

\[
N = 2n + |\ell| + 1,
\]  (6)

the real functions \( A \) and \( \Phi \) define the amplitude and phase, \( k \) is the beam wavenumber, \( w_0 \) is the beam waist (minimum beam width), \( R(z) \) is the radius of curvature of the wavefront, \( \Phi_G(z) \) is the Gouy phase, \( z_R \) is the Rayleigh diffraction length, \( L_n^{(\ell)} \) is the generalized Laguerre polynomial, and \( n = 0, 1, 2, \ldots \) is the radial quantum number. The quantities \( C_{n\ell} \) and \( \eta \) are given by Eqs. (2) and (3), respectively. For electrons, \( \Psi \) is a spinor. Evidently, \( \Psi \) is not an eigenfunction of the operator \( p_z \). Therefore, the free-space wave function (5), (6) characterizes a beam formed by partial waves with different \( p_z \).

A correspondence between the relativistic quantum-mechanical equations in the FW representation and the paraxial wave equations has been established in Refs. [28, 31]. The correspondence is very similar for photons and electrons. In connection with this similarity, we can mention the existence of bosonic symmetries of the standard Dirac equation [32–38].

Advanced results obtained in optics allow us to rigorously derive a general formula for the paraxial wave function of a relativistic twisted Dirac particle in a uniform magnetic field. In this case, the exact relativistic FW Hamiltonian is given by [25, 39, 41]

\[
i \frac{\partial \Psi_{FW}}{\partial t} = \mathcal{H}_{FW} \Psi_{FW},
\]

\[
\mathcal{H}_{FW} = \beta \sqrt{m^2 + \pi^2} - e \mathbf{\Sigma} \cdot \mathbf{B},
\]  (7)
where $\pi = p - eA$ is the kinetic momentum and $\beta$ and $\Sigma$ are the Dirac matrices. This Hamiltonian acts on the bispinor $\Psi_{FW} = \begin{pmatrix} \Phi_{FW} \\ 0 \end{pmatrix}$. The zero lower spinor of the bispinor can be disregarded. Eigenfunctions (more precisely, an upper spinor) of the relativistic FW Hamiltonian coincide with the nonrelativistic Landau solution (2) because the operator $\pi^2 - e\Sigma \cdot B$ commutes with the Hamiltonian in both cases (see Refs. [25, 39, 40]). The FW representation is important for obtaining a classical limit of relativistic quantum mechanics [42] and establishing a connection between relativistic and nonrelativistic quantum mechanics [43, 44].

Let us denote $P = \sqrt{E^2 - m^2} = \hbar k$, where $E$ is an energy of a stationary state. A transformation of Hamiltonian equations in the FW representation to the paraxial form has been considered in Refs. [28, 31, 45]. Squaring Eq. (7) for the upper spinor, applying the paraxial approximation for $p_z > 0$, and the substitution $\Phi_{FW} = \exp (ikz)\Psi$ lead to the paraxial equation [45]

$$\left( \nabla^2_{\perp} - i eB \frac{\partial}{\partial \phi} - \frac{e^2B^2r^2}{4} + 2es_zB + 2ik \frac{\partial}{\partial z} \right) \Psi = 0,$$

where $s_z$ is the spin projection onto the field direction. The above-mentioned substitution is equivalent to shifts of the zero energy level and of the squared particle momentum in Schrödinger quantum mechanics. When $B = 0$, Eq. (8) takes the form of the paraxial wave equation for free electrons [4].

The paraxial form of the Landau wave function is an eigenfunction of Eq. (8) and is given by [45]

$$\Psi = A \exp (i\ell \phi) \exp [-i\zeta_G(z)],$$

$$\zeta_G(z) = (2n + 1 + |\ell| + \ell + 2s_z) \frac{2z}{kw_m^2}, \quad w_m = \frac{2}{\sqrt{|e|B}},$$

where $\zeta_G(z)$ is the Gouy phase. Amazingly, the probability and charge densities defined by the nonrelativistic Landau wave function (2) and by the relativistic paraxial wave function (9) coincide. This property follows from the Lorentz boost along the $z$ axis ($x' = x$, $y' = y$) and takes place because a transversal motion in paraxial waves is always nonrelativistic.

While Eq. (9) is similar to Eqs. (5) and (6), there is a substantial difference between them. The paraxial Landau wave function (9) describes a wave with a fixed value of $p_z$, while the free-space LG beam is formed by partial waves with different $p_z$. Thus, the use of the function (9) for a general description of a twisted paraxial electron in a uniform magnetic
field means that even a weak magnetic field leads to destroying the longitudinal structure of LG beams. However, any partial wave forming the beams does not change its energy during the beam penetration from the free space into a magnetic field region. Therefore, the above-mentioned meaning is not reasonable and the Landau solution of Eq. (8) is not general. To obtain the general solution of this equation, we use its similarity to Eq. (4) and utilize optical approach [27, 46–48] applied for the free-space paraxial equation. The subsequent derivation shows that an electron state is described by the matter wave beam (5) but three functions on $z$ should be redefined. It is convenient to present $A$ in Eq. (5) in the more general form and to denote

$$A = \frac{C_n}{w(z)}\eta^{|l|/2}F(\zeta)\exp\left(-\frac{\zeta}{2}\right), \quad \zeta = \frac{2r^2}{w^2(z)},$$

where $w(z)$ and $F(\zeta)$ are not yet specified. The power and exponential functions are defined by an asymptotic behavior of Eq. (8) at $\zeta \to 0$ and $\zeta \to \infty$, respectively (see Ref. [20]). These functions cannot be totally specified a priori because of the presence of the last operator in Eq. (8). The substitution of $\Psi$ into Eq. (8) results in

$$\exp [i(\Phi - l\phi)]\nabla^2_\perp \Psi_0 + \left\{-\frac{4(\ell + 2s_z)}{w_m^2} - \frac{4r^2}{w_m^4}\right\}\Psi_0 - \frac{k^2r^2}{R^2(z)} - k^2r^2\left[\frac{1}{R(z)}\right]^\prime + 2k\Phi_G(z)\Psi_0 + 2ik\Upsilon(z)\left[1 + |\ell| - \frac{2r^2}{w^2(z)} + \frac{4r^2F'(\zeta)}{w^2(z)F(\zeta)}\right]\Psi_0 = 0,$

$$\nabla^2_\perp \Psi_0 = \frac{2}{w^2(z)}$$

\[4\zeta F''(\zeta) + 4(\zeta + |\ell| + 1)F'(\zeta) + (\zeta - 2|\ell| - 2)F(\zeta)\] \left[\frac{\Psi_0}{F(\zeta)}, \quad \Upsilon(z) = \frac{1}{R(z)} - \frac{w'(z)}{w(z)},

where $\Psi_0 = A\exp (i\ell\phi)$. This equation shows that appropriate functions $\Psi_i$ forming a set of orthogonal eigenfunction are proportional to the generalized Laguerre polynomials $L^{|l|}_n(\zeta)$. In this case, $F(\zeta) = L^{|l|}_n(\zeta)$.

In this case, $F(\zeta) = L^{|l|}_n(\zeta)$,

$$\nabla^2_\perp \Psi_0 = \left[\frac{\Psi_0}{w^2(z)} - N\right]$$

$\Psi_0$ coincides with the Landau wave eigenfunction, and the following conditions should be satisfied:

$$\frac{1}{R(z)} = \frac{w'(z)}{w(z)}, \quad \frac{k^2}{R^2(z)} + k^2\left[\frac{1}{R(z)}\right]^\prime = \frac{4}{w^4(z)} - \frac{4}{w_m^4}, \quad 2k\Phi_G(z) = \frac{4(\ell + 2s_z)}{w_m^2} + \frac{4N}{w^2(z)}.$$
The straightforward solution of these differential equations is based on known integrals \[49\] and has the form

\[ w(z) = w_0 \sqrt{\frac{1}{2} \left[ 1 + \frac{w_m^4}{w_0^4} - \left( \frac{w_m^4}{w_0^4} - 1 \right) \cos \frac{2z}{z_m} \right]} \]

\[ R(z) = kw_m^2 \cos^2 \frac{z}{z_m} + \frac{w_m^4}{w_0^4} \sin^2 \frac{z}{z_m}, \]

\[ \Phi_G(z) = N \arctan \left( \frac{w_m^2}{w_0^2} \tan \frac{z}{z_m} \right) + (\ell + 2s_z)z. \]

The normalization constant $C_{n\ell}$ is given by Eq. (2).

In the cases of $w_m > w_0$ and $w_m < w_0$ (for a relatively weak and strong magnetic field, respectively), the derivations are very different but the corresponding formulas for $w(z)$, $R(z)$, and $\Phi_G(z)$ coincide. $w(z)$ oscillates between $w_0$ and $w_m^2/w_0$. In the case of $B \to 0$ ($w_m >> w_0$), $z << z_m$, there is a full compliance with the solution for a free twisted particle and the beam parameters \[14\] take the form \[6\]. Our result coincides with the Landau solution when $w_0 = w_m$. In this case, the general wave function \[5\], \[14\] takes the form \[9\] and $w(z) = w_m = \text{const}$. However, the paraxial form \[9\] of the Landau wave eigenfunction cannot explain a transition to the free-space solution \[5\], \[6\] at $B \to 0$. The inconsistency of the weak-field limits of the Landau wave eigenfunction and its relativistic generalizations with the well-known equation for free twisted electron beams is rather natural because Refs. \[16\] \[19\] \[24\] describe only unstructured electrons.

Unlike the wave function in the free space, the wave function defined by Eq. \[14\] is spatially periodic. Amazingly, its period $\xi = \pi z_m = \pi kw_m^2/2 = 2\pi P/(\omega_c E)$ is equal to the pitch of the helix characterizing the classical motion of electrons ($\omega_c$ is the cyclotron frequency). Equations \[5\] and \[14\] show that the wave function of a twisted electron in a uniform magnetic field depends only on the total OAM $\hbar \ell$ but not on intrinsic and extrinsic OAMs separately. Therefore, the two latter OAMs cannot be separated.

The LG beam described by Eqs. \[5\], \[14\] is formed by partial waves with the same $E$ and $P$ but slightly different directions of the kinetic momentum. Figures \[1\] \[2\] clearly show
FIG. 1. The beam width, $w(z)$, of a twisted electron beam in a uniform magnetic field for different values of the ratio $w_0/w_m$. The black line describes the case of $w(z) = w_0 = w_m$, when the beam width is equal to the transverse magnetic width of Landau levels, $w_m$. The blue and green lines demonstrate the beam width defined by our general solution for $w_0 = 0.5w_m$ and $w_0 = 2w_m$, respectively. The red line shows the beam width of a free twisted electron beam for $w_0 = 0.5w_m$.

The mean square of the beam radius can be obtained by an integration of the operator $r^2$ over the transversal coordinates $r, \phi$ and reads (cf. Refs. [13, 50])

$$< r^2 > = \int \Psi^\dagger \Psi r^3 dr d\phi = \frac{w^2(z)}{2} (2n + |\ell| + 1).$$

The electric quadrupole moment of twisted electrons introduced in Ref. [50] is measured in
FIG. 2. The transverse probability density defined by our solution for different values of the longitudinal coordinate $z$ and the ratio $w_0/w_m$. In the case (a), $w_0 = w_m$ and our general solution coincides with the Landau solution and is independent of the longitudinal position. In the case (b), $w_0 = 0.5w_m$ and $z = 0$. In this case, our solution coincides with the corresponding one for a free twisted electron. In the case (c), $w_0 = 0.5w_m$ and $z = z_m$. All the plots presented correspond to the quantum numbers $n = 1$, $\ell = 2$.

The focal plane $z = 0$ and is given by

$$Q_0 = \frac{|e|w_0^2}{2} (2n + |\ell| + 1).$$

(16)

The relativistic magnetic moment and the tensor magnetic polarizability are defined in Refs. [51] and [50], respectively (see also Refs. [52, 53]). We note that integrating over the longitudinal coordinate results in

$$\frac{1}{2\pi z_m} \int_0^{2\pi z_m} w^2(z)dz = \frac{w_0^2}{2} \left( 1 + \frac{w_m^4}{w_0^4} \right)^2$$

(17)

Equation (2), its relativistic generalizations [16, 21, 22], and Eq. (9) do not describe twisted electrons which constitute \textit{structured} beams even in the free space. The necessity to use the general equations (5), (14) should substantially change the present theoretical description [3, 7, 8, 13, 15] of twisted electron beams in uniform magnetic fields.

Energies of all partial waves which manifold defines a twisted or a untwisted structured state conserve when a beam penetrates from the free space into a magnetic field region.
Therefore, final energies of such partial waves also coincide. This property remains valid for any nonuniform magnetic field. We predict the effect of a different behavior of two LG beams with opposite OAM directions penetrating from the free space into the magnetic field. Due to a helical motion in the magnetic field, both twisted and untwisted electrons acquire extrinsic OAMs with positive projections onto the field direction (cf. Ref. [45]). When the initial intrinsic OAMs of electrons in the two beams are antiparallel ($\ell_1 = -\ell_2 = |\ell_2|$), an appearance of the extrinsic OAMs conditions the relation $\ell_1' + \ell_2' > 0$ for the final OAMs. The change of total OAMs leads to the difference of magnetic moments of electrons which is observable. The transversal velocities of twisted electrons are nonzero and the Lorentz force turns electrons inwards and outwards for the beams with the intrinsic OAMs $\ell_1 > 0$ and $\ell_2 < 0$, respectively. When the initial beam waists coincide ($w_1 = w_2$), the final beam waists differ and $w_1' < w_2'$. The difference should be of the order of $w_m$. In the general case, the radial quantum numbers will also be changed ($n_1' \neq n_2'$). The effect is observable and the predicted properties can be discovered in a specially designed experiment which is in principle similar to that fulfilled in Ref. [54].

In Ref. [28], the effect of a quantization of the velocity and the effective mass of structured photons and electrons has been predicted. A similar effect should take place for twisted and other structured electrons in the uniform magnetic field. Expectation values of the group velocity are obtained by integrating the operator $v = \partial H_{FW}/(\partial p)$ over the transversal coordinates $r, \phi$ and are defined by (cf. Ref. [28])

$$<v_z> = \frac{ck}{E} \left[ 1 - \frac{<\pi_+^2> - 2es_zB}{2P^2} \right],$$

$$= \frac{ck}{\sqrt{k^2 + K^2}} \left( 1 + \frac{1}{k} \left< \frac{\partial \Phi}{\partial z} \right> \right), \quad K = \frac{mc}{\hbar}.$$

The effective electron mass is equal to (cf. Refs. [28, 55])

$$m_{eff} = \sqrt{m^2 + <\pi_+^2> - 2es_zB} = \sqrt{m^2 - 2k \left< \frac{\partial \Phi}{\partial z} \right>}.$$  

(18)

Cumbersome but straightforward calculations result in

$$<v_z> = \frac{ck}{\sqrt{k^2 + K^2}} \left[ 1 - \frac{\Lambda}{k} \right], \quad m_{eff} = \sqrt{m^2 + 2k\Lambda},$$

$$\Lambda = -\left< \frac{\partial \Phi}{\partial z} \right> = \frac{N}{k} \left( \frac{1}{w_0^2} + \frac{w_0^4}{w_m^4} \right) + \frac{2(\ell + 2s_z)}{kw_m^2}.$$

(20)

In the uniform magnetic field, the effect of quantization of the velocity and the effective mass of structured electrons has some distinguishing features. In particular, its strong
enhancement takes place when $w_m \ll w_0$. However, it is difficult to satisfy this condition. When $B = 1$ T, $w_m = 5.1 \times 10^{-8}$ m. An estimate of the beam waist $w_0 \sim 10^{-9}$ m can be extracted from results obtained in Ref. [56]. Therefore, usually $w_m > w_0$ and a significant enhancement of the effect does not occur.

In summary, we have revisited the theory of twisted paraxial electrons and have fulfilled their general quantum-mechanical description in the uniform magnetic field. We have generalized the Landau theory and its relativistic extensions. The results obtained establish fundamental properties of twisted and other structured electrons and substantially change the common view on the considered problem. In the weak-field limit, our solution agrees with the well-known equation for free twisted electron beams. To the contrary, the weak-field limits of the Landau wave function and its relativistic generalizations are inconsistent with this equation. We have predicted the important observable effect of the different behavior of LG beams with the same beam waist and opposite OAM directions penetrating from the free space into the magnetic field. When $\ell_1 = -\ell_2 = |\ell_2|$, the final beam waists differ ($w'_1 < w'_2$) and the final OAMs satisfy the relation $\ell'_1 + \ell'_2 > 0$. Distinguishing features of the quantization of the velocity and the effective mass of structured electrons in the uniform magnetic field have been analyzed.

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