

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

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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. Unlike all precedent investigations, the present study describes structured electron states which are not plane waves along the magnetic field direction. 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 the Laguerre-Gauss and Landau electrons in the uniform magnetic field are analyzed.

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The discovery of twisted (vortex) electron states with a nonzero intrinsic orbital angular momentum (OAM) [1] has confirmed their theoretical prediction [2] 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 $1000\hbar$) 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 $\hbar = 1$, $c = 1$. We include \hbar 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, $\mathbf{B} = B\mathbf{e}_z$. 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

$$\mathcal{H} = \frac{\pi^2 - e\sigma \cdot \mathbf{B}}{2m}, \quad \pi^2 = -\nabla^2 + ieB\frac{\partial}{\partial\phi} + \frac{e^2 B^2 r^2}{4} \quad (1)$$

reads

$$\begin{aligned} \psi &= \mathcal{A} \exp(i\ell\phi) \exp(ip_z z), \quad \int \psi^\dagger \psi r dr d\phi = 1, \\ \mathcal{A} &= \frac{C_{n\ell}}{w_m} \left(\frac{\sqrt{2}r}{w_m} \right)^{|\ell|} L_n^{|\ell|} \left(\frac{2r^2}{w_m^2} \right) \exp\left(-\frac{r^2}{w_m^2}\right) \eta, \\ C_{n\ell} &= \sqrt{\frac{2n!}{\pi(n+|\ell|)!}}, \quad w_m = \frac{2}{\sqrt{|e|B}} \end{aligned} \quad (2)$$

Here $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}$ is the kinetic momentum, the real function \mathcal{A} defines the beam amplitude, $L_n^{|\ell|}$ is the generalized Laguerre polynomial, and $n = 0, 1, 2, \dots$ is the radial quantum number. When the cylindrical coordinates are used, $A_\phi = Br/2$, $A_r = A_z = 0$. For the electron, $e = -|e|$. The spin function η is an eigenfunction of the Pauli operator σ_z (cf. Ref. [25]):

$$\sigma_z \eta^\pm = \pm \eta^\pm, \quad \eta^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \eta^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (3)$$

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 ψ 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]:

$$\left(\nabla_\perp^2 + 2ik \frac{\partial}{\partial z} \right) \Psi = 0, \quad \nabla_\perp^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}. \quad (4)$$

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

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and reads [26,29,30]

$$\begin{aligned}\Psi &= \mathbb{A} \exp(i\Phi), \quad \int \Psi^\dagger \Psi r dr d\phi = 1, \\ \mathbb{A} &= \frac{C_{n\ell}}{w(z)} \left(\frac{\sqrt{2}r}{w(z)} \right)^{|\ell|} L_n^{|\ell|} \left(\frac{2r^2}{w^2(z)} \right) \exp\left(-\frac{r^2}{w^2(z)}\right) \eta, \\ \Phi &= \ell\phi + \frac{kr^2}{2R(z)} - \Phi_G(z),\end{aligned}\quad (5)$$

where

$$\begin{aligned}w(z) &= w_0 \sqrt{1 + \frac{z^2}{z_R^2}}, \quad R(z) = z + \frac{z_R^2}{z}, \quad z_R = \frac{kw_0^2}{2}, \\ \Phi_G(z) &= N \arctan\left(\frac{z}{z_R}\right), \quad N = 2n + |\ell| + 1,\end{aligned}\quad (6)$$

the real functions \mathbb{A} and Φ define the amplitude and phase, k is the beam wave number, w_0 is the beam waist (minimum beam width), $R(z)$ is the radius of curvature of the wave front, $\Phi_G(z)$ is the Gouy phase, and z_R is the Rayleigh diffraction length. The quantities $C_{n\ell}$ and η are given by Eqs. (2) and (3), respectively. For electrons, Ψ is a spinor. Evidently, Ψ is not an eigenfunction of the operator p_z . Therefore, the free-space wave functions (5) and (6) characterize 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]

$$i \frac{\partial \Psi_{\text{FW}}}{\partial t} = \mathcal{H}_{\text{FW}} \Psi_{\text{FW}}, \quad \mathcal{H}_{\text{FW}} = \beta \sqrt{m^2 + \boldsymbol{\pi}^2} - e \boldsymbol{\Sigma} \cdot \mathbf{B}, \quad (7)$$

where $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}$ is the kinetic momentum and β and $\boldsymbol{\Sigma}$ are the Dirac matrices. This Hamiltonian acts on the bispinor $\Psi_{\text{FW}} = \begin{pmatrix} \Phi_{\text{FW}} \\ 0 \end{pmatrix}$. The zero lower spinor of the bispinor can be disregarded. Eigenfunctions (more precisely, an upper spinor) of the *relativistic* FW Hamiltonian coincide with the *non-relativistic* Landau solution (2) because the operator $\boldsymbol{\pi}^2 - e\boldsymbol{\Sigma} \cdot \mathbf{B}$ 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 $\Phi_{\text{FW}} = \exp(ikz)\Psi$ lead to the paraxial

equation [45]

$$\left(\nabla_\perp^2 - ieB \frac{\partial}{\partial \phi} - \frac{e^2 B^2 r^2}{4} + 2es_z B + 2ik \frac{\partial}{\partial z} \right) \Psi = 0, \quad (8)$$

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]

$$\begin{aligned}\Psi &= \mathcal{A} \exp(i\ell\phi) \exp[-i\zeta_G(z)], \\ \zeta_G(z) &= (2n + 1 + |\ell| + \ell + 2s_z) \frac{2z}{kw_m^2}, \quad w_m = \frac{2}{\sqrt{|e|B}},\end{aligned}\quad (9)$$

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 paraxial approximation for the electron velocity, $|v_\perp| \ll v$, and takes place in the laboratory frame. In this frame, the transversal motion can be described by means of nonrelativistic quantum mechanics.

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 an optical approach [27,46–48] applied for the free-space paraxial equation (see Supplemental Material [49], Sec. I). The subsequent derivation shows that an electron state is described by the matter wave beam (5) but three functions on z should be overridden. The power and exponential functions are defined by an asymptotic behavior of Eq. (8) at $\zeta \rightarrow 0$ and $\zeta \rightarrow \infty$, respectively (see Ref. [20]). These functions cannot be totally specified *a priori* because of the presence of the last operator in Eq. (8). It is helpful to suppose that the general solution of Eq. (8) has the form (5), where $w(z)$, $R(z)$, and $\Phi_G(z)$ are not yet specified. First of all, we need to check that the corresponding wave functions Ψ form a set of orthogonal eigenfunctions. When we denote

$$\zeta = \frac{2r^2}{w^2(z)},$$

the substitution of Ψ into Eq. (8) results in

$$\begin{aligned} & \exp[i(\Phi - \ell\phi)] \nabla_{\perp}^2 \Psi_0 + \left\{ -\frac{4(\ell + 2s_z)}{w_m^2} - \frac{4r^2}{w_m^4} \right. \\ & \quad \left. - \frac{k^2 r^2}{R^2(z)} - k^2 r^2 \left[\frac{1}{R(z)} \right]' + 2k\Phi'_G(z) \right\} \Psi \\ & \quad + 2ik\Upsilon(z) \left[1 + |\ell| - \frac{2r^2}{w^2(z)} + \frac{4r^2 L_n^{|\ell|'}(\zeta)}{w^2(z) L_n^{|\ell|}(\zeta)} \right] \Psi \\ & = 0, \\ & \nabla_{\perp}^2 \Psi_0 = \frac{2}{w^2(z)} \left[4\zeta L_n^{|\ell|''}(\zeta) + 4(-\zeta + |\ell| + 1) L_n^{|\ell|'}(\zeta) \right. \\ & \quad \left. + (\zeta - 2|\ell| - 2) L_n^{|\ell|}(\zeta) \right] \frac{\Psi_0}{L_n^{|\ell|}(\zeta)}, \\ & \Upsilon(z) = \frac{1}{R(z)} - \frac{w'(z)}{w(z)}, \end{aligned} \quad (10)$$

where $\Psi_0 = \mathbb{A} \exp(i\ell\phi)$ and primes denote derivatives with respect to mentioned variables (ζ or z). We can check that properties of the generalized Laguerre polynomials confirm our supposition about the validity of wave functions (5) in the considered case. In this case,

$$\nabla_{\perp}^2 \Psi_0 = \frac{4}{w^2(z)} \left[\frac{r^2}{w^2(z)} - N \right] \Psi_0, \quad (11)$$

Ψ_0 coincides with the Landau wave eigenfunction, and the following conditions should be satisfied:

$$\begin{aligned} \frac{1}{R(z)} &= \frac{w'(z)}{w(z)}, \quad \frac{k^2}{R^2(z)} + k^2 \left[\frac{1}{R(z)} \right]' = \frac{4}{w^4(z)} - \frac{4}{w_m^4}, \\ 2k\Phi'_G(z) &= \frac{4(\ell + 2s_z)}{w_m^2} + \frac{4N}{w^2(z)}. \end{aligned} \quad (12)$$

The straightforward solution of these differential equations is based on known integrals [50] and has the form (Supplemental Material [49], Sec. II)

$$\begin{aligned} w(z) &= w_0 \sqrt{\frac{1}{2} \left[1 + \frac{w_m^4}{w_0^4} - \left(\frac{w_m^4}{w_0^4} - 1 \right) \cos \frac{2z}{z_m} \right]} \\ &= w_0 \sqrt{\cos^2 \frac{z}{z_m} + \frac{w_m^4}{w_0^4} \sin^2 \frac{z}{z_m}}, \quad z_m = \frac{kw_m^2}{2}, \\ R(z) &= kw_m^2 \frac{\cos^2 \frac{z}{z_m} + \frac{w_m^4}{w_0^4} \sin^2 \frac{z}{z_m}}{\left(\frac{w_m^4}{w_0^4} - 1 \right) \sin \frac{2z}{z_m}}, \\ \Phi_G(z) &= N \arctan \left(\frac{w_m^2}{w_0^2} \tan \frac{z}{z_m} \right) + \frac{(\ell + 2s_z)z}{z_m}. \end{aligned} \quad (13)$$

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

It is important that the exact FW Hamiltonian for a Dirac particle in a *nonuniform* but time-independent magnetic field $\mathbf{B}(\mathbf{r})$ has also the form (7) [39,41]. We expect that our approach can be useful for a general description of relativistic Dirac particle beams in some axially symmetric nonuniform magnetic fields, in particular, for the relativistic electron beams in round magnetic lenses and real solenoids. These

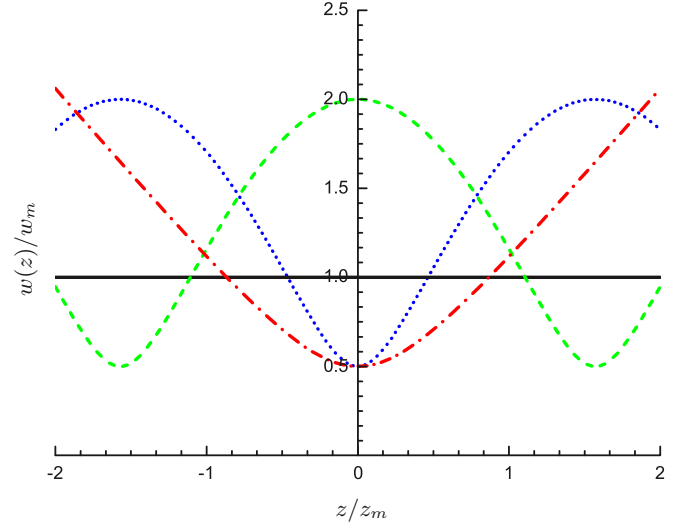


FIG. 1. The beam width, $w(z)$, of a twisted electron beam in a uniform magnetic field for different values of the ratio w_0/w_m . The solid black line describes the case of $w(z) = w_0 = w_m$, when the beam width is equal to the transverse magnetic width of Landau levels, w_m . The dotted blue and dashed green lines demonstrate the beam width defined by our general solution for $w_0 = 0.5w_m$ and $w_0 = 2w_m$, respectively. The dash-dotted red line shows the beam width of a *free* twisted electron beam for $w_0 = 0.5w_m$.

problems are of great practical importance (see Refs. [51,52], and references therein).

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 $B \rightarrow 0$ ($w_m \gg w_0$), $z \ll z_m$, there is a full compliance with the solution for a free twisted particle and the beam parameters (13) take the form (6). This important property is illustrated by Fig. 1 (the dotted blue and dash-dotted red lines at $z = 0$) and Fig. 2 (the middle plot). In the latter figure, the probability density distribution in the xy plane is shown. Our result coincides with the Landau solution when $w_0 = w_m$. The coincidence is shown by the

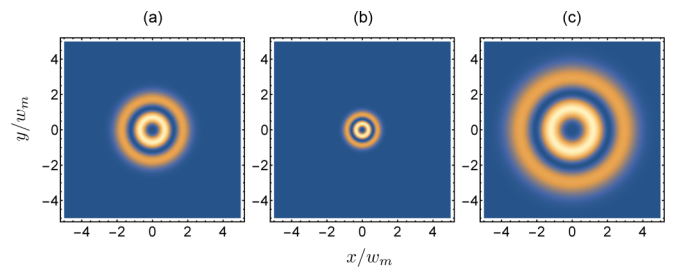


FIG. 2. The transverse probability density defined by our solution for different values of the longitudinal coordinate z and the ratio w_0/w_m . In case (a), $w_0 = w_m$ and our general solution coincides with the Landau solution and is independent of the longitudinal position. In case (b), $w_0 = 0.5w_m$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

solid black line in Fig. 1 and by Fig. 2 (the left plot). In this case, the general wave function (5), (13) 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 $B \rightarrow 0$. 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. (13) is spatially periodic. Amazingly, its period $\mathcal{L} = \pi z_m = \pi k w_m^2 / 2 = 2\pi P / (\omega_c E)$ is equal to the pitch of the helix characterizing the classical motion of electrons (ω_c is the cyclotron frequency). The spatially periodic behavior of the wave function is illustrated by Fig. 1. A similarity between the probability density distributions of the LG and Landau wave eigenfunctions is demonstrated by Fig. 2. Equations (5) and (13) 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) and (13) is formed by partial waves with the same E and P but slightly different directions of the kinetic momentum. Figures 1 and 2 clearly show differences between the Landau solution and ours. As follows from Eq. (13) and Fig. 1, our solution for $w(z)$ always crosses the Landau line.

The mean square of the beam radius can be obtained by an integration of the operator r^2 over the *transversal* coordinates r, ϕ and reads (cf. Refs. [13,53])

$$\langle r^2 \rangle = \int \Psi^\dagger \Psi r^2 dr d\phi = \frac{w^2(z)}{2} (2n + |\ell| + 1). \quad (14)$$

The electric quadrupole moment of twisted electrons introduced in Ref. [53] is measured in the focal plane $z = 0$ and is given by

$$Q_0 = \frac{|e|w_0^2}{2} (2n + |\ell| + 1). \quad (15)$$

The relativistic magnetic moment and the tensor magnetic polarizability are defined in Refs. [54] and [53], respectively (see also Refs. [55,56]). We note that integrating over the *longitudinal* coordinate results in

$$\begin{aligned} \frac{1}{2\pi z_m} \int_0^{2\pi z_m} w^2(z) dz &= \frac{w_0^2}{2} \left(1 + \frac{w_m^4}{w_0^4} \right) \\ &= w_m^2 \left[1 + \frac{1}{2} \left(\frac{w_m}{w_0} - \frac{w_0}{w_m} \right)^2 \right]. \end{aligned} \quad (16)$$

Equation (2), its relativistic generalizations [16,21,22], and Eq. (9) do not describe twisted electrons which constitute *structured* beams even in the free space. The necessity to use the general equations (5) and (13) 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 an 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. [57].

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 $\mathbf{v} = \partial \mathcal{H}_{\text{FW}} / (\partial \mathbf{p})$ over the *transversal* coordinates r, ϕ and are defined by (cf. Ref. [28])

$$\begin{aligned} \langle v_z \rangle &= \frac{cP}{E} \left(1 - \frac{\langle \pi_\perp^2 \rangle - 2es_z B}{2P^2} \right) \\ &= \frac{ck}{\sqrt{k^2 + K^2}} \left(1 + \frac{1}{k} \left\langle \frac{\partial \Phi}{\partial z} \right\rangle \right), \quad K = \frac{mc}{\hbar}. \end{aligned} \quad (17)$$

The effective electron mass is equal to (cf. Refs. [28,58])

$$m_{\text{eff}} = \sqrt{m^2 + \langle \pi_\perp^2 \rangle - 2es_z B} = \sqrt{m^2 - 2k \left\langle \frac{\partial \Phi}{\partial z} \right\rangle}. \quad (18)$$

Cumbersome but straightforward calculations similar to those fulfilled in Ref. [28] result in

$$\begin{aligned} \langle v_z \rangle &= \frac{ck}{\sqrt{k^2 + K^2}} \left[1 - \frac{\Lambda}{k} \right], \quad m_{\text{eff}} = \sqrt{m^2 + 2k\Lambda}, \\ \Lambda &= - \left\langle \frac{\partial \Phi}{\partial z} \right\rangle = \frac{N}{k} \left(\frac{1}{w_0^2} + \frac{w_0^2}{w_m^4} \right) + \frac{2(\ell + 2s_z)}{kw_m^2}. \end{aligned} \quad (19)$$

In the uniform magnetic field, the effect of quantization of the velocity and the effective mass of structured electrons strongly depends on a kind of the structured electron beam. A distance between neighboring quantum levels of these quantities defining the quantization is determined by Λ . Importantly, a similar quantization takes place for the Landau beams in the uniform magnetic field and the LG beams in the free space. In these cases, the formulas for $\langle v_z \rangle$ and m_{eff} presented in Eq. (19) remain the same and the corresponding formulas for Λ_L and Λ_{free} read

$$\Lambda_L = \frac{2(N + \ell + 2s_z)}{kw_m^2}, \quad \Lambda_{\text{free}} = \frac{N}{kw_0^2}. \quad (20)$$

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