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Dynamics of an orbital polarization of twisted electron beams in electric and magnetic fields

Alexander J. Silenko[1,2,3,*], *Pengming* Zhang[1,4,**], and *Liping* Zou[1,4,***]

[1]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[2]Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia
[3]Research Institute for Nuclear Problems, Belarusian State University, Minsk 220030, Belarus
[4]University of Chinese Academy of Sciences, Yuquanlu 19A, Beijing 100049, China

Abstract. Relativistic classical and quantum dynamics of twisted (vortex) Dirac particles in arbitrary electric and magnetic fields is constructed. The relativistic Hamiltonian and equations of motion in the Foldy-Wouthuysen representation are derived. Methods for the extraction of an electron vortex beam with a given orbital polarization and for the manipulation of such a beam are developed. The new effect of a radiative orbital polarization of a twisted electron beam in a magnetic field resulting in a nonzero average projection of the intrinsic orbital angular momentum on the field direction is predicted.

1 Introduction

The discovery of twisted (vortex) electron beams [1] has shown that particles can carry an intrinsic orbital angular momentum (OAM). Twisted electron beams with large intrinsic OAMs (up to $1000\hbar$) have been recently obtained [2]. Since twisted electrons possess large magnetic moments, this discovery opens new possibilities in the electron microscopy and investigations of magnetic phenomena [3–5]. The dynamics of the intrinsic OAM in external magnetic and electric fields has been previously studied in many works (see, e.g., [6–10]). However, the correct equation of motion of the intrinsic OAM in an electric field [11] differs from the equation found in [6]. In [11, 12], the general description of the relativistic dynamics of an intrinsic OAM in arbitrary electric and magnetic fields in the framework of relativistic quantum mechanics and classical physics has been made.

In the present work, the system of units $\hbar = 1$, $c = 1$ is used. We include $\hbar$ and c explicitly when this inclusion clarifies the problem. The curly brackets, $\{\ldots,\ldots\}$, denote anticommutators.

2 Relativistic centroid in the framework of the Dirac quantum mechanics

Since vortex electrons are relativistic quantum objects admitting also a semiclassical description, a construction of a *relativistic* Schrödinger-like dynamics of such particles is necessary.

*e-mail: alsilenko@mail.ru
**e-mail: zhpm@impcas.ac.cn
***e-mail: zoulp@impcas.ac.cn

It is important that one mainly observes a motion of charged centroids and it is instructive to mirror this circumstance in an appropriate quantum description. We present the general solution of this problem. We also notice the previous quantum-mechanical analysis mirrored in the reviews [3, 4].

A twisted electron is a single pointlike particle. However, its wave function is a superposition of states with different momentum directions. While the twisted electron in vacuum has a nonzero intrinsic OAM and a nonzero component of the momentum in the plane orthogonal to the direction of its resulting motion, it can be described by the Dirac equation for a free particle. Quantum mechanics (QM) of the twisted electron in external electromagnetic fields is also governed by the usual Dirac equation. We can disregard the anomalous magnetic moment of the electron because its g factor is close to 2. The Schrödinger form of the relativistic QM is provided by the relativistic Foldy-Wouthuysen (FW) transformation [13]. There are many methods of the relativistic FW transformation (see [14–18] and references therein). The results obtained by different methods agree because of the uniqueness of the FW representation [19]. The use of the nonrelativistic QM for a description of relativistic twisted electrons whose kinetic energy, 200 ÷ 300 keV, is comparable with their rest energy, 511 keV, is controversial.

The *exact* relativistic FW Hamiltonian for a Dirac particle in a magnetic field is given by

$$\mathcal{H}_{FW} = \beta\sqrt{m^2 + \boldsymbol{\pi}^2 - e\boldsymbol{\Sigma}\cdot\boldsymbol{B}}, \tag{1}$$

where $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}$ is the kinetic momentum, $\boldsymbol{B} = \nabla\times\boldsymbol{A}$ is the magnetic induction, and β and $\boldsymbol{\Sigma}$ are the Dirac matrices. This Hamiltonian has been first obtained in [20] and its validity has been confirmed in other works [15, 21, 22]. It is valid for a twisted and a untwisted particle. The spin angular momentum operator is equal to $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$. The magnetic field is, in general, nonuniform but time-independent. Our quantum description of a twisted Dirac particle is fully relativistic and correctly defines both electric and magnetic interactions. The precedent study [11] has shown the importance of the electric field.

The FW Hamiltonian acts on the bispinor wave function $\Psi_{FW} = \begin{pmatrix}\phi\\ 0\end{pmatrix}$. Since both the nonrelativistic and the relativistic FW Hamiltonians commute with the operators $\boldsymbol{\pi}^2$ and s_z, their eigenfunctions coincide. It is convenient to present the exact energy spectrum obtained by different methods [20–26] as follows:

$$E = \sqrt{m^2 + (2n + 1 + |l_z| + l_z + 2s_z)|e|B}, \tag{2}$$

where $n = 0, 1, 2, \ldots$ is the radial quantum number and $\boldsymbol{l} = \boldsymbol{r}\times\boldsymbol{p} = \boldsymbol{L} + \boldsymbol{L}^{(e)}$ is the total OAM operator being the sum of the intrinsic ($\boldsymbol{L}$) and extrinsic ($\boldsymbol{L}^{(e)}$) OAMs.

It is necessary to take into account that a twisted electron is a charged centroid [3, 6]. To describe observable quantum-mechanical effects, we need to present the Hamiltonian in terms of the centroid parameters. The centroid as a whole is characterized by the center-of-charge radius vector $\boldsymbol{R}$ and by the kinetic momentum $\boldsymbol{\pi}' = \boldsymbol{P} - e\boldsymbol{A}(\boldsymbol{R})$, where $\boldsymbol{P} = -i\hbar\partial/(\partial\boldsymbol{R})$. The intrinsic motion is defined by the kinetic momentum $\boldsymbol{\pi}'' = \mathfrak{p} - e[\boldsymbol{A}(\boldsymbol{r}) - \boldsymbol{A}(\boldsymbol{R})]$. Here $\mathfrak{p} = -i\hbar\partial/(\partial\mathfrak{r})$, $\mathfrak{r} = \boldsymbol{r} - \boldsymbol{R}$, $\boldsymbol{\pi}' + \boldsymbol{\pi}'' = \boldsymbol{\pi}$, $\boldsymbol{P} + \mathfrak{p} = \boldsymbol{p}$. Since

$$\boldsymbol{A}(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{R}) + \frac{1}{2}\boldsymbol{B}(\boldsymbol{R})\times\mathfrak{r},$$

the operator $\boldsymbol{\pi}^2$ takes the form

$$\boldsymbol{\pi}^2 = \boldsymbol{\pi}'^2 + \mathfrak{p}^2 - \frac{e}{2}\left[\boldsymbol{L}\cdot\boldsymbol{B}(\boldsymbol{R}) + \boldsymbol{B}(\boldsymbol{R})\cdot\boldsymbol{L}\right] + \boldsymbol{\pi}'\cdot\boldsymbol{\pi}'' + \boldsymbol{\pi}''\cdot\boldsymbol{\pi}'.$$

After summing over partial waves with different momentum directions, $<\boldsymbol{\pi}'\cdot\boldsymbol{\pi}''+\boldsymbol{\pi}''\cdot\boldsymbol{\pi}'>=0$. More precisely, the operator $\boldsymbol{\pi}'\cdot\boldsymbol{\pi}''+\boldsymbol{\pi}''\cdot\boldsymbol{\pi}'$ has zero expectation values for any eigenstates of the operator $\boldsymbol{\pi}^2$ and, therefore, it can be omitted.

The FW Hamiltonian summed over the partial waves [3] takes the form

$$\mathcal{H}_{FW}=\beta\epsilon-\beta\frac{e}{4}\left[\frac{1}{\epsilon}\boldsymbol{\Lambda}\cdot\boldsymbol{B}(\boldsymbol{R})+\boldsymbol{B}(\boldsymbol{R})\cdot\boldsymbol{\Lambda}\frac{1}{\epsilon}\right],\quad \epsilon=\sqrt{m^2+\boldsymbol{\pi}'^2+\mathfrak{p}^2},\quad \boldsymbol{\Lambda}=\boldsymbol{L}+\boldsymbol{\Sigma}. \tag{3}$$

The momentum and the intrinsic OAM can have different mutual orientations in different Lorentz frames. As a rule, the intrinsic OAM and the momentum of the twisted electron are collinear in the laboratory (lab) frame. However, it does not take place in other frames. The Lorentz transformation of the OAM from the lab frame ($\boldsymbol{L}=L_z\boldsymbol{e}_z$) to the rest frame results in $\boldsymbol{L}_0=\boldsymbol{L}$. The OAM in the frame moving with the arbitrary velocity $\boldsymbol{V}$ relative to the particle rest frame is given by [11, 12]

$$\boldsymbol{L}=\frac{\epsilon}{mc^2}\boldsymbol{L}^{(0)}-\frac{(\boldsymbol{L}^{(0)}\cdot\boldsymbol{\pi}')\boldsymbol{\pi}'}{m(\epsilon+mc^2)},\qquad \epsilon=\frac{mc^2}{\sqrt{1-\frac{V^2}{c^2}}}. \tag{4}$$

3 Twisted electrons in external electric and magnetic fields

The operators of the magnetic and electric dipole moments, $\boldsymbol{\mu}$ and $\boldsymbol{d}$, are defined by

$$\mathcal{H}_{FW}^{(int)}=-\frac{1}{2}[\boldsymbol{\mu}\cdot\boldsymbol{B}(\boldsymbol{R})+\boldsymbol{B}(\boldsymbol{R})\cdot\boldsymbol{\mu}+\boldsymbol{d}\cdot\boldsymbol{E}(\boldsymbol{R})+\boldsymbol{E}(\boldsymbol{R})\cdot\boldsymbol{d}], \tag{5}$$

where $\mathcal{H}_{FW}^{(int)}$ is the interaction Hamiltonian. In the weak-field approximation, the operator of the magnetic dipole moment of a moving centroid obtained from Eq. (3) is given by

$$\boldsymbol{\mu}=\beta\frac{e(\boldsymbol{L}+2\boldsymbol{s})}{2\epsilon}. \tag{6}$$

This equation agrees with [9, 11, 27, 28].

Now we can take into account that the quantities $\boldsymbol{L}^{(0)}$ and $\boldsymbol{\mu}^{(0)}$ are connected with the nonrotating instantaneous inertial frame and can perform the relativistic transformation of the dipole moments to the lab frame (see [29]):

$$\boldsymbol{d}=\boldsymbol{\beta}\times\boldsymbol{\mu}^{(0)},\qquad \boldsymbol{\mu}=\boldsymbol{\mu}^{(0)}-\frac{\gamma}{\gamma+1}\widetilde{\boldsymbol{\beta}}(\widetilde{\boldsymbol{\beta}}\cdot\boldsymbol{\mu}^{(0)}),\qquad \widetilde{\boldsymbol{\beta}}=\frac{\boldsymbol{V}}{c},\qquad \gamma=(1-\widetilde{\boldsymbol{\beta}}^2)^{-1/2}, \tag{7}$$

where the relation $\boldsymbol{d}^{(0)}=0$ is used and γ is the Lorentz factor. The centroid velocity operator can be obtained from the FW Hamiltonian: $\boldsymbol{V}=i[\mathcal{H}_{FW},\boldsymbol{R}]=(\beta/2)\{\epsilon^{-1},\boldsymbol{\pi}'\}$.

The general FW Hamiltonian for a relativistic twisted particle in electric and magnetic fields is given by [12]

$$\begin{aligned}\mathcal{H}_{FW}=&\beta\epsilon+e\Phi-\beta\frac{e}{4}\left[\frac{1}{\epsilon}\boldsymbol{L}\cdot\boldsymbol{B}(\boldsymbol{R})+\boldsymbol{B}(\boldsymbol{R})\cdot\boldsymbol{L}\frac{1}{\epsilon}\right]\\&+\frac{e}{4}\left\{\frac{1}{\epsilon^2}\boldsymbol{L}\cdot[\boldsymbol{\pi}'\times\boldsymbol{E}(\boldsymbol{R})]-[\boldsymbol{E}(\boldsymbol{R})\times\boldsymbol{\pi}']\cdot\boldsymbol{L}\frac{1}{\epsilon^2}\right\}.\end{aligned} \tag{8}$$

In this equation, spin effects are disregarded because they can be neglected on the condition that $L\gg 1$. The term $e\Phi$ does not include the interaction of the intrinsic OAM with the electric field. The corresponding classical Hamiltonian [11] is similar:

$$\begin{aligned}H=\epsilon+e\Phi+H^{(int)},\qquad H^{(int)}=&-\frac{e}{2mc}\Big[\boldsymbol{B}\cdot\boldsymbol{L}^{(0)}-\frac{\gamma}{\gamma+1}(\widetilde{\boldsymbol{\beta}}\cdot\boldsymbol{B})(\widetilde{\boldsymbol{\beta}}\cdot\boldsymbol{L}^{(0)})\\&-(\widetilde{\boldsymbol{\beta}}\times\boldsymbol{E})\cdot\boldsymbol{L}^{(0)}\Big]=-\frac{e}{2mc\gamma}\left[\boldsymbol{B}\cdot\boldsymbol{L}-(\widetilde{\boldsymbol{\beta}}\times\boldsymbol{E})\cdot\boldsymbol{L}\right].\end{aligned}$$

Equation (8) exhaustively describes the quantum dynamics of the intrinsic OAM in the general case of arbitrary electric and magnetic fields. The intrinsic-OAM motion is given by

$$\begin{gathered}\frac{d\boldsymbol{L}}{dt} = i[\mathcal{H}_{FW},\boldsymbol{L}] = \frac{1}{2}\left(\boldsymbol{\Omega}\times\boldsymbol{L}-\boldsymbol{L}\times\boldsymbol{\Omega}\right),\\ \boldsymbol{\Omega} = -\beta\frac{e}{4}\left\{\frac{1}{\epsilon},\boldsymbol{B}(\boldsymbol{R})\right\}+\frac{e}{4}\left[\frac{1}{\epsilon^2}\boldsymbol{\pi}'\times\boldsymbol{E}(\boldsymbol{R})-\boldsymbol{E}(\boldsymbol{R})\times\boldsymbol{\pi}'\frac{1}{\epsilon^2}\right].\end{gathered} \tag{9}$$

The relativistic quantum dynamics of the kinetic momentum is defined by the force operator:

$$\boldsymbol{F} = \frac{d\boldsymbol{\pi}'}{dt} = \frac{\partial\boldsymbol{\pi}'}{\partial t}+i[\mathcal{H}_{FW},\boldsymbol{\pi}'] = e\boldsymbol{E}(\boldsymbol{R})+\beta\frac{e}{4}\left\{\frac{1}{\epsilon},\left(\boldsymbol{\pi}'\times\boldsymbol{B}(\boldsymbol{R})-\boldsymbol{B}(\boldsymbol{R})\times\boldsymbol{\pi}'\right)\right\}+\boldsymbol{F}_{SGl}, \tag{10}$$

where $\boldsymbol{F}_{SGl}$ is the Stern-Gerlach-like force operator [12].

4 Manipulations of twisted electron beams

The obtained results provide a basis for developing methods for the manipulation of twisted electron beams [11]. These methods are similar to those governing the spin while formulas defining dynamics of the intrinsic OAM and the spin differ.

Separation of beams with opposite directions of the OAM.— For this separation, a longitudinal magnetic field can be applied. This field can be nonuniform [3] and even uniform. The nonuniform longitudinal magnetic field leads to a force acting on the OAM. The direction of this force depends on that of the OAM. As a result, accelerations of particles with oppositely directed OAMs have different signs. Since this leads to different velocities of particles with the opposite directions of the OAMs, the beam with a given OAM direction can be extracted.

Even a uniform longitudinal magnetic field leads to a dependence of a particle velocity on the OAM direction. If particles have equal energies beyond the field, their velocities in this field differ [11]. This effect either decreases or increases the beam separation caused by the *nonuniform* longitudinal magnetic field. The use of a transversal magnetic field is less convenient. This field can lead to loss of beam coherence due to the Larmor precession.

Freezing the intrinsic OAM in electromagnetic fields.— As in spin physics [30], it is important to determine a condition of freezing the intrinsic OAM relative to the momentum direction [$(\boldsymbol{L}\cdot\boldsymbol{\pi}') = const$]. In this case, the angular velocity of the Larmor precession (9) is equal to the angular velocity of the rotation of the momentum direction $\boldsymbol{N}=\widetilde{\boldsymbol{\beta}}/\widetilde{\beta}$ [31]:

$$\frac{d\boldsymbol{N}}{dt} = \boldsymbol{\omega}\times\boldsymbol{N}, \qquad \boldsymbol{\omega} = -\frac{e}{mc\gamma}\left(\boldsymbol{B}-\frac{\boldsymbol{N}\times\boldsymbol{E}}{\widetilde{\beta}}\right). \tag{11}$$

The standard geometry is $\boldsymbol{E}\perp\boldsymbol{B}\perp\widetilde{\boldsymbol{\beta}}$. When the condition $\boldsymbol{\Omega}_L=\boldsymbol{\omega}$ is satisfied,

$$\boldsymbol{B} = \left(\frac{2}{\widetilde{\beta}^2}-1\right)\widetilde{\boldsymbol{\beta}}\times\boldsymbol{E}, \qquad \boldsymbol{\Omega}_L = \boldsymbol{\omega} = -\frac{e\boldsymbol{B}}{mc\gamma(\gamma^2+1)}. \tag{12}$$

For a usual beam energy of the order of 10^2 keV, the beam deflection is rather effective.

The use of the proposed beam deflector after or together with the longitudinal magnetic field considered above allows one to separate out electrons with oppositely directed OAMs.

Rotator of the intrinsic OAM.— Another important beam manipulation is a rotation of the intrinsic OAM relative to the momentum direction. This manipulation is desirable and even necessary when the beam is confined in a storage ring or trap. In this case, the vertical OAM direction is preferable because it is not affected by the main vertical magnetic field and can

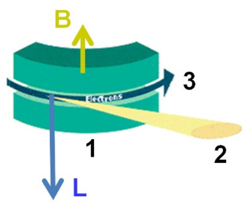

Figure 1. Radiative OAM polarization of twisted electrons: 1 – magnet, 2 – synchrotron light, 3 – twisted electron beam. The directions of the main magnetic field, $\boldsymbol{B}$, and the final orbital polarization of electrons, $\boldsymbol{L}$, are opposite

be conserved. A Wien filter frequently used in accelerator physics as a spin rotator can also be applied as an OAM rotator. In this case, $\boldsymbol{E}\perp\boldsymbol{B}\perp\widetilde{\boldsymbol{\beta}}$ and the Lorentz force is equal to zero ($\boldsymbol{E} = -\widetilde{\boldsymbol{\beta}} \times \boldsymbol{B}$). The angular velocity of precession of the intrinsic OAM is given by

$$\boldsymbol{\Omega}^{(W)} = -\frac{e(m^2 + \mathfrak{p}^2)}{2\epsilon^3}\boldsymbol{B} \approx -\frac{e}{2m\gamma^3}\boldsymbol{B}. \tag{13}$$

When beams with oppositely directed OAMs have different velocities, the Wien filter allows one to extract electrons with one of orbital polarizations.

Flipping the intrinsic OAM.— If twisted electrons with an upward or a downward orbital polarization are confined in a storage ring, the direction of the intrinsic OAM can be flipped. A flip of the OAM is similar to that of the spin and can be fulfilled by the method of the magnetic resonance. A significant difference between the flips of the OAM and the spin consists in different dependences of the resonance frequencies on the electric and magnetic fields. A spin flip frequency in a storage ring is defined by the Thomas-Bargmann-Mishel-Telegdi equation (see [32] for details) whose distinction from Eq. (9) is evident. The OAM flip can be forced by a longitudinal (azimuthal) magnetic field oscillating with the resonance frequency. A Wien filter with a vertical electric field and a radial magnetic field oscillating with the resonance frequency [32, 33] can also be used for the OAM flip.

5 Sokolov-Ternov-like effect of a radiative orbital polarization of twisted electron beams in a magnetic field

We predict the new effect of a *radiative orbital polarization of twisted electron/positron beams in a magnetic field – orbital Sokolov-Ternov effect* [12]. The well-known effect is the radiative spin polarization of electron/positron beams in storage rings caused by the synchrotron radiation (Sokolov-Ternov effect [24]). The spin polarization is acquired by unpolarized electrons and is opposite to the direction of the main magnetic field. The reason of the effect is a dependence of spin-flip transitions from the initial particle polarization. We can notice the evident similarity between interactions of the spin and the intrinsic OAM with the magnetic field [see Eq. (3)]. In particular, energies of stationary states depend on projections of the spin and the intrinsic OAM on the field direction. This similarity validates the existence of the effect of the radiative orbital polarization. As well as the radiative spin polarization, the corresponding orbital polarization acquired by unpolarized twisted electrons should be opposite to the direction of the main magnetic field (see Fig. 1). The effect is conditioned by transitions with a change of a projection of the intrinsic OAM. The probability of such transitions is large enough if the electron energy is not too small. Similarly to the spin polarization, the orbital one is observable when electrons are accelerated up to the energy of the order of 1 GeV. The acceleration can depolarize twisted electrons but cannot vanish L. During the process of the radiative polarization, the average energy of the electrons should be kept unchanged.

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