Relativistic electron vortices beyond the paraxial approximation

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A paraxial approximation in optics:

$$\sigma_\perp \gg \lambda,$$
$$k_\perp \ll k_z$$

Naively, for massive wave-packets:

$$\sigma_\perp \gg \lambda_{dB} = 2\pi/p,$$
$$p_\perp \ll p_z$$

An example:
The Laguerre-Gaussian beams
of electrons [see e.g., K. Y. Bliokh, et al., Physics Reports **690**, 1 (2017)]

The problem: the lack of Lorentz invariance!

A Lorentz invariant condition of paraxiality:

$$\sigma_\perp \gg \lambda_c = \hbar/mc,$$
$$\sigma \sim 1/\sigma_\perp \ll m,$$

← The vacuum is stable!

That is, $\lambda_{dB}(\neq \text{inv}) \to \lambda_c = \hbar/mc(= \text{inv})$

A *non-paraxial* Gaussian scalar packet is
[D. V. Naumov, V. A. Naumov, J. Phys. G **37**, 105014 (2010)]:

$$\psi(p) = \frac{2^{3/2}\pi}{\sigma}\frac{e^{-m^2/\sigma^2}}{\sqrt{K_1(2m^2/\sigma^2)}}\exp\left\{\frac{(p-\bar{p})^2}{2\sigma^2}\right\}$$

$$\int \frac{d^3p}{(2\pi)^3}\frac{1}{2\varepsilon}\,|\psi(p)|^2 = 1,$$

$$p^2 = \bar{p}^2 = m^2 \qquad \varepsilon = \sqrt{\boldsymbol{p}^2 + m^2}.$$

And when $\sigma \ll m$, one has:

$$\frac{(p-\bar{p})^2}{2\sigma^2} = -\frac{1}{2\sigma^2}\left(\delta_{ij} - \bar{u}_i\bar{u}_j\right)(\boldsymbol{p}-\bar{\boldsymbol{p}})_i(\boldsymbol{p}-\bar{\boldsymbol{p}})_j$$

Is the non-paraxial description really necessary?

$$\sim \sigma^2/m^2 \sim \lambda_c^2/\sigma_\perp^2 \ll 1$$

For an LHC beam, it is less than 10^{-22}

For modern electron accelerators: 10^{-14} (and some 2-3 orders larger for ILC and CLIC)

For electron microscopes: 10^{-6} (!) J. Verbeeck, et al., Appl. Phys. Lett. **99**, 203109 (2011).

However, these estimates are valid *only for Gaussian packets*!

The condition of paraxiality is different

for vortex electrons with orbital angular momentum ℓ :

$$\sigma^2/m^2 \ll 1 \to |\ell|\sigma^2/m^2 \ll 1,$$
$$\text{or, alternatively, } \lambda_c \to \sqrt{|\ell|}\,\lambda_c \gg \lambda_c \text{ when } \ell \gg 1$$

$$|\ell|\frac{\sigma^2}{m^2} = |\ell|\frac{\lambda_c^2}{\sigma_\perp^2(0)} \approx \ell^2\frac{\lambda_c^2}{\langle\rho\rangle^2}$$ ← Grows with the OAM!

The current record is
[E. Mafakheri, et al., Appl. Phys. Lett. **110**, 093113 (2017)]:

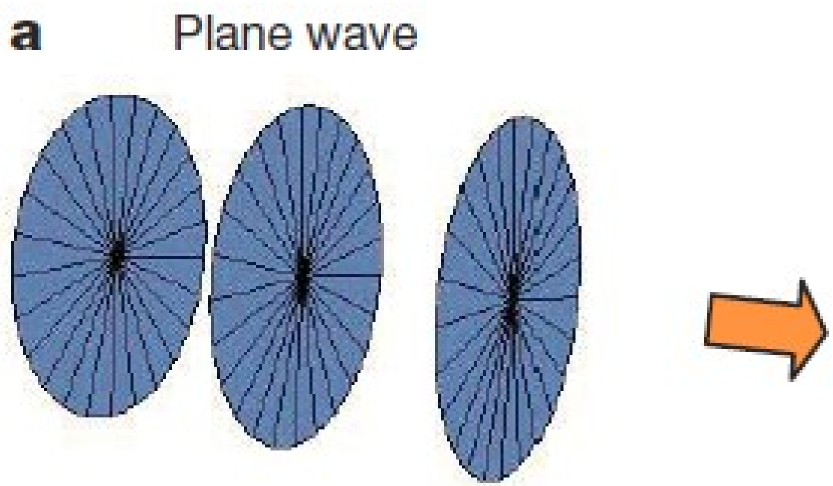
$$\ell \sim 10^3$$

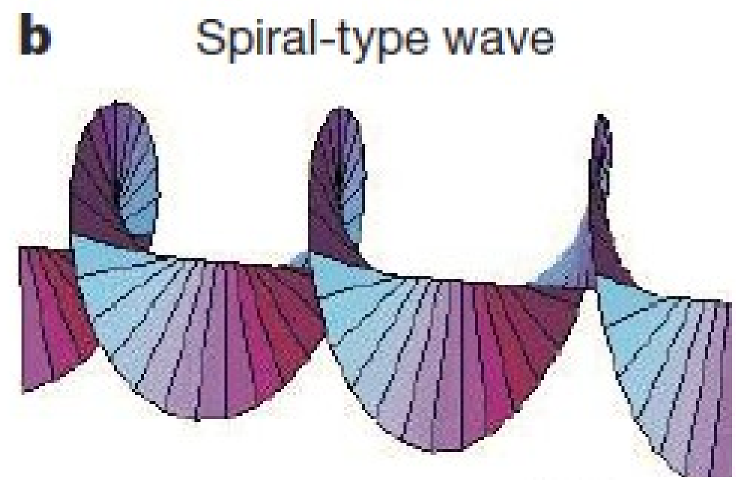
As a result,

$$|\ell|\sigma^2/m^2 \;\; \text{can reach} \;\; \sim 10^{-3}(!)$$

Vortex particles with orbital angular momentum (OAM)

Twisted photons: Allen, et al. 1992



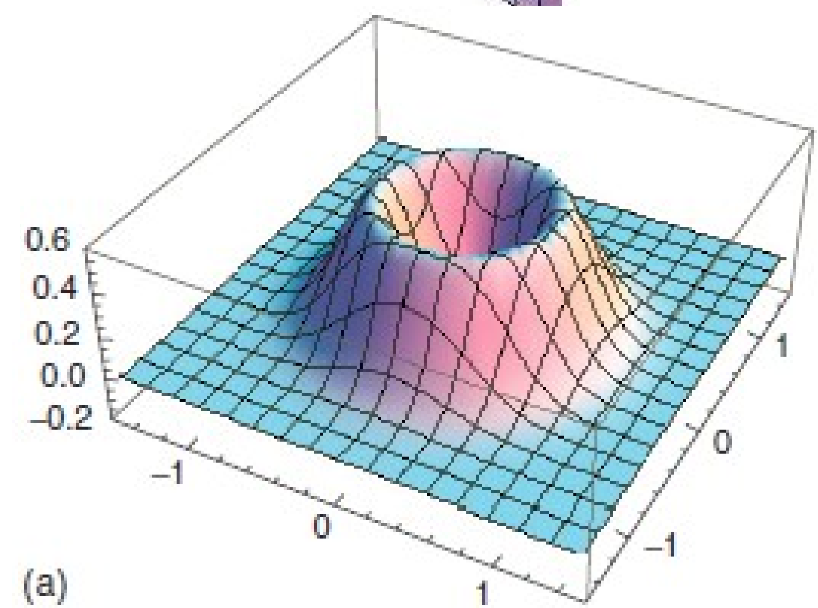


M. Uchida and A.Tonomura, Nature **464**, 737 (2010)

A Bessel state of a free scalar particle:

$$\psi(r) = N\ J_\ell(\kappa\rho)e^{-i\varepsilon t+ip_\parallel z+i\ell\phi_r}$$

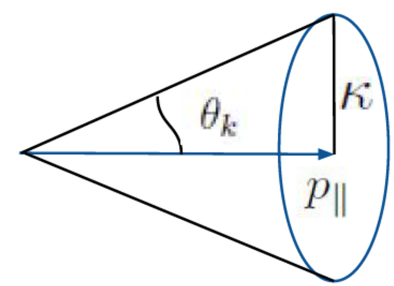
Probability density



Vortex particles with orbital angular momentum (OAM)

They form a complete and orthogonal set:

$$\langle p'_{\|},\kappa',\ell'|p_{\|},\kappa,\ell\rangle = (2\pi)^2 2\varepsilon(p)\,\delta(p_{\|}-p'_{\|})\frac{\delta(\kappa-\kappa')}{\kappa}\,\delta_{\ell\ell'}$$



$$\hat{\psi}(x) = \sum_{\ell}\int \frac{dp_{\|}\kappa d\kappa}{(2\pi)^2 2\varepsilon}(\langle x|p_{\|},\kappa,\ell\rangle\, \hat{a}_{\{p_{\|},\kappa,\ell\}} + \text{H.c.})$$

$$= \sum_{\ell}\int \frac{dp_{\|}\kappa d\kappa}{(2\pi)^2\sqrt{2\varepsilon}}\,(J_{\ell}(\kappa\rho)e^{-i\varepsilon t+ip_{\|}z+i\ell\phi_r}\hat{a}_{\{p_{\|},\kappa,\ell\}} + \text{H.c.})$$

$$[\hat{a}_{\{p_{\|},\kappa,\ell\}},\hat{a}^{\dagger}_{\{p'_{\|},\kappa',\ell'\}}] = (2\pi)^2\delta(p_{\|}-p'_{\|})\frac{\delta(\kappa-\kappa')}{\kappa}\,\delta_{\ell\ell'}$$

$$[\hat{\psi}(x),\hat{\psi}^{\dagger}(x')] = \sum_{\ell}\int \frac{dp_{\|}\kappa d\kappa}{(2\pi)^2 2\varepsilon}J_{\ell}(\kappa\rho)J_{\ell}(\kappa\rho')\,(e^{-i\varepsilon(t-t')+ip_{\|}(z-z')+i\ell(\phi_r-\phi'_r)} - \text{c.c.}).$$

*D.K., PRA **91** (2015) 013847*

Why do the Bessel beams *not* describe the non-paraxial effects for large OAM?

1. The packet's width, length, and energy-momentum uncertainties are ignored (unlocalized orthogonal states)

2. The mean transverse momentum *is independent* of the OAM

Why do the Laguerre-Gaussian beams *not* describe the non-paraxial effects for large OAM?

1. They are intrinsically paraxial

Non-paraxial relativistic wave packets with OAM are needed!

There are two recent papers where an attempt to achieve this was made:

Selected for a Viewpoint in *Physics*
PRL **118**, 114801 (2017) PHYSICAL REVIEW LETTERS week ending 17 MARCH 2017

Relativistic Electron Wave Packets Carrying Angular Momentum

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(Received 1 November 2016; published 13 March 2017)

There are important differences between the nonrelativistic and relativistic description of electron beams. In the relativistic case the orbital angular momentum quantum number cannot be used to specify the wave functions and the structure of vortex lines in these two descriptions is completely different. We introduce analytic solutions of the Dirac equation in the form of exponential wave packets and we argue that they properly describe relativistic electron beams carrying angular momentum.

DOI: 10.1103/PhysRevLett.118.114801

Selected for a Viewpoint in *Physics*
PRL **118**, 114802 (2017) PHYSICAL REVIEW LETTERS week ending 17 MARCH 2017

Relativistic Electron Vortices

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(Received 25 November 2016; published 13 March 2017)

The desire to push recent experiments on electron vortices to higher energies leads to some theoretical difficulties. In particular the simple and very successful picture of phase vortices of vortex charge ℓ associated with $\ell\hbar$ units of orbital angular momentum per electron is challenged by the facts that (i) the spin and orbital angular momentum are not separately conserved for a Dirac electron, which suggests that the existence of a spin-orbit coupling will complicate matters, and (ii) that the velocity of a Dirac electron is not simply the gradient of a phase as it is in the Schrödinger theory suggesting that, perhaps, electron vortices might not exist at a fundamental level. We resolve these difficulties by showing that electron vortices do indeed exist in the relativistic theory and show that the charge of such a vortex is simply related to a conserved orbital part of the total angular momentum, closely related to the familiar situation for the orbital angular momentum of a photon.

DOI: 10.1103/PhysRevLett.118.114802

Massive scalar packets with the OAM:

$$\psi_\ell(p) = \frac{2^{3/2}\pi}{\sigma^{|\ell|+1}\sqrt{|\ell|!}}\, p_\perp^{|\ell|}\, \frac{e^{-m^2/\sigma^2}}{\sqrt{K_{|\ell|+1}(2m^2/\sigma^2)}} \exp\left\{\frac{(p-\bar{p})^2}{2\sigma^2} + i\ell\phi_p\right\}$$

They are orthogonal in OAM: $$\int \frac{d^3p}{(2\pi)^3}\frac{1}{2\varepsilon}\,[\psi_{\ell'}(p)]^*\,\psi_\ell(p) = \delta_{\ell,\ell'}$$

An exact solution to the Klein-Gordon equation:

$$\psi_\ell(x) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2\varepsilon}\,\psi_\ell(p)e^{-ipx} = \frac{(i\rho)^{|\ell|}}{\sqrt{2|\ell|!}\,\pi}\,\frac{\sigma^{|\ell|+1}}{\varsigma^{|\ell|+1}}\,\frac{K_{|\ell|+1}(\varsigma m^2/\sigma^2)}{\sqrt{K_{|\ell|+1}(2m^2/\sigma^2)}}\,e^{i\ell\phi_r}$$

$$\varsigma = \frac{1}{m}\sqrt{(\bar{p}_\mu + i x_\mu \sigma^2)^2} = \text{inv},\ \operatorname{Re}\varsigma > 0$$

And analogously for a fermion with $\langle \hat{j}_z \rangle = \ell + \lambda$

The mean 4-momentum is

$$\langle p^{\mu}_{\ell}\rangle = \{\langle\varepsilon_{\ell}\rangle, \langle\boldsymbol{p}_{\ell}\rangle\} = \{\bar{\varepsilon}, \bar{\boldsymbol{p}}\}\,\frac{K_{|\ell|+2}\,(2m^2/\sigma^2)}{K_{|\ell|+1}\,(2m^2/\sigma^2)} \simeq \{\bar{\varepsilon}, \bar{\boldsymbol{p}}\}\left(1 + \left(\frac{3}{4} + \frac{|\ell|}{2}\right)\frac{\sigma^2}{m^2}\right)$$

An invariant mass of this packet:

$$m_{\ell}^2 = \langle p_{\ell}\rangle^2 \simeq m^2\left(1 + \left(\frac{3}{2} + |\ell|\right)\frac{\sigma^2}{m^2}\right)$$

An enhancement due to the OAM!

What can already be achieved: $\dfrac{\delta m_{\ell}}{m_{\text{inv}}} \simeq \dfrac{\delta m_{\ell}}{m} \lesssim 10^{-3}$ $\quad |\ell| \sim 10^3 \quad \sigma_{\perp} \gtrsim 0.1\ \text{nm}$

For the vortex electron's magnetic moment:

$$\mu_f = \frac{1}{2}\int d^3r\, \mathbf{r} \times \bar{\psi}_f(x)\gamma\psi_f(x) \simeq \frac{1}{2\bar{\varepsilon}}(\zeta + \hat{z}\,\ell)\Big(1 + \mathcal{O}(|\ell|\sigma^2/m^2)\Big)$$

A Bohr magneton

A large magnetic moment due to the OAM [K.Yu. Bliokh, et al., PRL 107, 174802 (2011)] (described by the Bessel beam)

An enhancement of the spin-orbit interaction due to the OAM!

(*not* described by the Bessel beam)

$$\mu_f = \mu_s + \mu_b$$

Bosonic (OAM) contribution:

$$\mu_b = \frac{1}{2}\left\langle u \times \frac{\partial \varphi_\ell(p)}{\partial p}\right\rangle = \hat{z}\,\ell\left\langle \frac{1}{2\varepsilon}\right\rangle \simeq$$
$$\simeq \hat{z}\,\ell\,\frac{1}{2\bar{\varepsilon}}\left(1 - \frac{\sigma^2}{2m^2}\left(|\ell| + \frac{1}{2} + \frac{m^2}{\bar{\varepsilon}^2}\right)\right).$$

Spin contribution:

$$\mu_s = \left\langle \frac{1}{(2\varepsilon)^2}\left(\zeta(\varepsilon+m) + \frac{\mathbf{p}(\mathbf{p}\zeta)}{\varepsilon+m}\right)\right\rangle \simeq$$
$$\simeq \zeta\,\frac{1}{2\bar{\varepsilon}}\Bigg(1 - \frac{\sigma^2}{2m^2}\Bigg[\frac{1}{2} + \frac{3}{2}\frac{m}{\bar{\varepsilon}} + \frac{1}{2}\frac{m^2}{\bar{\varepsilon}^2} - \frac{3}{2}\frac{m^3}{\bar{\varepsilon}^3} -$$
$$-\frac{m}{\bar{\varepsilon}+m}\left(\frac{3}{2} - 2\frac{m^2}{\bar{\varepsilon}^2} - \frac{3}{2}\frac{m^3}{\bar{\varepsilon}^3}\right) +$$
$$+|\ell|\left(1 + \frac{m}{\bar{\varepsilon}} - \frac{m}{\bar{\varepsilon}+m}\right)\Bigg]\Bigg)$$

The spin-orbit interaction is also $|\ell|$ times enhanced compared to the Bessel beam!

Non-invariant corrections

The reason: $\langle p_\perp\rangle \simeq \sigma\sqrt{|\ell|}$ when $|\ell| \gg 1$

The conical angle now *grows* with the OAM:

$$|\ell|\frac{\sigma^2}{m^2} \simeq \frac{\langle p_\perp\rangle^2}{m^2} = \left(\frac{\bar{\varepsilon}^2}{m^2} - 1\right)\tan^2\theta_0 \approx \ell^2\frac{\lambda_c^2}{\langle\rho\rangle^2}$$

In the paraxial regime, these packets reduce to the invariant Laguerre-Gaussian beams with n = 0:

$$\psi_\ell^{\rm par}(x) = \frac{i^\ell}{\sqrt{|\ell|!}}\frac{1}{\sqrt{2m}}\left(\frac{\sigma}{\sqrt{\pi}}\right)^{3/2}\frac{(\rho/\sigma_\perp(t))^{|\ell|}}{(1+(t/t_d)^2)^{3/4}}\exp\Big\{i\ell\phi_r - i\bar{p}^\mu x_\mu -$$
$$-i\,(|\ell|+3/2)\arctan(t/t_d) - \frac{1}{2\sigma_\perp^2(t)}\Big(1 - it/t_d\Big)\Big(\rho^2 + \frac{\bar{\varepsilon}^2}{m^2}(z-\bar{u}t)^2\Big)\Big\},$$

- $\sigma_\perp(t) = \sigma^{-1}\sqrt{1+(t/t_d)^2}$
- t/t_d (where $t_d = \bar{\varepsilon}/\sigma^2$ is a diffraction time)
- $\rho^2 + \bar{\varepsilon}^2(z-\bar{u}t)^2/m^2$

← are all Lorentz invariant together with the wave function!

A Gouy phase $(|\ell|+3/2)\arctan(t/t_d)$:

- Is also Lorentz invariant
- In contrast to twisted photons, it depends on *t* rather than on *z*
- It has 3/2 instead of 1 (= 2/2) due to localization in a 3D space

The Laguerre-Gaussian beams with $n \neq 0$:

$$\psi^{\text{par}}_{\ell,n}(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\varepsilon} \psi^{\text{par}}_{\ell,n}(p)\, e^{-ipx} = \sqrt{\frac{n!}{(|\ell|+n)!}} \frac{i^{2n+\ell}}{\pi^{3/4}\sqrt{2m}} \frac{(\rho/\sigma_\perp(t))^{|\ell|}}{\sigma_\perp^{3/2}(t)} L_n^{|\ell|}\left(\rho^2/\sigma_\perp^2(t)\right)$$

$$\times \exp\left\{i\ell\phi_r - i\bar{p}_\mu x^\mu - i(2n+|\ell|+3/2)\arctan(t/t_d) - \frac{1}{2\sigma_\perp^2(t)}\left(1 - i\frac{t}{t_d}\right)\left(\rho^2 + \bar{\varepsilon}^2(z-\bar{u}t)^2/m^2\right)\right\},$$

$$\int d^3r\, 2\bar{\varepsilon}\, |\psi^{\text{par}}_{\ell,n}(x)|^2 = 1,$$

← Invariant normalization

A mean radius of the beam:

$$\langle\rho\rangle = \sigma_\perp(t)\frac{\Gamma(n+|\ell|+3/2)}{\Gamma(n+|\ell|+1)} \approx \sigma_\perp(t)\sqrt{|\ell|}, \qquad |\ell| \gg n$$

The beam width grows with the OAM
and the corresponding effects can be described
only beyond the paraxial approximation!

The differences of these packets
from those of Barnett
[S. M. Barnett, PRL **118**, 114802 (2017)]:

These packets	Those of Barnett
1.) Applicable beyond the paraxial regime	1.) Not applicable beyond the paraxial regime
2.) Lorentz invariant (scalar)	2.) Non-invariant
3.) The Gouy phase depends on *t* (applicable also for non-relativistic particles!)	3.) The Gouy phase depends on *z* (*only* for ultra-relativistic particles with *z* = *t*)
4.) Correct description of spin (no issues with the spin operators)	4.) Incorrect description of spin (see *K. Bliokh et al., Physics Reports* ***690****, 1 (2017) and Phys. Rev. A* ***96****, 023622 (2017)*)

$$u_{\ell,n} = \sqrt{\frac{2n!}{\pi(n+|\ell|)!}}\frac{(\rho\sqrt{2})^{|\ell|}}{w^{|\ell|+1}(z)}\exp\left(-\frac{p_0\rho^2}{2(z_R+iz)}\right) \times L_n^{|\ell|}\left(\frac{2\rho^2}{w^2(z)}\right)e^{i\ell\phi}\exp[-i(2n+|\ell|+1)\tan^{-1}(z/z_R)], \quad (12)$$

The differences of these packets
from those of Bialynicki-Birula and Bialynicka-Birula
[I. Bialynicki-Birula, Z. Bialynicka-Birula, PRL **118**, 114801 (2017)]:

These packets	Those of Bialynicki-Birula
1.) Applicable beyond the paraxial regime	1.) Also applicable ...
2.) Lorentz invariant (scalar)	2.) Not invariant
3.) At large distances decay as	3.) At large distances decay as (see Eq.(15))
$\psi_\ell(x) \propto \exp\left\{-\sqrt{-x_\mu^2}/\lambda_c\right\}$	$\psi_\ell(x) \propto \exp\left\{-\frac{\varepsilon}{m}\rho/\lambda_c\right\}$

The troubles with this behavior:

1. The decay is *not* Lorentz invariant

2. Worse: in relativistic case, the beam width *is smaller than the Compton wavelength* – impossible!

Summary

1) We put forward the wave packets of vortex bosons and fermions
that preserve Lorentz invariance and are applicable beyond the paraxial regime

2) In the paraxial approximation, these packets reduce
to *the invariant Laguerre-Gaussian beams*

3) There are notable differences of the latter from the twisted photons,
relevant especially for non-relativistic particles

4) Compared to packets with the *non-singular* phases (Gaussian, Airy, etc.),
the non-paraxial effects turn out to be drastically enhanced
for large orbital angular momenta

So what?

I. Unlike the Bessel states, the wave packets *do interfere*,
which is crucial for potential applications with entangled beams
(interaction-free measurements, probing of Coulomb/hadronic phases, etc.)

II. The non-paraxial corrections can be important for describing:

- The spin-orbit interaction in relativistic highly twisted beams
- Scattering of wave packets by atoms, including quantum superpositions thereof (Schroedinger cats of electrons)
- Beam-beam collisions of the highly energetic twisted beams (say, the Compton effect)

These corrections can already compete
with a contribution of the 2nd loop in QED:

$$d\sigma^{(1)}/d\sigma_{\text{pw}} \sim |\ell|\sigma^2/m^2 \gtrsim \alpha_{em}^2 = 1/137^2$$