Semiclassical Dynamics of Electron Wave Packet States with Phase Vortices

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We consider semiclassical higher-order wave packet solutions of the Schrödinger equation with phase vortices. The vortex line is aligned with the propagation direction, and the wave packet carries a well-defined orbital angular momentum (OAM) $\hbar l$ (l is the vortex strength) along its main linear momentum. The probability current coils around the momentum in such OAM states of electrons. In an electric field, these states evolve like massless particles with spin l. The magnetic-monopole Berry curvature appears in momentum space, which results in a spin-orbit-type interaction and a Berry/Magnus transverse force acting on the wave packet. This brings about the OAM Hall effect. In a magnetic field, there is a Zeeman interaction, which, can lead to more complicated dynamics.

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Introduction.—The phase front singularities of a wave field, vortices, and related nonintegrable phases have been introduced and examined in seminal papers [1–5]. Phase vortices appear naturally in the electron eigenstates in atoms, quantum Hall fluids, supermedia, ferromagnets, Bose-Einstein condensates, and classical wave fields (e.g., in optics). While 2D vortices in condensed matter physics are pointlike objects, with vorticity being orthogonal to the plane of motion [6], the optical vortices are mainly considered as linear objects in 3D space, with vorticity being aligned with the wave momentum. Wave beams with vortices constitute a fundamental set of modes with well-defined orbital angular momentum (OAM) [5]. Recently, these beams have found numerous applications both in classical and quantum optics [3,5].

Simultaneously, topological phenomena related to the semiclassical wave packet dynamics of quantum particles have motivated intensive investigations in various areas of physics: condensed matter, high energy physics, optics, etc. [6–12]. This has resulted in the revisiting of the semiclassical equations of motion, but now with the Berry-phase terms taken into account, and the discovery of such phenomena as the spin Hall effect, with potential applications. In most cases, the topological Berry terms are due to the (pseudo)spin of particles, whereas the particle's phase front is implicitly assumed to be locally smooth, i.e., without singularities.

The dynamics of various types of vortices also undergo the action of the topological Berry force, which can be associated with the Magnus force [13–15]. Both vortex and spin dynamics relate to such fundamental concepts as magnetic monopoles, Berry phase, space noncommutativity, and generalized Hamiltonian dynamics [1,2,4,6–16]. It has been shown very recently that the dynamics of optical beams with vortices reveals all the topological phenomena previously associated with spin, but now they are related to the intrinsic OAM carried by the vortex [15,17]. In contrast to spin effects, these phenomena are polarization-independent and can be much larger in magnitude, since the OAM (the vortex strength) can take arbitrarily large values [15]. The OAM Hall effect (an analogue of the spin Hall effect) has also drawn attention in semiconductor physics [18], but there it is assumed that the wave packet states of the electrons have *zero intrinsic* OAM.

While confined electron states with vortices are well-studied in molecules and 2D structures [19], here we aim to analyze the semiclassical dynamics of a 3D propagating electron wave packet or beam with intrinsic OAM due to a phase vortex. For simplicity, we will consider nonrelativistic scalar electrons without spin. As we will show, electron wave packets with OAM manifest fundamental topological and dynamical features which were associated so far mostly with spin dynamics.

OAM states of a free electron.—The Schrödinger equation in free space reads $(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2)\psi = 0$. Let us construct semiclassical (paraxial) wave packet solutions propagating along the z axis and characterized by a narrow distribution in $(\mathbf{p}, E)$ space around some center at $(\mathbf{p}_c, E_c) = (p_c\mathbf{e}_z, p_c^2/2m)$. Usually, one assumes Gaussian-type wave packets with the maximal probability density and nearly-plane phase front in its center [8]. However, this is not the case for higher-order modes. By making the ansatz $\psi = \exp[i\hbar^{-1}(p_c z - E_c t)]u$, where u is a smooth function with respect to z and t, and neglecting the second-order derivative $\partial^2 u/\partial z^2$, we arrive at the parabolic-type equation

$$\left(i\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla_\perp^2\right)u = 0. \quad (1)$$

Here, $\nabla_\perp^2 = \nabla_x^2 + \nabla_y^2$ and $\partial/\partial\tau = \partial/\partial t + (p_c/m)\partial/\partial z$ is the time derivative in the coordinate frame (x, y, ζ, τ) moving with the wave packet center ($\zeta = z - p_c t/m$, $\tau = t$). Since the operator in Eq. (1) is ζ-independent, such modes allow factorization so that one can choose the transverse and longitudinal parts in the form of the known in optics Laguerre-Gaussian (LG) beams (with an azimuthally-symmetric intensity profile) and Hermite-Gaussian (HG) wave packets:

$$u_{l,\mathrm{m,n}}(r, \varphi, \zeta, \tau) = u^{\mathrm{LG}}_{l,\mathrm{m}}(r, \varphi, \tau) u^{\mathrm{HG}}_{\mathrm{n}}(\zeta). \qquad (2)$$

Here (r, φ) are polar coordinates in the (x, y) plane, whereas $l = 0, \pm 1, \pm 2, \ldots$ and $\mathrm{m}, \mathrm{n} = 0, 1, 2, \ldots$ are the quantum numbers corresponding to the azimuthal, radial, and longitudinal directions. The zeroth mode, $l = \mathrm{m} = \mathrm{n} = 0$, is a usual Gaussian wave packet.

The explicit form of standard LG and HG solutions can be found in the optics literature [5], while here we will only emphasize their most significant features. First, they represent wave packets with Gaussian envelopes and constitute a complete orthonormal set of modes, so that $\langle u_{l,\mathrm{m,n}} | u_{l',\mathrm{m}',\mathrm{n}'} \rangle = \delta_{ll'} \delta_{\mathrm{mm}'} \delta_{\mathrm{nn}'}$, and any localized wave function can be represented as a superposition $|u\rangle = \sum_{l,\mathrm{m,n}} a_{l,\mathrm{m,n}} |u_{l,\mathrm{m,n}}\rangle$. Second, LG modes with $l \neq 0$ contain a screw dislocation of the phase front on the wave packet axis, $u^{\mathrm{LG}}_{l,\mathrm{m}} \propto \exp(il\varphi)$; in other words, they contain a *phase vortex* of strength l at $r = 0$. Owing to this, the solutions (2) have a well-defined z-component of the OAM. Indeed, $\hat{L}_z |u_{l,\mathrm{m,n}}\rangle = \hbar l |u_{l,\mathrm{m,n}}\rangle$ ($\hat{L}_z = -i\hbar \partial/\partial\varphi$), and, effectively, the electron possesses an *intrinsic angular momentum* $\mathbf{L} \equiv \hbar \boldsymbol{l} = \hbar l \mathbf{e}_z$. The wave packets (2) also have a *magnetic moment* $\boldsymbol{\mu} = g\mu_B \boldsymbol{l}$ ($\mu_B = e\hbar/2m$, $e = -|e|$, $c = 1$), where $g = 1$ for classical orbital motion, but the g-factor can be different in general (e.g., $g = 2$ for electron spin).

The transverse distribution of the probability density, $\rho = |u|^2$, for LG modes with $l \neq 0$, represents $(\mathrm{m} + 1)$ concentric circles and vanishes at $r = 0$. At the same time, the probability current coils around z: $\mathbf{j} = m^{-1}[\rho \mathbf{p}_c + \hbar \mathrm{Im}(u^* \nabla u)] \simeq m^{-1} \rho(\mathbf{p}_c + \hbar l \mathbf{e}_\varphi / r)$, Fig. 1. (The same behavior is characteristic for the Pointing vector of optical LG beams [5].) This implies that the electron trajectories are effectively *spiral* in *free* space. This effect disappears in the classical limit $\hbar = 0$, and can be regarded as a *Zitterbewegung* due to the intrinsic OAM. In what follows, we will consider only trajectories of the *center* of the wave packet (2), which is a sort of guiding center, propagating rectilinearly in free space.

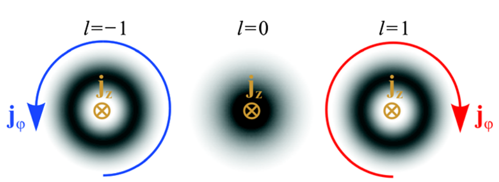

FIG. 1 (color online). Transverse distribution of the probability density ρ in LG beams with $\mathrm{m} = 0$ and different values of OAM, l. Shown are the directions of common z component and different φ components of the probability current $\mathbf{j}$.

Dynamics in external fields.—In an external electromagnetic potential $(\mathbf{A}, \Phi)$ generating the field $(\mathbf{E}, \mathbf{B})$, the Schrödinger equation reads $[i\hbar \frac{\partial}{\partial t} - e\Phi - \frac{1}{2m}(-i\hbar \nabla - e\mathbf{A})^2]\psi = 0$. The potentials are assumed to be smoothly space- and time-dependent (the fields are weak) to ensure the independent adiabatic evolution of the modes (2). We assume that the wave packet center $(\mathbf{p}_c, \mathbf{r}_c)$ (in what follows, the subscripts "c" are omited), moves in the vicinity of classical electron trajectory, $\dot{\mathbf{p}} = e\mathbf{E} + e\dot{\mathbf{r}} \times \mathbf{B}$, $\dot{\mathbf{r}} = \mathbf{p}/m$, and approximately conserves its form (2) in the accompanying coordinate system with the z axis locally directed along $\mathbf{p}$ ($\zeta = z - \int p dt/m$). This means that, effectively, we deal with a "relativistic" configuration where $\boldsymbol{l} = l\mathbf{p}/p$ and the "helicity," $\boldsymbol{l} \cdot \mathbf{p}/p = l$, is conserved (see below). The local coordinate frame is transported along a curved trajectory. This produces a phase shift due to the Berry phase [4] and a deflection of the wave packet center due to the geometrical force [6–12,15], both described by the effective Berry gauge potential (connection) and field (curvature).

Geometrically, the Berry connection provides for the parallel transport of the state vector over the phase space [4,7]. Since the z axis is attached now to $\mathbf{p}$, the solution (2) becomes essentially momentum-dependent. The parallel transport of the wave packet over momentum space implies the covariant derivative $D/D\mathbf{p} = \partial/\partial\mathbf{p} + \boldsymbol{\mathcal{A}}^{(l)}(\mathbf{p})$, where $\boldsymbol{\mathcal{A}}^{(l)} = i\langle u_{l,\mathrm{m,n}} | \partial/\partial\mathbf{p} | u_{l,\mathrm{m,n}} \rangle$ is the Berry connection, whereas the corresponding curvature is $\boldsymbol{\mathcal{B}}^{(l)} = \partial/\partial\mathbf{p} \times \boldsymbol{\mathcal{A}}^{(l)}$. As will be seen, only the quantum index l noticeably contributes to the Berry connection. Furthermore, $\langle u_{l,\mathrm{m,n}} | \partial/\partial\mathbf{p} | u_{l',\mathrm{m}',\mathrm{n}'} \rangle \propto \delta_{ll'} \delta_{\mathrm{mm}'} \delta_{\mathrm{nn}'}$, which evidences the independent evolution of the modes (2). As in the relativistic case of massless particles with spin, the Berry gauge field takes the form of a "magnetic monopole," which originates from the local vortex structure $\exp(il\varphi)$ in the wave packet [15]. Indeed, $\exp(il\varphi) = (e_x + ie_y)^l$, where $\mathbf{e}$ is a unit vector orthogonal to $\mathbf{p}$. Under variations of $\mathbf{p}$, $\mathbf{e}$ moves on the unit sphere $\mathbf{p}/p$, which leads to the magnetic-monopole-type connection $\boldsymbol{\mathcal{A}} = i(e_x - ie_y)\partial/\partial\mathbf{p}(e_x + ie_y)$ and corresponding curvature $\boldsymbol{\mathcal{B}} = -\mathbf{p}/p^3$ [4,11,12]. As a result, we have $\boldsymbol{\mathcal{A}}^{(l)} = l\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}}^{(l)} = l\boldsymbol{\mathcal{B}}$, so that each mode is characterized by the "charge" l in the "magnetic monopole" field in the momentum space.

The semiclassical dynamics of the wave packet center can be described involving the minimal coupling prescription for the electromagnetic and Berry's gauge fields. This results in the Lagrangian [8]

$$\mathcal{L} = -\mathcal{H} + \mathbf{p} \cdot \dot{\mathbf{r}} + e\mathbf{A} \cdot \dot{\mathbf{r}} + \hbar l \boldsymbol{\mathcal{A}} \cdot \dot{\mathbf{p}}. \qquad (3)$$

Here, the Hamiltonian acquires the energy correction due to the *Zeeman interaction* of the intrinsic OAM with the magnetic field [8,9,12]: $\mathcal{H} = \frac{p^2}{2m} + e\Phi + \Delta = E$, $\Delta = -\boldsymbol{\mu} \cdot \mathbf{B}$, where the magnetic moment $\boldsymbol{\mu} = g\mu_B \boldsymbol{l}$ is also momentum-dependent now. The Berry phase term, last in Eq. (3), is of the form of the relativistic spin-orbit interaction [12], but now this is the *orbit-orbit interaction* between the intrinsic OAM and the external degrees of freedom. Equation (3) yields the common phase of the wave packet:

$$\theta = \hbar^{-1}\int(\mathbf{p}d\mathbf{r} - Edt) + \hbar^{-1}e\int\mathbf{A}d\mathbf{r} + l\int\boldsymbol{\mathcal{A}}d\mathbf{p}, \quad (4)$$

which substitutes for the free-space phase, $\hbar^{-1}(pz - Et)$. The three terms in Eq. (4) are, respectively, the dynamical phase, the Dirac (Aharonov-Bohm) phase [1,2], and the Berry phase [4,7,8]. The latter provides for the parallel transport of the transverse structure of the wave packet along the curved trajectory [15,17].

Considering the Euler-Lagrange equations for $\mathcal{L} = \mathcal{L}(\mathbf{p}, \dot{\mathbf{p}}, \mathbf{r}, \dot{\mathbf{r}})$, Eq. (3), we arrive at the semiclassical equations of motion for the wave packet center [6–16]:

$$\dot{\mathbf{p}} = e\mathbf{E} - \frac{\partial\Delta}{\partial\mathbf{r}} + e\dot{\mathbf{r}}\times\mathbf{B}, \qquad \dot{\mathbf{r}} = \frac{\mathbf{p}}{m} + \frac{\partial\Delta}{\partial\mathbf{p}} - \hbar l\dot{\mathbf{p}}\times\boldsymbol{\mathcal{B}}. \quad (5)$$

These equations follow from the Hamiltonian formalism as well, where the minimal coupling with the electromagnetic and Berry's fields implies a deformation of the symplectic structure $\Omega = g^{ij}dX_i \wedge dX_j/2$ [7,16]:

$$\Omega = dp_i\wedge dr_i + e\frac{\epsilon_{ijk}}{2}B_k dr_i\wedge dr_j + \hbar l\frac{\epsilon_{ijk}}{2}\mathcal{B}_k dp_i\wedge dp_j. \quad (6)$$

Here, $\mathbf{X} = (\mathbf{r}, \mathbf{p})$, and g^{ij} is the symplectic metric tensor. The equations of motion (5) take the simple form $g^{ij}\dot{X}_j = \partial\mathcal{H}/\partial X_i$, whereas the Poisson brackets of the dynamical variables (or commutators of the corresponding operators) become nontrivial, $\{X_i, X_j\} = g_{ij}$ (cf. [7,12,16,20]):

$$\{p_i, p_j\} = D^{-1}e\epsilon_{ijk}B_k, \qquad \{r_i, r_j\} = D^{-1}\hbar l\epsilon_{ijk}\mathcal{B}_k,$$
$$\{r_i, p_j\} = D^{-1}(\delta_{ij} - e\hbar lB_i\mathcal{B}_j), \qquad D = \sqrt{\det g^{ij}}. \quad (7)$$

Here, $D = 1 - e\hbar l\mathbf{B}\cdot\boldsymbol{\mathcal{B}}$ is a correction to the phase space volume which modifies the density of states [20].

Let us briefly analyze the most remarkable features of Eqs. (5). The last term in the second Eq. (5), given by $\hbar l\dot{\mathbf{p}}\times\mathbf{p}/p^3$, represents the anomalous velocity ($\dot{\mathbf{r}} \not\parallel \mathbf{p}$) or the "Lorentz force" from Berry's "magnetic monopole" in momentum space [6–12]. It causes the transverse deflection of the wave packet trajectory, which is proportional to the intrinsic OAM $\hbar l$ [15]. This results in the transverse orbital current, or *OAM Hall effect*, similar to the spin current in the spin Hall effect [10–12]. For instance, when $\mathbf{B} = \mathbf{0}$, $\mathbf{E} = \text{const}$, Eqs. (5) take the simple form: $\dot{\mathbf{p}} = e\mathbf{E}$, $\dot{\mathbf{r}} = \mathbf{p}/m + e\hbar l\mathbf{E}\times\mathbf{p}/p^3$, and can be readily integrated analytically (see [10]). They show the transverse shift of the trajectories, equaling $\hbar l/p_0$ when $\mathbf{p}_0 \perp \mathbf{E}$, Fig. 2. The OAM Hall effect can be much stronger than the spin one since it is proportional to l, which formally can take

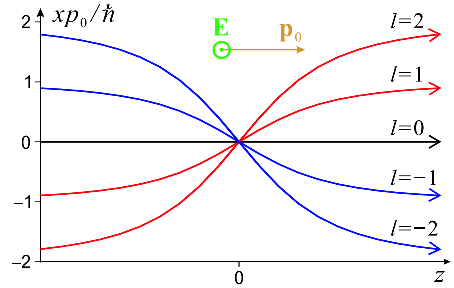

FIG. 2 (color online). Central trajectories, Eqs. (5), of the electron states with different values of OAM, l, moving in a uniform electric field $\mathbf{E} = E\mathbf{e}_y$ ($\mathbf{p}_0 = p_0\mathbf{e}_z$, $\mathbf{r}_0 = \mathbf{0}$, and $l = 0$ line corresponds to the classical trajectory).

arbitrarily large values. At the same time, the anomalous velocity is a counterpart of the Magnus force for 2D vortices which also appears due to the Berry curvature term, but in coordinate rather than momentum space [13,14]. In an external magnetic field, $\mathbf{E} = \mathbf{0}$, $\mathbf{B} = \text{const}$ (for simplicity, let $\mathbf{B} \perp \mathbf{p}$), Eqs. (5) are reduced, in the linear approximation in $\hbar$, to $\dot{\mathbf{p}} = \frac{e}{m}\mathbf{p}\times\mathbf{B}$, $\dot{\mathbf{r}} = m^{-1}[\mathbf{p} + e\hbar l(1 - \frac{g}{2})\mathbf{B}/p]$. Thus, at $g \neq 2$, an OAM-dependent transport of electrons can appear in a constant magnetic field.

The intrinsic OAM, $\boldsymbol{l}$, can also be considered as an independent intrinsic dynamical variable. It can be shown that the helicity $\boldsymbol{l}\cdot\mathbf{p}/p$ is conserved during the evolution, Eqs. (5), if $\boldsymbol{l}$ obeys the equation

$$\dot{\boldsymbol{l}} = -\left(\frac{e}{m}\mathbf{B} + \frac{e\mathbf{E}\times\mathbf{p}}{p^2}\right)\times\boldsymbol{l}. \quad (8)$$

Equation (8) is of the form of the well-known BMT equation for the electron spin precession [12,21], where the Berry phase (spin-orbit) term is taken in the relativistic limit (because intrinsic OAM reveals topological features similar to the spin of a massless particle), while all other terms are nonrelativistic. Equation (8) is compatible with Lagrangian (3) only if either $g = 2$ or $\mathbf{B} = \mathbf{0}$. Under evolution of the OAM with $g \neq 2$ in a magnetic field, $\boldsymbol{l}$ does not follow $\mathbf{p}$ (the precession frequency of OAM differs from the cyclotron frequency), and thus the initial assumption of this study is not valid. In this case, the problem becomes much more complicated and requires an independent study.

Discussion. Comparison with optics.—Electron states with vortices can appear in both bulk solids and in free space. These may open new avenues of research in condensed matter physics (OAM Hall effect) as well as in electron microscopy and holography [22] (similarly to singular optics). A comparative analysis of the electron OAM states and their optical counterparts is summarized in Table I. The dynamics of optical beams with vortices is described by equations similar to Eqs. (5), where the refractive index of the medium, n, plays the role of the external scalar potential Φ [15]. At the same time, there is no counterpart of the external curl potential and magnetic

TABLE I. Comparison between electron OAM states and their optical counterparts.

	Optics	Electrons
wave field	**E**	ψ
external potential field	n, ∇n	Φ, **E**
external curl field	...	**A**, **B**
generation of	hologram (grating with dislocation)	crystal plate with dislocation
phase vortex	spiral-thickness lens	spiral-thickness plate
	...	magnetic monopole
common features	orbit-orbit interaction: Berry phase and Magnus/Berry force	
distinctive features	Lorentz force, Dirac phase, Zeeman interaction [23], modified density of states	

field in optics. Therefore, all electric-field-related features are absolutely similar in electron and optical systems, while the magnetic-field-related effects are inherent to the evolution of charged particles only [23].

It is important to find some ways for creating electron phase vortices. On the one hand, the phase vortex *cannot* be created from a plane wave by a large-scale electromagnetic potential. Indeed, the phase incursion at the closed contour around the vortex line equals $2\pi l$. A Dirac phase of this kind can appear only due to a real magnetic monopole [1,22] or in the presence of an infinite Aharonov-Bohm solenoid [2]. On the other hand, a phase vortex can be created by a short-scale potential. For instance, an optical vortex can be produced using a diffracting grating with an edge dislocation (''fork'') [3,5]. For electrons, such a grating can be provided by a real thin crystal plate with a dislocation. This offers the opportunity of using phase vortices in electron or neutron crystallography. One can also use a bulk solid as an effective refractive medium for free electrons because the electron changes its effective mass there [22]. Then, a spiral-thickness solid plate will create an electron phase vortex similarly to the analogous optical lens [3,5].

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