Aharonov-Bohm and Berry Phases for a Quantum Cloud of Charge

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We investigate the phase accumulated by a charged particle in an extended quantum state as it encircles one or more magnetic fluxons, each carrying half a flux unit. A simple, essentially topological analysis reveals an interplay between the Aharonov-Bohm phase and Berry's phase.

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The Aharonov-Bohm (AB) phase [1] $\Phi_{AB} = (q/\hbar)\oint_C \mathbf{A}\cdot d\mathbf{r}$ collected by a charge q, moving in a closed path C about a line of magnetic flux ϕ, is purely topological: $\Phi_{AB} = 2\pi n(q/e)\phi/\phi_0$, with n the winding number of C around the fluxon, e the elementary charge, and ϕ_0 the corresponding flux unit $\phi_0 = 2\pi\hbar/e$. The AB phase is independent of the shape of the path C and of the history of motion along it. If the charge is not pointlike, or the fluxon is not linelike, they may overlap; what then happens to the AB phase? As long as the charge and flux are distributed classically, the answer is straightforward: A system of charges moving in a closed path through a classical magnetic field collects an AB phase $\Phi_{AB} = (1/\hbar)\sum q_i\phi_i$, with ϕ_i the flux enclosed by the path of the ith charge. Here, however, we consider charges distributed by quantum smearing. The phase of a *quantum* charge is no simple sum over the undeformed charge distribution. If we compute it via the Born-Oppenheimer approximation, we find a remarkable interplay between the AB phase and Berry's phase that determines the overall topological phase.

Consider a single electron bound to a heavy "nucleus" (assumed neutral, for simplicity) in the presence of an infinitely long and narrow flux line (fluxon). Both the nucleus and the fluxon may move. If the fluxon moves around the nucleus and returns to its initial configuration, it sweeps out a sheet which generally encloses only part of the quantum charge distribution (the electron "cloud"). Suppose that the time in which the fluxon crosses the "atom" is much shorter than typical electronic time scales (period). In this limit, the initial electronic wave function Ψ_0 transforms into $\Psi_1 = e^{i\Phi_{AB}}\Pi_C\Psi_0 + (1-\Pi_C)\Psi_0$, where Π_C projects onto the enclosed region. But, except in this limit, we cannot assign distinct phases to parts of the wave function. Consider now the opposite limit, of adiabatic motion. In this limit, another phase effect comes into play. Berry's phase [2] arises when parameters for a quantum system vary adiabatically in a closed path. Applying the Born-Oppenheimer approximation to the fluxon-atom system, and for definiteness fixing the nucleus, we obtain *both* an AB phase and a Berry phase. An AB phase arises as the fluxon moves though the vector potential of the instantaneous charge distribution [3], while Berry phase arises from rearrangement of the electronic wave function. There is a subtle interplay of these two phases, which is purely topological for special values of the flux ϕ carried by the fluxon. For example, when $\phi = n\phi_0$, the phases completely cancel [4] as expected since the fluxon is a pure gauge artifact. Here, we consider the more interesting case of fluxons carrying half a flux unit ("semifluxons") where topological analysis, with no computations, reveals the interplay of the AB phase and Berry's phase.

Let us begin with the electron (mass m_1) bound by a potential $V(\mathbf{r}_1)$ and the fluxon (mass m_2) free to move but constrained to remain parallel to the z axis. The relevant Hamiltonian is [5]

$$H = \frac{(\mathbf{p}_1 + e\mathbf{A})^2}{2m_1} + V(\mathbf{r}_1) + \frac{(\mathbf{p}_2 - e\mathbf{A})^2}{2m_2}. \quad (1)$$

For a semifluxon we take

$$\mathbf{A} = (\hbar/2e)\nabla_2\varphi_{12}, \quad (2)$$

with φ_{12} defined as the polar angle of the fluxon in a coordinate system where the electron is at the origin. Consider a limited time reversal operation T sending $\mathbf{p}_i \to -\mathbf{p}_i$ but leaving $\mathbf{A}$ unchanged. T sends $(\mathbf{p}_i \pm e\mathbf{A})^2 \to (\mathbf{p}_i \mp e\mathbf{A})^2$; since $\mathbf{A} \neq -\mathbf{A}$, T seems not to be a symmetry of H. However, for the special case of a *semifluxon,* the difference between $\mathbf{A}$ and $-\mathbf{A}$ amounts to a pure gauge transformation: $\mathbf{A} = -\mathbf{A} + \nabla_2\Lambda$ with $\Lambda \equiv (\hbar/e)\varphi_{12}$; so T *is* a symmetry of H. Thus there is a gauge in which we can choose the eigenstates of H real [6]. Suppose $m_2 \gg m_1$. If we apply the Born-Oppenheimer approximation to Eq. (1), the effective

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Hamiltonian for the fluxon will contain an induced vector potential due to adiabatic transport of a *real* electron wave function, thus it will preserve the time reversal symmetry. Suppose that an initial state of the semifluxon evolves adiabatically around a loop C, according to this effective Hamiltonian H_{eff}. The state accumulates a phase factor which may include a geometric as well as a dynamical phase. The latter is given by the time integral of the instantaneous effective Hamiltonian, $-\int H_{\text{eff}} dt/\hbar$. Time reversal symmetry implies that the state acquires the *same* phase factor if it moves around C in the opposite direction. The dynamical phase is the same in the two cases, but the geometric phase changes sign. Since the overall phase factor remains unchanged, we conclude that the geometric phase acquired by the electron-fluxon system, $\Phi(C)$, can be only 0 or π.

What, then, becomes of the geometrical phase $\Phi(C)$ as we deform the path C? Let us assume the electronic wave function to be restricted to a finite region S. Figure 1 shows a closed fluxon path C_1 which lies completely outside the region S without encircling it. For this path, the AB phase is zero. Furthermore, Berry's phase also vanishes. Now let us gradually distort the path C_1 until it becomes a large loop C_2 that encircles the region S without touching it. For this loop Berry's phase vanishes, but the AB phase is $\Phi_{\text{AB}}(C_2) = \pi$, since all the charge has been encircled once [7]. We can distort C_1 into C_2 by many steps which enlarge the loop by an infinitesimal region. Naively, we would expect the phase Φ of the loop to vary smoothly from 0 to π but, as noted, Φ can only be 0 or π. Thus, we conclude that some infinitesimal region contains a "singular point" $\mathcal{P}$ so that Φ "jumps" when this infinitesimal region is annexed. The electronic wave function yields a vector potential that is always bounded, and so an infinitesimal region cannot lead to a jump in the AB phase. Therefore, the jump in Φ is due to Berry's phase. The significance of $\mathcal{P}$ is clear: $\mathcal{P}$ is a point such that if a semifluxon is introduced there, the electron wave function becomes degenerate. (Only a degeneracy can cause such a jump in Berry's phase.) The feature that we exhibit with this indirect argument, namely, that such a point $\mathcal{P}$ exists [even if $V(\mathbf{r}_1) \neq V(r_1)$], would be hard to see from a direct study of Schrödinger's equation.

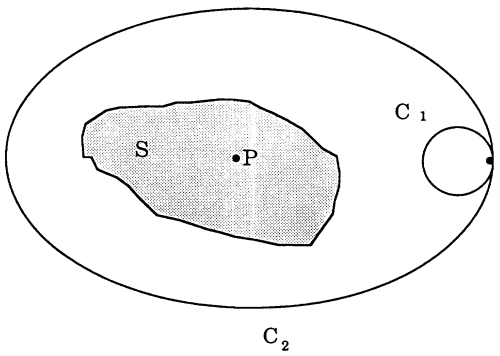

FIG. 1. The shaded region S indicates where the wave function is nonzero, and C_1 and C_2 are limiting paths. Insertion of a semifluxon at point P induces degeneracy.

Conversely, suppose we suspect that two states become degenerate at a point $\mathcal{P}$. Near $\mathcal{P}$, we can truncate that Hilbert space for the system to the subspace spanned by the two states, and write the effective Hamiltonian as a sum of Pauli matrices (plus a constant) $H_0(x,y) + H_1(x,y)\sigma_1 + H_2(x,y)\sigma_2 + H_3(x,y)\sigma_3$. For a generic fluxon, the degeneracy condition involves *three* equations with two parameters x, y (the coordinates of the fluxon), so that, in general, there are no solutions. However, for the special case of a semifluxon, the eigenstates and thus the effective Hamiltonian can always be chosen real. Then $H_2(x,y)$ vanishes. The degeneracy point $\mathcal{P} = (x^*, y^*)$ is fixed by requiring $H_1(x^*, y^*) = H_3(x^*, y^*) = 0$; these two equations naturally lead to isolated points of degeneracy.

The actual location of $\mathcal{P}$ depends on the state Ψ_0 and the relevant potential. When the potential is spherically symmetric, $V(\mathbf{r}) = V(r)$, the point $\mathcal{P}$ is at the origin. The Hamiltonian retains azimuthal symmetry. If states depend on φ as $e^{im\varphi}$ for integer m, introducing the fluxon is equivalent to shifting the angular momentum L_z by half a unit: $-i(\partial/\partial\varphi) \rightarrow -i(\partial/\partial\varphi) - 1/2$ or $L_z \rightarrow L_z - \hbar/2$. Initially the energy is proportional to m^2. All the energy levels are doubly degenerate except for the ground state. The shift $m \rightarrow m' = m - 1/2$ rearranges *all* the levels into degenerate pairs. In particular, the ground state $m = 0$ becomes degenerate with $m = 1$ (since $m = 0 \rightarrow m' = -1/2$ and $m = 1 \rightarrow m' = 1/2$). This degeneracy occurs only for a semifluxon.

There could be any odd number of degeneracy points. Indeed, consider the $m' = \pm 3/2$ (degenerate) states of a rotationally symmetric potential with a semifluxon at the center. By adding a perturbation $V' = \lambda \cos 3\varphi$ which connects these two states, the degeneracy is lifted. To restore the degeneracy, we must move the semifluxon away from the origin. The problem is now invariant under rotations of $2\pi/3$ and so, by symmetry, there will be three degeneracy points. A similar argument with $m' = \pm(2k + 1)/2$ and $V' = \lambda \cos(2k + 1)\varphi$ leads to $2k + 1$ symmetrically situated points [8]. In a spherically symmetric potential, however, only one degeneracy point can appear.

Let us now determine the phase collected by an atom which slowly moves in the presence of *two* semifluxons. If the atomic ground state in the absence of any semifluxons would be spherically symmetric, and if the fluxons are fixed, we can map this problem to an equivalent one, replacing the spherical charge distribution by a point charge located at its center, and the fluxons by "shadow" fluxons. The shadow fluxons are defined as points such that when the center of the atom coincides with one of them, a degeneracy results. The winding number of the path of the

point charge around the shadow fluxons gives the phase accumulated by the atom. Consider two straight and parallel semifluxon lines situated a distance L apart. Two extreme cases are easily solved. When the distance between the fluxons is much larger than the size of the atom, we can move the atom in the vicinity of one of the fluxons without the electron cloud crossing the other fluxon. In this case the atom collects a phase of π each time its center encircles the fluxon, exactly as if the other fluxon were not present. The shadow fluxons coincide therefore with the original fluxons. On the other hand, for $L = 0$ the two semifluxons are at the same point, adding up to an integer fluxon with no effect on the energy levels of the electron, and therefore no shadow fluxons can exist. When the fluxons are slightly separated, they do not affect the energy. However, by continuity, an infinitesimal separation of the fluxons cannot produce a degeneracy; rather, a minimal distance L^* is required. Thus we arrive at the conclusion that in an adiabatic quantum process (say, an atom in a specific state moving slowly) the geometric phase due to two semifluxons will always be zero once their separation L is less than some nonvanishing distance L^*.

We may now interpolate between $L = L^*$ and $L \to \infty$. Instead of considering the atom as moving by fixed semifluxons, let us fix the atom and one semifluxon and allow the second semifluxon to move. Let the center of the atom be at $\mathcal{O}$ and a fluxon F_1 at $\mathcal{P}_1$, and let us determine the phase accumulated by a second fluxon F_2 as it slowly moves along various closed paths (Fig. 2). Again, this phase can only be 0 or π; thus there must be a point $\mathcal{P}_2$ such that when F_2 encircles $\mathcal{P}_2$, the phase "jumps" by π. Insertion of the fluxon F_2 at the point $\mathcal{P}_2$ produces a degeneracy. The connection with the "shadows" is that here the point $\mathcal{O}$ corresponds to a shadow fluxon. Let us assume that the points $\mathcal{P}_1$ and $\mathcal{P}_2$ are related by a continuous function. By symmetry, $\mathcal{P}_1$, $\mathcal{P}_2$, and $\mathcal{O}$ must form a straight line. We claim that $\mathcal{P}_1$ and $\mathcal{P}_2$ lie on opposite sides of $\mathcal{O}$. Let us examine $\mathcal{P}_1$ as a function of $\mathcal{P}_2$. If $\mathcal{P}_2$ is located in the region where the wave function vanishes, $\mathcal{P}_1$ must be situated at the atom's center $\mathcal{O}$. As $\mathcal{P}_2$ enters the electron cloud and moves towards $\mathcal{O}$, $\mathcal{P}_1$ must move either towards $\mathcal{P}_2$ or in the opposite direction. The first possibility must be discarded: in this case either $\mathcal{P}_1$ and $\mathcal{P}_2$ will collide or $\mathcal{P}_1$ will reverse direction and eventually return to $\mathcal{O}$ to avoid collision with $\mathcal{P}_2$. Both alternatives are inconsistent. If the two semifluxons collide, they form an integer fluxon with no degeneracy. If $\mathcal{P}_1$ reverses direction, we obtain an "accidental" degeneracy with $\mathcal{P}_1$ at $\mathcal{O}$ and $\mathcal{P}_2$ inside the electron cloud, where a degeneracy cannot arise [9]. As claimed, then, the points $\mathcal{P}_1$ and $\mathcal{P}_2$ lie on opposite sides of $\mathcal{O}$. Thus, the shadow fluxon associated with each semifluxon is shifted towards the other semifluxon.

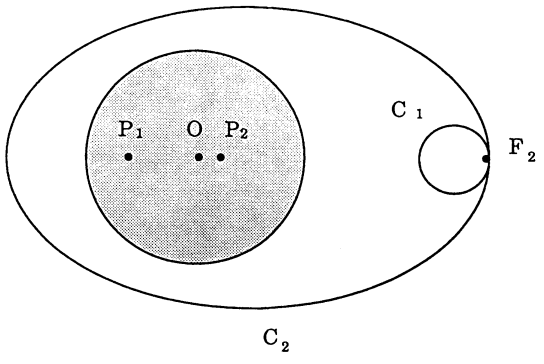

FIG. 2. The center of the atom is $\mathcal{O}$; at points P_1, P_2 simultaneous insertion of semifluxons induces degeneracy. C_1 and C_2 are limiting paths of the semifluxon F_2.

It is amusing to consider more general patterns of semifluxons and resulting shadows. Even in the case of a single semifluxon, the shadow need not coincide with the original, if the semifluxon is not straight. For example, a semifluxon in the form of a ring radius much smaller than the characteristic length of the electron cloud does not have a shadow fluxon at all. Just as there is a critical distance between two straight semifluxons, there is a critical (smallest) radius for a degeneracy in the state of the electron to appear. For two semifluxons intersecting at an acute angle, we expect to find shadow fluxons in the plane of the semifluxons, located near the latter but shifted towards a more acute angle. Then from continuity, we expect "hyperbolic" shadow fluxons as shown in Fig. 3. For the case of n semifluxons in a plane intersecting symmetrically at one point, the shadow fluxons will be identical with the semifluxons and will induce simple degeneracies. The intersection could be a point of higher degeneracy.

Finally, we discuss the case of N semifluxons and an electron cloud of arbitrary shape. For simplicity we consider a two-dimensional problem. The set of points $(\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N)$ such that if in each of them a semifluxon is introduced, the initial wave function of the electron becomes degenerate, constitutes a $(2N - 2)$-dimensional hypersurface Σ. Indeed, for *any* given points $\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_{N-1}$ there always exists at least one corresponding point $\mathcal{P}_N$. As proof, we introduce a semifluxon in each of the $N - 1$ points $\mathcal{P}_1, \ldots, \mathcal{P}_{N-1}$ and consider the phase accumulated by the Nth semifluxon as

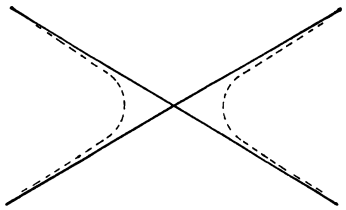

FIG. 3. Two semifluxons intersecting at an acute angle and the resulting shadow fluxons.

it takes various paths. Similar arguments to those above for one and two semifluxons lead to the conclusion that at some point $\mathcal{P}_N$, the Berry phase jumps by π. Introducing semifluxons at $\mathcal{P}_1, \ldots, \mathcal{P}_{N-1}, \mathcal{P}_N$ therefore results in a degeneracy.

We may describe the locations of the N fluxons by a point $(x_1, y_1, \ldots, x_N, y_N)$. To every configuration of $N-1$ fluxons there corresponds a location x_N, y_N where the Nth fluxon induces a degeneracy:

$$x_N = f(x_1, y_1, \ldots, x_{N-1}, y_{N-1}),$$
$$y_N = g(x_1, y_1, \ldots, x_{N-1}, y_{N-1}). \quad (3)$$

Equation (3) then defines the $(2N-2)$-dimensional hypersurface Σ. Suppose that N semifluxons move slowly and after a certain time all return to their initial positions. What is the topological phase in this case? The fluxons describe a closed path C in the $2N$-dimensional space $(x_1, y_1, \ldots, x_N, y_N)$. The phase accumulated by the fluxons as they move through the charge distribution is simply $n\pi$, where n is the winding number of the closed path C around Σ.

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[1] Y. Aharonov and D. Bohm, Phys. Rev. **115**, 485 (1959).

[2] M. V. Berry, Proc. R. Soc. London A **392**, 45 (1984).

[3] The AB effect is often illustrated by an electron that encircles a fluxon. Here, a fluxon encircles an electron. Whether we consider the adiabatic motion in the frame of the electron or in the frame of the fluxon, the phase is the same. Occasionally, the phase obtained by a fluxon encircling a charge is called the Aharonov-Casher (AC) phase (see Ref. [5] below), but we find this name more appropriate for the Aharonov-Casher effect, dual to the AB effect, which applies to a point magnetic dipole moving around a line of charge instead of a point charge moving around a line of flux. All results derived in our Letter hold for the dual system of an infinitely narrow line of charge interacting with a polarized magnetic dipole cloud (interplay of AC and Berry phases).

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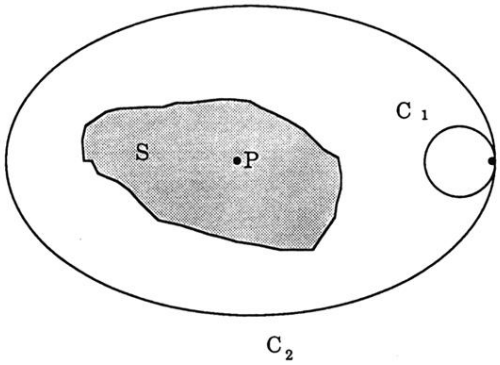
[5] Y. Aharonov and A. Casher, Phys. Rev. Lett. **33**, 319 (1984).

[6] The connection between semifluxons and time reversal was pointed out by M. Berry, R. Chambers, M. Large, C. Upstill, and J. Walmsley, Eur. J. Phys. **1**, 154 (1980); M. Berry and M. Robnik, J. Phys. A **19**, 649 (1986).

[7] An explicit proof that the total phase accumulated in this case is π is as follows. Consider a solution $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$ of Schrödinger's equation [for the Hamiltonian given by Eqs. (1) and (2)] that represents a localized fluxon state encircling the region S. It is easy to verify that $\Psi = e^{(i/2)\varphi_{12}}\Psi'$, where Ψ' is a solution of the Schrödinger equation without vector potential. (Note that Ψ' is single valued as long as the fluxon is localized and does not enter the region of S.) No geometrical phase arises with $\mathbf{A} = 0$, and so the sole contribution to the phase acquired by Ψ comes from the factor $e^{(i/2)\varphi_{12}}$, and it is π for a circuit around S.

[8] By contrast, $V' = \lambda \cos(2k\varphi)$ does not connect any degenerate pair and this argument fails—as it must, since the number of degeneracy points cannot be even.

[9] P. A. M. Dirac, Proc. R. Soc. London A **133**, 60 (1931), showed that the wave function for a charged particle, in the presence of a magnetic monopole, must have a line of zeros extending from the monopole to an antipole or to infinity. An analogous argument shows that, in the presence of a semifluxon, a nondegenerate state Ψ_0 must have a line of zeros extending from the semifluxon to another semifluxon or to infinity. (A *surface* of zeros issues from a three-dimensional fluxon, but we refer to a line for the effective two-dimensional problem.) In the ground state only one such null line issues from each semifluxon. We can choose the vector potential $\mathbf{A}$ to be singular on the null line and zero elsewhere. Approaching the "accidental" degeneracy configuration, the semifluxons carry null lines which, by symmetry, must lie along their common line. A null line can connect the fluxons, or two null lines can issue from them in opposite directions. As the atom approaches from infinity, the corresponding wave functions are not degenerate because the two null lines are more constraining than one.



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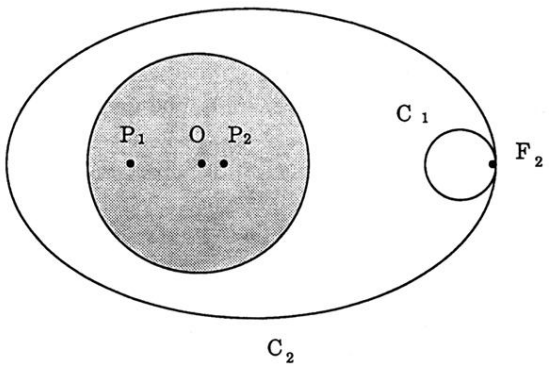

FIG. 2. The center of the atom is $\mathcal{O}$; at points P_1, P_2 simultaneous insertion of semifluxons induces degeneracy. C_1 and C_2 are limiting paths of the semifluxon F_2.