A-B AND BERRY PHASES FOR A QUANTUM CLOUD OF CHARGE

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ABSTRACT

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 is purely topological: $\Phi_{AB} = \left(\frac{q}{\hbar}\right) \oint_C \vec{A} \cdot d\vec{r}$ collected by a charge $q$, moving in a closed path $C$ about a line of magnetic flux $\phi$, is $2\pi n \left(\frac{q}{e}\right) \left(\frac{\phi}{\phi_0}\right)$, with $n$ the winding number of $C$ around the fluxon, $e$ the elementary charge, and $\phi_0$ the corresponding flux unit $\phi_0 = \frac{2\pi}{\hbar/e}$. 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 $\Phi_{AB} = \left(\frac{1}{\hbar}\right) \sum q_i \phi_i$, with $\phi_i$ the flux enclosed by the path of the $i$-th 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 flux line. Both the nucleus and the fluxon may move. If the fluxon makes a closed path around the nucleus, it may encircle some parts of the quantum charge distribution (the electron “cloud”) and not others. Suppose that the time in which the fluxon crosses the “atom”, multiplied by typical electronic frequencies, is much smaller than 1. In this limit, the initial electronic wave function $\Psi_0$ transforms into $\Psi_1 = e^{i\Phi_{AB}} \Pi_C \Psi_0 + (1 - \Pi_C) \Psi_0$, where $\Pi_C$ projects onto the part of $\Psi_0$ that the fluxon encircles. The electron has no time to move between the two parts of $\Psi_0$. But, except in this limit, we cannot assign parts of the wave function distinct phases. Consider now the opposite limit, of adiabatic motion. In this limit, another phase effect comes into play. Berry’s phase 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 from motion of the fluxon with respect to the instantaneous charge distribution, while a 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 $\phi$ carried by the fluxon. For example, when $\phi = n\phi_0$, the phases completely cancel\[^3\] as expected since the fluxon is a pure gauge artifact. Here, we consider the more interesting case of fluxons carrying half a flux unit (“half-fluxons” or “semifluxons”). 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 at the origin with a potential $V(\vec{r}_1)$ and the fluxon (mass $m_2$) free to move but constrained to remain parallel to the $z$-axis. The Hamiltonian is

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

for a half-fluxon we take $\vec{A} = (\hbar/2e)\nabla_2 \varphi_{12}$ with $\varphi_{12}$ the angle of the fluxon in polar coordinates with the electron at the origin.\[^4\] Consider a limited time reversal operation $T$ sending $\vec{p}_i \rightarrow -\vec{p}_i$ but leaving $\vec{A}$ unchanged. $T$ sends $(\vec{p}_i \pm e\vec{A})^2 \rightarrow (\vec{p}_i \mp e\vec{A})^2$; since $\vec{A} \neq -\vec{A}$, $T$ seems not to be a symmetry of $H$. However, for the special case of a half-fluxon, the difference between $\vec{A}$ and $-\vec{A}$ amounts to a pure gauge transformation: $\vec{A} = -\vec{A} + \nabla_2 \Lambda$ 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. Suppose $m_2 >> m_1$. If we apply the Born-Oppenheimer approximation to Eq. (1), the effective 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. Let an initial state for the half-fluxon evolve according to this effective Hamiltonian and move adiabatically around a loop $C$. The state accumulates a phase factor which may include a geometric as well as a dynamical phase. Time reversal symmetry implies that the state acquires the same phase factor if it moves around $C$ in the opposite sense. The dynamical phase is the same in the two cases but the geometric phase $\Phi(C)$ changes sign. Since the overall phase factor remains unchanged, we conclude that the geometric phase acquired by the electron-fluxon system can be only 0 or $\pi$. 
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 \( S \). Fig. 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 \( \Phi_{AB}(C_2) = \pi \), since all the charge has been encircled once.\(^5\) 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 \( \Phi \) of the loop to vary smoothly from 0 to \( \pi \) but, as noted, \( \Phi \) can only be 0 or \( \pi \). Thus, we conclude that some infinitesimal region contains a “singular point” \( \mathcal{P} \) so that \( \Phi \) 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 \( \Phi \) is due to Berry’s phase. The significance of \( \mathcal{P} \) is clear: \( \mathcal{P} \) is a point such that if a half-fluxon 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 \( V(\vec{r}_1) \neq V(r_1) \)), would be hard to see from a direct study of Schrödinger’s equation.

Conversely, suppose we suspect that two states become degenerate at a point \( \mathcal{P} \). Near \( \mathcal{P} \), we can truncate the 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 there are no solutions. However, for the special case of a half-fluxon, 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 \( \Psi_0 \) and relevant potential. When
the potential is spherically symmetric, $V(\vec{r}) = V(r)$, the point $P$ corresponds to a fluxon through the $z$-axis. The Hamiltonian retains azimuthal symmetry. If states depend on $\varphi$ 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 half-fluxon.

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 half-fluxon 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 half-fluxon 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.

Let us now determine the phase collected by an atom which slowly moves in the presence of two semifluxons. When the undisturbed ground state is spherically symmetric and 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 $\pi$ 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
affect the energy. However, by continuity, an infinitesimal separation of the fluxons
cannot produce a degeneracy; rather, a minimal distance $L^* > 0$ 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 half-fluxons will
always be zero once their separation $L$ is less than some $L^* > 0$.

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 $\pi$; thus there must be a point $\mathcal{P}_2$ such that when $F_2$ encircles $\mathcal{P}_2$, the phase
jumps by $\pi$. 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 half-fluxons 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.\[7\] 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.
It is amusing to consider various patterns of half-fluxons and resulting shadows. Even in the case of a single half-fluxon, the shadow need not coincide with the original, if the fluxon line is not straight. For two half-fluxon lines intersecting at an acute angle, we expect to find shadow fluxons in the plane of the half-fluxons, 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 \( n \) half-fluxon lines in a plane intersecting symmetrically at one point, the shadow fluxons will be identical with the half-fluxons 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 \( \Sigma \). 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 \( N \)-th semifluxon as 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 \( \pi \). 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 \( N \)-th fluxon induces a degeneracy:

\[
x_N = f(x_1, y_1, \ldots, x_{N-1}, y_{N-1}) \quad y_N = g(x_1, y_1, \ldots, x_{N-1}, y_{N-1}).
\] (2)

Eq. (2) then defines the \((2N-2)\)-dimensional hypersurface \( \Sigma \). 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 $\Sigma$.

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4. See Y. Aharonov and A. Casher, *Phys. Rev. Lett.* **33**, 319 (1984). The Aharonov-Casher (AC) effect is dual to the AB effect: a neutron interacting with a line of charge is equivalent to an electron interacting with a fluxon. Eq. (1) is an effective two-dimensional Hamiltonian for both the AB and AC effects, and all our conclusions hold for both cases.

5. Let $\Psi(\vec{r}_1, \vec{r}_2)$ represent a localized fluxon wave packet encircling the electron without entering $S$. Since the wave packet is localized, the wave function $\Psi'$ defined by $\Psi = e^{(i/2)\varphi_{12}} \Psi'$ is single-valued. Note $\Psi'$ solves Eq. (1) with $\vec{A} = 0$. The remaining factor $e^{(i/2)\varphi_{12}}$ in $\Psi$ yields the phase $\pi$ for a circuit about $S$.

6. 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.

7. P. A. M. Dirac, *Proc. Roy. Soc.* **A133**, 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 $\Psi_0$ 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 $\vec{A}$ 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. The corresponding wave functions are not degenerate because the two null lines are more constraining than one.
FIGURE CAPTIONS

Fig 1. The shaded region $S$ indicates where the wave function is non-zero, and $C_1$ and $C_2$ are limiting paths. Insertion of a half-fluxon at point $P$ induces degeneracy.

Fig. 2. The center of the atom is $O$; at points $P_1$, $P_2$ simultaneous insertion of half-fluxons induces degeneracy. $C_1$ and $C_2$ are limiting paths of the half-fluxon $F_2$.

Fig. 3. Two half-fluxons intersecting at an acute angle and the resulting shadow fluxons.
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