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Letter

Gauge-invariant Aharonov–Bohm streamlines

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Abstract

The phase gradient of the wave describing the Aharonov–Bohm effect (AB) is proportional to the local canonical momentum. This vector field contains vortices (phase singularities), whose strengths cannot be detected in quantum mechanics because they increase (discontinuously) with the magnetic flux, violating gauge invariance. The analogous quantity which is gauge-invariant is the kinetic momentum field, proportional to the local electron velocity. Investigation of the streamlines (integral curves) of this velocity field reveals that as the flux line, accompanied by a stagnation point (saddle) S that emerges from V and then collapses back into V. The VS pair is always small: the maximum distance between V and S is approximately 0.0209 de Broglie wavelengths. The VS phenomenon survives generalization to a superposition of AB waves. If the flux is confined within an impenetrable tube of radius *R*, S persists if R < 0.004 de Broglie wavelengths, and is swallowed by the tube for larger *R*. An experiment is envisaged.

Keywords: singularities, vortices, vector potential, momentum, quantum

(Some figures may appear in colour only in the online journal)

1. Introduction

One way to represent the geometry of a wave field is by displaying its streamlines. Usually these are the trajectories (integral curves) of the gradient of phase of the wave, or equivalently, the local expectation of the canonical momentum density or the local current (see [1] for several other interpretations). In one-particle quantum physics, these streamlines descibe the flow of the fluid in the Madelung representation [2] of the Schrödinger wavefunction, or, what is formally the same, the paths of particles in the Bohm–De Broglie interpretation [3]. In optics, the streamlines are the trajectories of the Poynting vector—a concept whose germ can be traced back to Isaac Newton [4, 5].

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But in quantum physics the phase gradient is not physically observable, because it depends on the choice of gauge. This is especially significant when there is a magnetic field: the phase gradient depends on the choice of vector potential. The quantity that is gauge-invariant, and therefore potentially physically observable, is not the canonical momentum density but the local kinetic momentum density, proportional to the local velocity $u(\mathbf{r})$. For momentum operator $\hat{\mathbf{p}}$ and vector potential \hat{A} and charge q, in the state $|\psi\rangle$, with $\langle \mathbf{r} |\psi\rangle = \psi(\mathbf{r})$, this can be written, ignoring uninteresting constants,

$$\boldsymbol{u}\left(\boldsymbol{r}\right) = \left\langle\psi\right|\frac{1}{2}\left[\delta\left(\boldsymbol{r}-\widehat{\boldsymbol{r}}\right)\left(\widehat{\boldsymbol{p}}-q\widehat{\boldsymbol{A}}\right) + \left(\widehat{\boldsymbol{p}}-q\widehat{\boldsymbol{A}}\right)\delta\left(\boldsymbol{r}-\widehat{\boldsymbol{r}}\right)\right]\left|\psi\right\rangle$$

$$= \hbar\operatorname{Im}\left[\psi^{*}\left(\boldsymbol{r}\right)\nabla\psi\left(\boldsymbol{r}\right)\right] - q\boldsymbol{A}\left(\boldsymbol{r}\right)\left|\psi\left(\boldsymbol{r}\right)\right|^{2}$$

$$= \left|\psi\left(\boldsymbol{r}\right)\right|^{2}\left[\hbar\nabla\operatorname{arg}\psi\left(\boldsymbol{r}\right) - q\boldsymbol{A}\left(\boldsymbol{r}\right)\right].$$
(1)

(The connection between velocity and kinetic momentum can be seen most directly from the Hamilton equation $\boldsymbol{u} = \boldsymbol{r} = \nabla_{\boldsymbol{p}} H = (\boldsymbol{p} - \boldsymbol{A}) / m$.) When $\psi(\boldsymbol{r})$ satisfies the Schrödinger equation with vector and scalar potentials $\boldsymbol{A}(\boldsymbol{r})$ and $V(\boldsymbol{r})$, namely

$$\left(\frac{1}{2m}(-i\hbar\nabla - q\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}), \qquad (2)$$

then, for any singlevalued scalar function $U(\mathbf{r})$, $u(\mathbf{r})$ is invariant under the gauge transformation $A(\mathbf{r}) \rightarrow A(\mathbf{r}) + \nabla U(\mathbf{r})$.

A context in which the canonical/kinetic distinction matters is the Aharonov–Bohm effect (AB), whose wave, in the simplest idealised case [6], describes quantum particles influenced by an inaccessible line of magnetic flux Φ . The canonical streamlines, defined by (1) with A = 0, violate gauge invariance in two ways. First, as just discussed, they are not invariant under $A(\mathbf{r}) \rightarrow A(\mathbf{r}) + \nabla U(\mathbf{r})$. The second violation is of the principle [7] that physically observable quantities must be periodic in the quantum flux

$$\alpha = \frac{q\Phi}{2\pi\hbar}.$$
(3)

The violation occurs because, as was shown long ago [8], there is a phase singularity (=wave vortex = wave dislocation = nodal point) at the flux line, whose phase increment (accumulated in a circuit of the origin) is $2\pi \times$ nearest integer to $\alpha = 2\pi$ int $\left(\alpha + \frac{1}{2}\right)$, which jumps by 1 as α passes through 1/2 (mod 1). This initially unexpected phase jump was observed in a classical analogue experiment, in which ripples on the surface of water are scattered by a bathtub vortex [8]—an experiment in which this aspect of gauge invariance does not apply because the analogue of $A(\mathbf{r})$ is the fluid velocity. The fact that this secular increase of vortex strength with α is quantum-mechanically unobservable stimulated the present study, whose aim is to understand the kinetic momentum streamlines in the AB wave.

The main calculation is carried out in section 2, for the idealised case where the flux is confined within a region of zero radius. The result is that when for $\alpha \neq$ integer and $\alpha \neq 1/2$ (mod 1), the AB streamlines possess a vortex V at the magnetic flux line, whose circulation extends until interrupted by a stagnation point (saddle) S. The unexpected result is that V and S are very close for all α ; seeing this distinctive topological feature of the AB wave requires high magnification.

Extension of the basic theory for flux confined within a region of finite radius R is carried out in section 3. The result is that for extremely small R the VS geometry occurs in essentially the same way as for R = 0. But as R increases through very small value, S gets swallowed by the tube.

Section 4 considers the more general situation where ψ is a superposition of AB waves, and speculates on the possibility of observing the VS pair.

2. Vortex-stagnation point pairs

With distances measured in units of wavelength $\lambda/2\pi$, energy scales out of the Schrödinger equation (2), which can be written, using polar coordinates $\mathbf{r} = \{x, y\} = r\{\cos\theta, \sin\theta\}$ and the circular gauge for $A(\mathbf{r})$,

$$\left(\nabla + i\alpha \frac{\boldsymbol{e}_{\theta}}{\boldsymbol{r}}\right)^{2} \psi\left(\boldsymbol{r}\right) + \psi\left(\boldsymbol{r}\right) = 0.$$
(4)

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The solution, corresponding to a plane wave incident from $x = -\infty$, i.e. $\theta = \pi$, on an infinitely thin flux line, is the AB wave [6]

$$\psi\left(\boldsymbol{r}\right) = \sum_{-\infty}^{\infty} \left(-\mathrm{i}\right)^{|\boldsymbol{m}-\boldsymbol{\alpha}|} (-1)^{\boldsymbol{m}} J_{|\boldsymbol{m}-\boldsymbol{\alpha}|}(\boldsymbol{r}) \exp\left(\mathrm{i}\boldsymbol{m}\boldsymbol{\theta}\right).$$
(5)

The gauge-invariant kinetic momentum density (1) (proportional to the local velocity), whose integral curves are the desired streamlines, is

$$\boldsymbol{u}(\boldsymbol{r}) = u_{\mathbf{r}}(\boldsymbol{r}) \boldsymbol{e}_{r} + u_{\theta}(\boldsymbol{r}) \boldsymbol{e}_{\theta}$$

$$u_{\mathbf{r}}(\boldsymbol{r}) = \operatorname{Im} \left[\psi^{*}(\boldsymbol{r}) \partial_{r} \psi(\boldsymbol{r}) \right]$$

$$u_{\theta}(\boldsymbol{r}) = \frac{1}{r} \left(\operatorname{Im} \left[\psi^{*}(\boldsymbol{r}) \partial_{\theta} \psi(\boldsymbol{r}) \right] - \alpha |\psi(\boldsymbol{r})|^{2} \right).$$
(6)

It is easy to show from (1) and (2) that u(r) is divergenceless, implying that one way to calculate the streamlines is as the contours of a stream function S(r) given by

$$\boldsymbol{u}(\boldsymbol{r}) = \nabla \times (S(\boldsymbol{r}) \boldsymbol{e}_{z}),$$

$$S(\boldsymbol{r}) = -\int_{0}^{r} \mathrm{d}\boldsymbol{r}' \boldsymbol{u}_{\theta}(\boldsymbol{r}', 0) + r \int_{0}^{\theta} \mathrm{d}\boldsymbol{\theta}' \boldsymbol{u}_{r}(\boldsymbol{r}, \theta').$$
(7)

But although the relevant integrations can be performed analytically, this is awkward, and it is easier to integrate the vector field u(r) directly. This can be done automatically using the StreamPlot function in MathematicaTM. It is necessary to calculate the stream function only for $0 \le \alpha \le 1/2$, because the pattern for $1 - \alpha$ is the same as that for α with $y \rightarrow -y$, and for $\alpha + 1$ it is the same as for α .

The results are shown in figures 1 through 4, on which the values of flux α and the scales plotted are indicated, and calculations of u(r) are carried out using the exact AB wave (5). Figure 1 shows the start and end of the interval $0 \le \alpha \le 1/2$. For $\alpha = 0$ there is no AB effect and the streamlines are simply those of a plane wave. For $\alpha = 1/2$, the pattern is symmetric in *y* and there is no vortex at the flux line (for this case, the sum (5) can be expressed compactly in terms of the Fresnel integral [6]).

In figure 2, the left panel shows that for the small flux $\alpha = 1/128$ the streamlines appear slightly deformed over the range plotted. The magnification in the right panel reveals that the deformation consists of a vortex (V) at the origin and a stagnation point (S) slightly below it. The existence of the vortex for $\alpha \neq 0$ is confirmed by a leading small *r* analysis of (6) using (5): as $r \rightarrow 0$, the radial component $u_r \rightarrow \text{constant}$, while the azimuthal component $u_{\theta} \rightarrow O(r^{2\alpha-1})$, from the vector potential term in (6) (the term involving $\partial_{\theta}\psi$ is of higher order), so the flow asymptotically close to the flux line is azimuthal and the streamlines are circles.

In figure 3, the left panel shows that for $\alpha = 1/4$ S has receded from V and swung clockwise. In the right panel, the slightly larger value of α corresponds to the maximum distance between V and S (see below). Figure 4 shows that on the approach to $\alpha \rightarrow 1/2$ both V and S persist, but the distance between them shrinks to zero.

The location r_s of the stagnation point S can be calculated numerically from (6) and

$$u_r(\mathbf{r}_s) = 0, \quad u_\theta(\mathbf{r}_s) = 0. \tag{8}$$



Figure 1. Streamlines of the vector field (6) for $\alpha = 0$ and $\alpha = 1/2$.



Figure 2. Streamlines of the vector field (6) for $\alpha = 1/128$, and magnification $25 \times$.

Figures 5(a) and (c) confirm that that, as α increases from zero, S initially recedes from V and then collapses back into it when $\alpha = 1/2$. The flux for which the maximum separation between V and S occurs, and its radius and azimuth, are

$$\alpha = 0.312\ 78, \quad \mathbf{r}_{s} = 0.131\ 549 = 0.020\ 937\lambda, \quad \theta_{s} = -128.119^{\circ}.$$
 (9)

Figure 5(b) indicates that as α increases from zero S emerges from V on the negative y axis $(\theta_s = -90^\circ)$ reaches its maximum azimuth of $\theta_s = -136.90^\circ$ near $\alpha = 0.446$, then swings back into the origin near $\theta_s = -126.6^\circ$.

The existence of S, with Poincaré index -1, is not surprising: if it were absent, the Poincaré index +1 of V would be uncompensated, leading to a net circulation reaching infinity, contradicting the scattering boundary conditions. The nonexistence of S for $\alpha = 1/2$ follows from the fact that for this value there is no V and therefore no Poincaré index requiring compensation.

In the next section, we will see that S does not survive if the flux is confined within a tube of sufficiently large radius. It is easy to find simpler gauge-invariant solutions of (4) without a stagnation point, for solutions of the Schrödinger equation that do not represent the scattering of a plane wave. A class of such solutions, parameterised by an integer n, is



Figure 3. Streamlines of the vector field (6) for $\alpha = 1/4$ and the value $\alpha = 0.31278$ corresponding to the maximum separation between V and S.



Figure 4. Streamlines of the vector field (6) for α near 1/2, and its magnification 25×.

$$\psi_n (\mathbf{r}) = J_{|n+m(\alpha)-\alpha|}(r) \exp\left(\mathrm{i}\theta \left(n+m(\alpha)\right)\right)$$

$$m(\alpha) = \mathrm{int}\left(\alpha + \frac{1}{2}\right) = \mathrm{nearest\ integer\ to}\ \alpha.$$
(10)

From (6) it follows that the streamlines are circles: the radial component $u_r(r)$ vanishes, and

$$\boldsymbol{u}_{n}\left(\boldsymbol{r}\right) = \left(n + m\left(\alpha\right) - \alpha\right) \left(J_{|n+m(\alpha)-\alpha|}(\boldsymbol{r})\right)^{2} \boldsymbol{e}_{\theta}.$$
(11)

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This possesses a vortex at the origin, even when the wave (10) does not depend on θ , for example when n = 0 and $0 < \alpha < 1/2$.

Although the existence of S was not surprising, its closeness to V—always less that 1/50 of the de Broglie wavelength, was unexpected. S and V lie well within the near field of the AB wave, suggesting that these geometric features can be reproduced by the corresponding solution of the gauge-invariant version of the Laplace equation. This is accomplished by replacing the Bessel



Figure 5. (a) Distance r_s of the stagnation point S from the vortex V at the flux line at r = 0, as a function of flux α ; (b) azimuth angle of S; (c) track of S as α varies from 0 to 1/2.

functions in (5) by their lowest-order approximations $J_{|m-\alpha|}(r) \sim (r/2)^{|m-\alpha|} / |m-\alpha|!$. Remarkably, the sum over *m* can be evaluated in closed form, with the result

$$\psi_{\text{near field}} = \exp\left(i\alpha\left(\theta - \pi\right)\right) \left(\exp\left(i\zeta\right)\frac{\gamma(1 - \alpha, i\zeta)}{\Gamma(1 - \alpha)} + \exp\left(i\zeta^*\right)\frac{\gamma(\alpha, i\zeta^*)}{\Gamma(\alpha)}\right)$$

$$\zeta = \frac{1}{2}\left(x + iy\right), \gamma\left(\mu, z\right) = \int_0^z dt t^{\mu - 1} \exp\left(-t\right) \text{(incomplete gamma function)}.$$
(12)

(This expression is valid in the interval $\frac{1}{2}\pi \le \theta \le 2\pi$, which includes the location of S; outside this interval, the formula must be modified to accomodate the branch cuts in the incomplete gamma function.) It is immediately clear from (12) that $\exp(-i\alpha\theta)\psi_{\text{near field}}$ satisfies the ordinary Laplace equation. When u(r) is calculated using this approximation, figures 1 through 5 are reproduced to visual accuracy, and the corresponding numbers differ from those in (9) by a few parts in 1000. The further approximation of retaining only the terms m = -1,0,1,2 in (5), in addition to replacing the Bessel functions by their leading terms, also reproduces the geometrical structure with S receding from V and collapsing back into V.

3. Finite-radius flux tube

In order for the stagnation point S to be accessible to observation, it must lie in the space outside the flux. So, whatever contains the flux should be significantly thinner than $r_s \sim \lambda/50$ in (9); in fact, as will now be shown, it must be significantly thinner still. To explore this, we calculate streamlines when the flux is confined within an impenetrable tube of radius *R*. The corresponding AB wave, replacing (5), with Dirichlet boundary conditions at r = R, is [8]



Figure 6. Streamlines of the vector field (6), generated by the wave (13), for flux $\alpha = 0.31278$ (corresponding to the maximum separation between V and S when R = 0), confined within tubes of the indicated radii: one (left) for which the stagnation point S has not been destroyed, and a larger radius (right) for which S has been swallowed by the tube.

$$\psi(\mathbf{r}) = \sum_{-\infty}^{\infty} (-\mathbf{i})^{|m-\alpha|} (-1)^m \exp(\mathbf{i}m\theta) \\ \times \left(J_{|m-\alpha|}(r) - \frac{J_{|m-\alpha|}(R)}{H_{|m-\alpha|}^{(1)}(R)} H_{|m-\alpha|}^{(1)}(r) \right).$$
(13)

For $R \ll r_s$ the geometry is, as expected, essentially the same as for the infinitely thin solenoid: the stagnation point S exists, and so does the vortex V, in the sense that u(r) circulates monotonically around the flux tube (figure 6, left panel). But as *R* increases, S approaches the flux tube and eventually gets swallowed by it. Moreover, V disappears, in the sense that u(r)no longer flows monotonically around the tube boundary; there are two stagnation points on the boundary, where the flow reverses (figure 6, right panel). The critical radius R_c , for which the S gets swallowed, can easily be found numerically. For the flux $\alpha = 0.31278$ where S for the infinitely thin tube lies at the maximum distance $r_s = 0.131459 = 0.021\lambda$, the critical radius $R_c = 0.0248 = 0.0040\lambda \sim r_s/5$. This shows that for a tube with finite radius the unexpected topological fine structure represented by S is even more delicate than for the infinitely thin tube.

4. Concluding remarks

This study of the streamlines of the kinetic momentum (velocity) vector field has revealed unxpectedly fine topological structure in the simplest AB wave, representing scattering of a plane wave by an infinitely thin flux line: a vortex V at the flux line and a stagnation point S very near it. One difference between V and the superficially similar and more familiar phase singularity at the flux line is that V exists even when there is no phase singularity, for example when $0 < \alpha < 1/2$. Another difference is in the circulation around any circuit enclosing the flux. A convenient quantity is the kinetic generalization of the phase gradient (equal to the local velocity when multiplied by \hbar/m), whose circulation is



$$C = \oint d\mathbf{r} \cdot \frac{\mathbf{u}(\mathbf{r})}{\left|\psi(\mathbf{r})^{2}\right|} = \oint d\mathbf{r} \cdot \left(\nabla \arg\psi(\mathbf{r}) - \alpha \frac{\mathbf{e}_{\theta}}{\mathbf{r}}\right) = 2\pi \left(\operatorname{int}\left(\alpha + \frac{1}{2}\right) - \alpha\right).$$
(14)

This is gauge-invariant, and differs by the term $-2\pi\alpha$ from the non-gauge-invariant phase itself. (The circulation of $u(\mathbf{r})$ itself is also gauge-invariant, but not circuit-independent because the vorticity $\nabla \times \mathbf{u}(\mathbf{r})$ is not zero.)

It is important to know whether the VS structure survives in more general AB waves involving a single flux line. These are superpositions of AB plane waves [9–11] initially travelling in directions θ_n :

$$\psi(\mathbf{r}) = \sum_{m=-\infty}^{\infty} (-\mathbf{i})^{|m-\alpha|} (-1)^m J_{|m-\alpha|}(r) \sum_n \exp(\mathbf{i}\alpha\theta_n) \exp(\mathbf{i}m(\theta - \theta_n)).$$
(15)

Such superpositions will typically contain additional phase singularities away from the flux line; when $\alpha = 0$, these are the much-studied wave vortices in typical complex scalar fields [12–14]. As α increases, these vortices move [11]. Although the pattern of phase and canonical streamlines in which they are embedded is gauge-dependent, the kinetic streamlines possess vortices at the same locations. This follows from the last equality in (1), because the shift in the vector field u(r) resulting from the kinetic contribution, proportional to A(r), vanishes on the phase singularities because $\psi(r)$ is zero there. (The streamlines of the superposition also contain stagnation points, but their locations are different from those of the phase saddles.)

In addition to the remote vortices, a nodal point appears at the flux line, corresponding to a phase singularity if $|\alpha| > 1/2$, and its strength is gauge-dependent. This nodal point corresponds to the one we have discussed for the simplest AB scattered plane wave. And as with AB plane waves it corresponds to a vortex in the pattern of kinetic velocity streamlines; this follows from an analogous leading-order small *r* analysis of (13). Moreover, as with the single AB wave, a slightly higher-order approximation suggests that the birth of a vortex as α increases from zero will also be accompanied by a stagnation point. Numerical simulations with the superposition (15), including plane waves in randomly chosen directions θ_n , confirm this expectation: the VS pair persists.

The emphasis in this paper has been on the VS pair close to the flux line. Although this is a complete description of the gauge-invariant singularities in the AB plane wave, further study can be envisaged for superpositions. In particular, the behaviour of the kinetic streamlines and the VS pair as one or more parameters in the superposition are varied so as to steer a remote vortex into the origin (as studied for the phase singularities in [11]) is not clear, expecially when α is close to 1/2.

Since the pattern of kinetic streamlines, including the vortex-stagnation point pair, is gaugeinvariant, it is in principle observable. An experiment to see it would involve AB plane-wave scattering of electrons by flux trapped inside a solenoid (as in [15]) or a magnetized whisker (as in the pioneering experiment [16]). The direction u(r) of the streamline could be detected by the momentum acquired from the electrons by an atom trapped near r, as envisaged for optical vortices [17]. An experiment would not be easy: even an electron with speed as slow as 1 ms^{-1} (energy $2.8 \times 10^{-12} \text{ ev}$) has de Broglie wavelength $\lambda = 727 \mu \text{m}$, so observing S would require an extremely thin solenoid—approximately $R < \lambda/250 \sim 3 \mu \text{m}$.

Finally, it is tempting to interpret the extraordinaily fine geometrical detail reported here (λ /250 in section 3) as an example of superoscillations [18, 19], that is, variation in a function faster than that corresponding to its highest Fourier component. The reason is that in (5) and (13) the waves exp ($-i\alpha\theta$) $\psi(\mathbf{r})$ are solutions of the free-space Helmholtz equation,



representable as a superposition of plane waves with the same wavenumber (in this case k = 1). But for AB the solution involves evanescent plane waves (as reflected in the fractional-order Bessel functions in (5) and (13)) and so is not band-limited. Nevertheless, the scale of the detail is much smaller than the wavelength and so falls into the same class as superoscillations, even though not conforming to the strict definition.

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