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Berry phase, Aharonov–Bohm effect and topology

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Abstract. The Berry phase for an electron in a one-dimensional box rotated around a magnetic flux line has contributions from the geometry and the magnetic flux, which gives an Aharonov–Bohm effect. For a circular box enclosing the magnetic flux, the Berry phase depends on the boundary conditions.

The phase discovered by Berry [1] has attracted a great deal of interest in the past few years because it occurs in a great variety of problems [2, 3]. Among other things, Berry [1] showed that his phase was related to the Aharonov–Bohm (AB) effect [4], the effect of the vector potential in a field-free region in quantum mechanics [5, 6]. This relationship was also investigated by Aharonov and Anandan [7], who say that a more careful investigation of the problem is needed. The geometry used in these two investigations was different. Berry [1] considered a particle in a box, which was rotated by an angle of 2π about an axis containing magnetic flux, and showed that the Berry phase was proportional to the magnetic flux. On the other hand, Aharonov and Anandan [7] considered a situation in which a beam of particles is divided into two, each going on different sides of a magnetic flux line, and finally being recombined. They use an approximate treatment, but obtain a Berry phase which depends on the flux.

In this paper we investigate further the relationship between the Berry phase [1] and the AB effect [4, 6] by solving a simple one-dimensional model of an electron which has an amplitude for being in a box of angular width θ_0 located at a distance R from a line with magnetic flux Φ. When the box is rotated by 2π about the axis with magnetic flux, a Berry phase is obtained which is the sum of a term that depends only on the geometry (i.e. θ_0) and a term that depends only on the magnetic flux. Physically, these two contributions have completely different origins, and it is interesting that they both contribute to give the total Berry phase. The Berry phase can give an observable interference effect if the single electron originally has a non-zero amplitude for being in each of two boxes, only one of which is rotated. After rotation of the one box by 2π, the two boxes are combined. The principle of superposition is used to obtain the resultant wavefunction. Because the Berry phase has a flux-dependent term, the interference effect depends on the flux.

This Berry phase flux-dependent interference effect is a new type of AB effect‡, since the two boxes can be separated by a *macroscopic* distance $2R$ before being

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‡ There are at least four different AB effects, which are (i) AB diffraction, (ii) the bound-state AB effect, (iii) AB scattering, and (iv) the Berry phase AB effect discussed here. Berry said [1] that the Berry phase is only another way of obtaining the AB effect by using only single-valued wavefunctions.

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recombined. (In the usual AB interference effect the flux is placed between two slits which are separated by a *microscopic* distance which is the order of the electron's wavelength.) To record an interference pattern on a photographic plate, the experiment must be repeated many times. Each time, the same photographic plate can be placed in contact with the combined boxes and exposed. In each experiment only *one* electron is involved, so that the principle of superposition is used with the amplitude $\psi^{(1)}$ for the electron to be in box 1 and $\psi^{(2)}$ for the same electron to be in box 2 to obtain the total wavefunction, $\psi^{(1)}+\psi^{(2)}$. When the square of the absolute value of the total wavefunction is taken, an interference term is obtained which depends on the relative phase between the rotated box and the box at rest. On the other hand, if *two* electrons, each in a different box, are used as suggested by Berry [1], the total wavefunction after rotation by 2π of box 2 would be an antisymmetrized product of the wavefunction $\psi^{(1)}(1)$ of box 1 and the wavefunction $\psi^{(2)}(2)$ of box 2, namely $[\psi^{(1)}(1)\psi^{(2)}(2)-\psi^{(1)}(2)\psi^{(2)}(1)]2^{-1/2}$. When the square of the absolute value of this total wavefunction is taken, the interference term does not involve the flux.

The topology of the problem is changed when the angular width θ_0 of the box is extended to 2π, so that it encompasses the whole circle enclosing the flux. If the wavefunction is chosen to be single valued, the energy eigenvalues depend on the enclosed flux, which is the 'bound state AB effect' [5, 6], but the Berry phase is *unobservable. If the wavefunction is multivalued in such a way that the energy* eigenvalues do not depend on the flux, then there is a non-trivial Berry phase which can in principle be determined by interference. The two solutions are, in principle, distinguishable by the experiment. The solution and the Berry phase, therefore, depend on the topology of the box.

The simple model considered here is an *electron of mass m and charge q constrained* to move in a box of angular width θ_0 located a distance R from the z-axis on which there is magnetic flux Φ. The box of angular width θ_0 is located an angular distance Θ from the x-axis. In a gauge in which the scalar potential A_0 of the electromagnetic field is zero, the Schrödinger equation is [8]

$$\{(\hbar^2/2I)(-\mathrm{i}\,\partial/\partial\theta-\alpha)^2+V(\theta)\}\psi_n=\varepsilon_n\psi_n \tag{1}$$

where $I=mR^2$ is the moment of inertia, $\alpha=q\Phi/2\pi\hbar c$ is a dimensionless flux parameter, and $V(\theta)$ is a potential energy. If the angular width of the box θ_0 is $0<\theta_0<2\pi$, then the energy of the particle should not depend on the flux on the z-axis because the path does not enclose the flux. The potential $V(\theta)$ can be chosen so that a solution to (1) is the eigenfunction

$$\psi_n(\theta)=\theta_0^{-1/2}\exp\{\mathrm{i}(\kappa_n+\alpha)(\theta-\Theta)\}u(\theta-\Theta)u(\Theta+\theta_0-\theta) \tag{2}$$

where the Heaviside step function u is defined as $u(x)=1$ for $x\geqslant 0$, and $u(x)=0$ for $x<0$. When (2) is substituted into (1), the eigenvalue obtained is

$$\varepsilon_n=\hbar^2\kappa_n^2/2I \tag{3}$$

which is real. The potential $V(\theta)$ in (1) must be chosen to cancel the contributions from the end-points and is

$$V(\theta)=(\hbar^2/2I)\{[\delta(0)+2\mathrm{i}\kappa_n]\delta(\theta-\Theta)+[\delta(0)-2\mathrm{i}\kappa_n]\delta(\Theta+\theta_0-\theta)$$
$$+\delta'(\theta-\Theta)+\delta'(\Theta+\theta_0-\theta)\} \tag{4}$$

which is complex, state (or velocity) dependent, and highly singular at the end points. The reason the potential is complex is that the solution in (2) is a wave travelling in a counterclockwise direction in the angular sector $(\Theta, \Theta+\theta_0)$. Therefore, there must be a source of probability at $\theta=\Theta$ and a sink of probability at $\theta=\Theta+\theta_0$ to account for the solution (2). Probability (and hence charge) is not conserved locally, which is an unphysical feature of this otherwise illustrative model. The solution in (2) is chosen to satisfy the boundary condition

$$\psi_n(\Theta+\theta_0)=\exp(\mathrm{i}\alpha\theta_0)\psi_n(\Theta) \tag{5}$$

which determines

$$\kappa_n=2\pi n/\theta_0 \tag{6}$$

where $n=0, \pm1, \pm2, \ldots$. The energy in (3) is therefore independent of the flux Φ, since the box containing the electron can be shrunk to a point without enclosing the flux. For this reason the wavefunction in (2) was chosen with the boundary condition in (5).

Even though the potential in (4) is complex and state dependent, the eigenfunctions in (2) are orthonormal

$$\langle\psi_n|\psi_m\rangle=\delta_{nm}. \tag{7}$$

The kinetic angular momentum operator $L_3=-\mathrm{i}\,\partial/\partial\theta-\alpha$ is Hermitian

$$\langle L_3\psi_n|\psi_m\rangle=\langle\psi_n|L_3\psi_m\rangle=\kappa_n\delta_{nm} \tag{8}$$

with the wavefunctions in (2). The Hamiltonian in (1) is also Hermitian

$$\langle H\psi_n|\psi_m\rangle=\langle\psi_n|H\psi_m\rangle=\varepsilon_n\delta_{nm}. \tag{9}$$

The values κ_n and ε_n in (6) and (3), respectively, are both real. It appears that the complexity and state dependence of the potential in (4) compensate each other in order to give real energy eigenvalues.

If Θ depends on the time, there is also a non-trivial Berry phase for this problem. The gauge-invariant Berry phase [7, 9, 10] at time T is

$$\gamma_n(T)=\hbar^{-1}\int_0^T \mathrm{d}t\langle\psi_n|(\mathrm{i}\hbar\,\partial/\partial t-qA_0)\psi_n\rangle. \tag{10}$$

This generalized Berry phase is invariant under gauge transformations, so no gauge can be found to make the Aharonov–Bohm flux-dependent contribution part of the dynamical phase, contrary to a statement in [7, p 1595]. In the gauge used here, in which the scalar potential A_0 is zero and the wavefunction is given by (2), the Berry phase is

$$\gamma_n(T)=(\kappa_n+\alpha)\Delta\Theta \tag{11}$$

where $\Delta\Theta=\Theta(T)-\Theta(0)$ is the angle by which one box is rotated with respect to the other. If the box of angular width θ_0 is rotated by 2π radians in the time T, then $\Delta\Theta=2\pi$, and the Berry phase is

$$\gamma_n(T)=2\pi(2\pi n/\theta_0)+2\pi\alpha \tag{12}$$

which is the relative phase between the rotated box and the box at rest. On the right-hand side of (12) the first term is purely geometrical because it depends only on θ_0. The second term depends only on the magnetic flux $\Phi=2\pi\hbar c\alpha/q$ enclosed by the orbit of the box when it is rotated by 2π radians. Since both θ_0 and Φ can be varied separately, it is possible to distinguish between the contribution of the flux and the contribution of the geometry to the Berry phase. For example, if $2\pi\{(2\pi n/\theta_0)-[2\pi n/\theta_0]\}\neq 0$ and $2\pi\{\alpha-[\alpha]\}=0$, where $[x]$ denotes the largest integer less than or equal to x, there is a non-trivial Berry phase due to the geometry of the box θ_0 which can be observed by interference. On the other hand, if $2\pi\{(2\pi n/\theta_0)-[2\pi n/\theta_0]\}=0$ and $2\pi\{\alpha-[\alpha]\}\neq 0$ there is a non-trivial Berry phase due to the magnetic flux that can be observed by interference. In general both the effect of the geometry of the box and the magnetic flux contribute in an additive way to the Berry phase, even though they are physically completely different.

The geometrical contribution (dependent on θ_0) to the Berry phase in (12) is the contribution of the second term on the right-hand side of (34) in Berry's original paper in [1]. In that paper [1] the term vanishes by normalization because he chose the wavefunction to be real. In our case the wavefunction in (2) is complex and hence contributes to the total Berry phase. The geometrical contribution to the Berry phase also appears in another guise in the second term on the right-hand side of (10) in [7]. If this term $\oint \boldsymbol{p}\cdot \mathrm{d}\boldsymbol{x}/\hbar$ is replaced by $\oint \hbar\kappa_n\, \mathrm{d}\theta/\hbar=2\pi\kappa_n$ we obtain the first term on the right-hand side of our (12). (See note 9 of [7] for a discussion of this point.)

When $\theta_0=2\pi$, the topology of the model changes, and the path of the particle can now no longer be shrunk to a point without crossing the magnetic flux on the z-axis. The boundary condition in (5) requires that the wavefunction be multivalued,

$$\psi_n(\theta)=(2\pi)^{-1/2}\exp[\mathrm{i}(n+\alpha)(\theta-\Theta)] \tag{13}$$

but there is no need for Heaviside step functions. Equation (13) is a solution of (1) with the potential $V=0$. In this case the flux-independent energy is also given by (3) with $\kappa_n=n$ from (6). When one box (circle) is rotated by an angle $\Delta\Theta=\Theta(T)-\Theta(0)$ with respect to the stationary one, the geometrical contribution to the Berry phase in (11) is $n\Delta\Theta$, while the magnetic flux contributes a phase $\alpha\Delta\Theta$. For the periodic case where $\Delta\Theta=2\pi$, the geometrical contribution to Berry's phase is trivial, while the contribution from the magnetic flux is $2\pi\alpha$, which is still observable by interference.

On the other hand, when $\theta_0=2\pi$ it is reasonable to use a single-valued wavefunction with the boundary condition

$$\psi_n(\Theta+2\pi)=\psi_n(\Theta). \tag{14}$$

The single-valued energy eigenfunction which satisfies (1) for $V=0$ is

$$\psi_n(\theta)=(2\pi)^{-1/2}\exp[in(\theta-\Theta)] \tag{15}$$

where $n=0,\pm 1,\pm 2,\ldots$. The energy eigenvalue in (1) for $V=0$ is

$$\varepsilon_n=\hbar^2(n-\alpha)^2/2I \tag{16}$$

which now depends on the magnetic flux. This dynamical effect, in which the energy eigenvalues of a particle in a region where there is no magnetic field depend on the enclosed magnetic flux, is called the 'bound-state AB effect' [5, 6]. The energy in (16) would contribute to the dynamical phase. The Berry phase when $\theta_0=2\pi$ is calculated from (10). When (15) in the gauge for which $A_0=0$ is used in (10), the Berry phase is

$$\gamma_n(T)=n[\Theta(T)-\Theta(0)]=n\Delta\Theta. \tag{17}$$

If one box (circle) is rotated by $\Delta\Theta=2\pi$ radians with respect to the other, the Berry phase is a trivial $2\pi n$, which is not observable.

When the topology of the system changes so that the path of the electron cannot be shrunk to a point without crossing the magnetic flux there are (at least) two solutions possible†. One is based on a multivalued wavefunction which gives a non-trivial flux-dependent Berry phase and no bound state AB effect. The other is based on a single-valued wavefunction which has a trivial non-observable Berry phase and exhibits a bound state AB effect. The two solutions can in principle be distinguished from each other by interference effects [11] or spectroscopic measurements.

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† By an appropriate choice of wavefunction for $\theta_0 = 2\pi$ it is possible to have solutions which interpolate between these two cases, for example, $\psi_n(\theta) = (2\pi)^{-1/2} \exp[i(n + c\alpha)(\theta - \Theta)]$, where c is a constant. When the constant $c = 0$ we obtain (15), and when $c = 1$ we have (13). There are thus an infinite number of solutions to (1), but these can be restricted by choosing the boundary conditions for physical reasons.