Aharonov - Bohm geometric phases for rotated rotators

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Abstract. On a ring threaded by a flux line moves a charged quantum particle whose rotation is hindered by an angle-dependent potential. When the potential is rigidly rotated through 2π, the particle (in the nth eigenstate of the potential on the ring) acquires a geometric phase γ_n. A general formula is $\gamma_n = 2\pi(\alpha + J_n)$, where α is the dimensionless quantum flux and J_n is a Schrödinger current associated with the state. Properties of J_n are obtained in terms of the transmission coefficient round the ring. J_n vanishes when the box is impenetrable or when α is integer or half-integer. Energy levels form bands, with α playing the role of Bloch pseudomomentum. For unhindered semiclassical states above the barrier, a WKB theory gives the geometric phase and hence the (previously calculated) classical Hannay angle Θ_H. This does not vanish when α is integer or half-integer, but these cases correspond to band edges where the semiclassical states are degenerate and differ greatly from the true asymptotic states. The theory is illustrated by the exact calculation of J_n for a model where the potential is a delta function.

1. Introduction

One of the earliest examples of a geometric phase is that acquired by charged particles near a line of magnetic flux Φ (Aharonov and Bohm 1959). Previously (Berry 1984b), I considered this in terms of a model where the charge q is in an eigenstate confined in a box that is transported round the flux line (see also de Polavieja and Sjöqvist 1997). The geometric phase is the same as the Aharonov–Bohm (AB) phase

$$\gamma_{AB} = 2\pi\alpha \qquad \text{where} \quad \alpha \equiv \frac{q\Phi}{h} \tag{1}$$

is the dimensionless flux. This phase is independent of the quantum state of the particle in the box, and so the Hannay angle Θ_H—its classical counterpart (Hannay 1985), given by the derivative of the phase with respect to quantum number (Berry 1985)—must be zero. It is possible to regard this version of the AB effect as a rotated rotator in the presence of a flux line, where the rotator is hindered by the confining potential of the box. But Θ_H has been calculated for a class of rotated rotators (Berry and Morgan 1996), and it is not zero (and moreover Θ_H is independent of Φ).

My purpose here is to resolve this discordance, by calculating the geometric phase γ exactly for a class of penetrable boxes, and examining several limits. It will emerge that (1) is an approximation, valid when the box is impenetrable—either because its potential walls are high or because the confined particles are nearly classical. In the opposite extreme, when the box is completely penetrable (that is, the particle can move unhindered round the flux line—because it is nearly classical and unconfined by potential barriers), Θ_H is equal to the previously calculated nonzero value, provided α is not an integer or a half-integer.

In these exceptional cases, $\Theta_H = 0$, that is, not the previously calculated value; this will be explained as a clash between the semiclassical limit and the long-time limit.

Only the motion round the flux line is important, so the particle can be restricted to a ring $(0 \leqslant \theta < 2\pi)$ on which there is a potential $V(\theta - X(t))$ that describes the box. X is the parameter describing the angular location of the box. If V has high walls, the box is impenetrable. Geometric phases are generated by transporting the box, that is forcing X to increase from 0 to 2π. The quantum eigenstates are determined by

$$H\psi_n = \left[\frac{\hbar^2}{2MR^2} (-i\partial_\theta - \alpha)^2 + V(\theta - X) \right] \psi_n = E_n \psi_n \tag{2}$$

where M is the mass of the particle and R the radius of the ring. These states are periodic (that is, single-valued on the ring) and, for this simple type of transport, are obtained for different X simply by translation:

$$\psi_n = \psi_n(\theta - X) = \psi_n(\theta + 2\pi - X). \tag{3}$$

Thus the geometric phase is

$$\gamma_n = -\mathrm{Im} \oint \langle \psi_n \mid d\psi_n \rangle$$

$$= -\mathrm{Im} \int_0^{2\pi} dX \int_0^{2\pi} d\theta\, \psi_n^*(\theta - X)\, \partial_X \psi_n(\theta - X)$$

$$= +2\pi \mathrm{Im} \int_0^{2\pi} d\theta\, \psi_n^*(\theta)\, \partial_\theta \psi_n(\theta). \tag{4}$$

2. Geometric phase calculation

We transfer the flux in (2) from the operator to the boundary condition by writing (for $X = 0$)

$$\psi_n(\theta) = \exp(i\alpha\theta)\, \chi_n(\theta) \tag{5}$$

so that

$$\left(\frac{\hbar^2}{2MR^2} \partial_\theta^2 + E_n - V(\theta) \right) \chi_n = 0 \qquad \chi_n(\theta + 2\pi) \exp(2\pi i\alpha) = \chi_n(\theta). \tag{6}$$

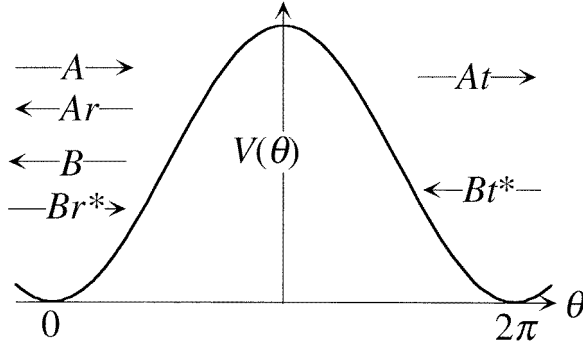Thus (2) is reduced to a Bloch problem, with pseudomomentum $2\pi\alpha$. The geometric phase (4) becomes

$$\gamma_n = 2\pi(\alpha + J_n) \tag{7}$$

where J_n is the current of the Hamiltonian (6), namely

$$J_n = 2\pi \mathrm{Im}\chi_n^* \partial_\theta \chi_n \tag{8}$$

which is conserved according to (6) and so can be evaluated at any θ. Only if J_n vanishes does γ_n take its AB value (1). From (6) it follows that

$$J_n(\alpha + 1) = J_n(\alpha) \qquad J_n(-\alpha) = -J_n(\alpha). \tag{9}$$

Figure 1. Superposed transmitted and reflected waves, and their conjugates, constituting the wavefunction on the ring.

To calculate J, it is convenient to choose $V = 0$ near $\theta = 0$, and write χ in terms of transmission and reflection coefficients t and r (figure 1), both dependent on energy E. This can be accomplished by writing

$$\chi(\theta) = A\chi_+(\theta) + B\chi_+^*(\theta) \qquad \text{where}$$

$$\left.\begin{array}{ll} \chi_+(\theta) = \exp(ik\theta) + r\exp(-ik\theta) & (\theta \approx 0) \\ \chi_+(\theta) = t\exp(ik\theta) & (\theta \approx 2\pi) \end{array}\right\} \tag{10}$$

where we have introduced the notation

$$k \equiv \frac{R}{\hbar}\sqrt{2ME}. \tag{11}$$

Thus (8) gives the current as

$$J = 2\pi |t|^2 k \left(|A|^2 - |B|^2\right). \tag{12}$$

Application of the boundary condition in (6) gives

$$A + r^*B = tA \exp\{2\pi i (k + \alpha)\}$$
$$rA + B = t^*B \exp\{2\pi i (-k + \alpha)\} \tag{13}$$

whence

$$\frac{B}{A} = \frac{t\exp\{2\pi i (k + \alpha)\} - 1}{r^*} \qquad \frac{A}{B} = \frac{t^*\exp\{2\pi i (-k + \alpha)\} - 1}{r}. \tag{14}$$

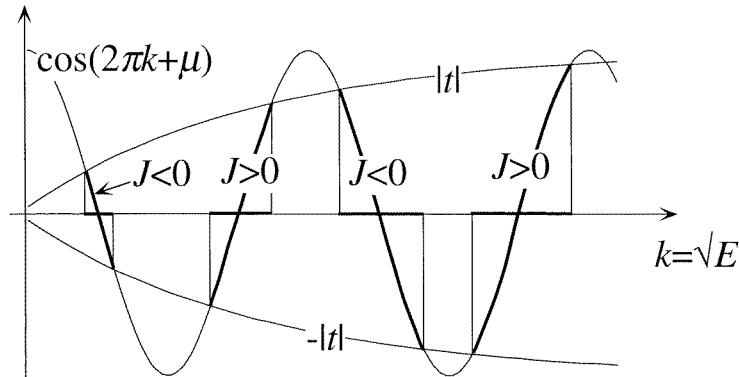Compatibility leads to a quantization condition, namely (restoring the energy dependence)

$$\cos\{2\pi k_n + \mu(E_n)\} = |t(E_n)| \cos\{2\pi\alpha\} \tag{15}$$

where μ is the phase of the transmission coefficient:

$$t = |t| \exp(i\mu). \tag{16}$$

This describes the familiar structure (figure 2) of narrow tight-binding bands when $|t| \ll 1$, near $2\pi k + \mu = (n + 1/2)\pi$, and nearly-free bands when $|t| \approx 1$, with narrow gaps near $2\pi k + \mu = n\pi$.

Some algebra based on (13) and (14) gives

Figure 2. Quantization condition for bands (bold), indicating signs of current J, drawn for $\sin \alpha > 0$.

$$\left|\frac{B}{A}\right|^2 = 1 + \frac{2|t|^2}{|r|^2}\sin^2(2\pi\alpha) + \frac{2|t|}{|r|}\sin(2\pi\alpha)\sin(2\pi k + \mu)$$

$$\left|\frac{A}{B}\right|^2 = 1 + \frac{2|t|^2}{|r|^2}\sin^2(2\pi\alpha) - \frac{2|t|}{|r|}\sin(2\pi\alpha)\sin(2\pi k + \mu). \tag{17}$$

Several conclusions follow from these equations. First, J vanishes if α is an integer or half-integer (corresponding to band edges), since then (cf. 12) $|A| = |B|$ and the wavefunctions χ can be chosen to be real (for an explanation of the half-integer case in terms of 'false time-reversal symmetry-breaking', see Robnik and Berry 1986). Second, J also vanishes when the box is impenetrable, that is in the classical limit where E is below the barrier top and $|t| \approx 0$, since then again $|A| = |B|$. In these cases, the geometric phase is simply γ_{AB}, given by (1). Third, the sign of J depends on the sign of $\sin(2\pi\alpha)\sin(2\pi k + \mu)$. When this quantity is positive, $|B| > |A|$ and $J < 0$; when it is negative, $|A| > |B|$ and $J > 0$. Thus for given flux α the sign of J alternates between bands (figure 2), and if α is replaced by $-\alpha$ all the signs reverse.

3. Semiclassical limit

For energies above the barrier, and small $\hbar$, the approximate solutions of (6) are given by the WKB method (Berry and Mount 1972) as the reflectionless distorted plane waves

$$\chi(\theta) \approx \chi_{sc}(\theta) = N\frac{\exp\left\{\pm(i/\hbar)\,R\sqrt{2M}\int_0^\theta d\phi\sqrt{E - V(\phi)}\right\}}{[E - V(\theta)]^{1/4}} \tag{18}$$

where the normalization constant is

$$N^2 = \left\{\int_0^{2\pi}\frac{d\theta}{\sqrt{E - V(\theta)}}\right\}^{-1}. \tag{19}$$

The continuation requirement (6) yields the approximate quantization rule

$$I(E_n) = \hbar(n \mp \alpha) \qquad (n = \ldots -2, -1, 0, 1, 2, 3 \ldots) \tag{20}$$

where the action is defined by

$$I(E) = \frac{R}{2\pi} \sqrt{2M} \int_0^{2\pi} d\theta \sqrt{E - V(\theta)}. \tag{21}$$

The angular frequency $\omega(E)$ of the classical motion is related to N by

$$\frac{1}{\omega(E)} = \partial_E I = \frac{R}{2\pi N^2} \sqrt{\frac{M}{2}}. \tag{22}$$

Now (7) and (8) give the geometric phase as

$$\gamma_{\mathrm{sc},n} = 2\pi \left[\alpha \pm \frac{MR^2 \omega(E_n)}{\hbar} \right]. \tag{23}$$

The $+$ and $-$ correspond to the two solutions (18). Here the phase arises entirely from the normalization condition. The Hannay angle is

$$\Theta_{\mathrm{H}} = -\partial_n \gamma_{\mathrm{sc},n} = -\hbar \partial_I \gamma_{\mathrm{sc},n} = \mp 2\pi MR^2 \partial_I \omega(E(I)). \tag{24}$$

This is exactly the result previously calculated classically (Berry and Morgan 1996) (apart from a physically insignificant term 2π arising from the definition of the origin of the angle variable, with the extra lower sign corresponding to particles circulating negatively).

As expected, Θ_{H} is independent of the flux α (because this is classically unobservable), but the fact that Θ_{H} is not zero gives rise to a discordance with the results of the last section, according to which J_n, and therefore also Θ_{H}, must vanish when α is integer ($\gamma_n = 0$) or half-integer ($\gamma_n = \pi$). In precisely these cases, however, the solutions (18) do not correspond to eigenstates, because the semiclassical quantization condition (20) predicts—wrongly—that the $+$ and $-$ states are degenerate; they are not modes but 'quasimodes' (Arnold 1972, Berry 1978). The semiclassically weak above-barrier reflection generates an exponentially small splitting between the levels (20). In this situation we must represent the semiclassical states more accurately by a linear combination of the solutions (18), namely

$$\chi(\theta) \approx \frac{N}{[E - V(\theta)]^{1/4}} \times \left[C \exp\left\{ \frac{\mathrm{i}}{\hbar} R\sqrt{2M} \int_0^\theta d\phi \sqrt{E - V(\phi)} \right\} \right.$$

$$\left. + D \exp\left\{ -\frac{\mathrm{i}}{\hbar} R\sqrt{2M} \int_0^\theta d\phi \sqrt{E - V(\phi)} \right\} \right]. \tag{25}$$

C and D are proportional to A and B in (10) apart from phase factors, so that $|C/D| = |A/B|$. (C and D are not quite constant, but this does not affect the results now to be obtained.)

Now we can repeat the argument leading to (23) (neglecting a semiclassically small term arising from interference oscillations in the normalization integral) and thereby obtain the corrected formula

$$\gamma_{\mathrm{sc},n} = 2\pi \left[\alpha \pm \frac{MR^2 \omega(E_n)}{\hbar} \left(\frac{1 - |B/A|^2}{1 + |B/A|^2} \right) \right]. \tag{26}$$

For the ratios of coefficients we can use (17), in which $|r|$ is exponentially small (in $\hbar$), $|t|$ is exponentially close to unity, and the phase μ of t is given by comparing (18) with (10):

$$2\pi k + \mu = \frac{2\pi}{\hbar} I(E). \tag{27}$$

Unless α is integer or half-integer, $|A/B|$ is either much greater or much less than unity (this follows from (17)). Then (26) reduces to the previous formula (23). Exponentially close to a band edge, however, $|A/B|$ is close to unity and (23) and (26) differ. At a band edge, $|A/B| = 1$ and the corrected semiclassical geometric phase is a multiple of π (as is the exact geometric phase).

This discordance between semiclassical and exact geometric phases near a band edge persists as $\hbar \to 0$. It can be interpreted in terms of the familiar clash between the semiclassical and long-time limits (for other examples, see Berry 1984a, Robbins and Berry 1992). The approximate solutions (18) differ radically from the true eigenstates near band edges, but in view of the small energy splitting this difference becomes apparent only after times that are exponentially long in $\hbar$. Then, a state initially given by (18) with the positive sign would, being nonstationary, transform by above-barrier tunnelling into the state with the negative sign, that is, the particles would reverse their direction of circulation. Therefore, if the adiabatic transport of the potential is carried out in a time shorter than $O(\exp(1/\hbar))$— but still long in comparison with the orbital period $2\pi/\omega$—the formula (23) would give the geometric phase correctly for the states (18), even near band edges.

4. Exactly-solvable model

Let the potential be

$$V(\theta) = \frac{\hbar^2}{2MR^2} K\delta(\theta).$$ (28)

If $K > 0$, this represents a wide potential well with a thin barrier, and if $K < 0$ the barrier is wide and the well is narrow. The coefficients r and t are determined by continuity of χ across the δ spike, which gives $r + 1 = t$, together with the discontinuity of $\partial_\theta \chi$ that results from integrating (6) across the spike, namely

$$\lim_{\varepsilon \to 0} (\partial_\theta \chi(\varepsilon) - \partial_\theta \chi(-\varepsilon)) = K\chi(0).$$ (29)

Thus follows

$$t = \frac{1}{1 - K/2ik} \qquad r = \frac{K/2ik}{1 - K/2ik}.$$ (30)

From (15) follows the quantization condition

$$\cos(2\pi\alpha) = \cos(2\pi k) + \frac{K}{2k}\sin(2\pi k).$$ (31)

As α varies from 0 to $1/2$ this generates the bands, as illustrated in figure 3. For positive K, all the bands have positive energy (for this non-smooth potential, the gap widths decrease asymptotically as K/k rather than exponentially). For negative K there is also one band with negative energy. With $k = i\sigma$, this is determined by

$$\cos(2\pi\alpha) = \cosh(2\pi\sigma) - \frac{|K|}{2\sigma}\sinh(2\pi\sigma).$$ (32)

If $-2/\pi < K < 0$ the negative-energy band passes though $E = 0$ (at flux $\cos(2\pi\alpha) = 1 - \pi|K|$). For large negative K, the negative-energy band is very narrow (tight-binding limit), and given approximately by

$$\sigma = \frac{|K|}{2}\left[1 + 2\exp(-\pi|K|)\cos(2\pi\alpha)\right].$$ (33)
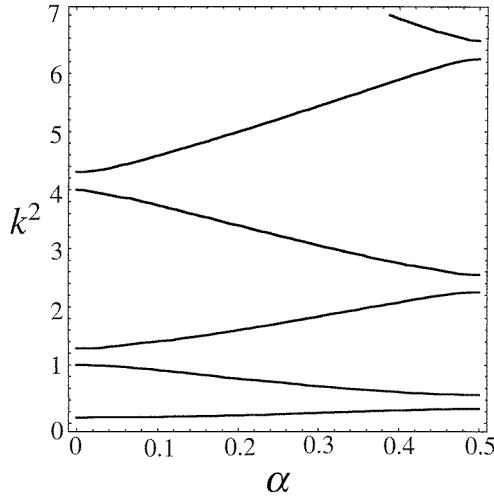
Figure 3. Energy bands generated by (31) for the potential (28) with $K = 1$.

To calculate the geometric phase for this model, we use (7) and (12). The current J can be determined by calculating the normalization integral using (10), and the fact that for this model the solution χ_+ written there for $\theta \approx 2\pi$ holds in the range $0 < \theta \leqslant 2\pi$. It follows that

$$J = k \frac{\left(1 - |B/A|^2\right)}{\left(1 + |B/A|^2 + (\sin(2\pi k) / \pi k) \operatorname{Re}\left((Bt^*/At) \exp(-2\pi i k)\right)\right)}. \qquad (34)$$

A convenient expression for Bt^*/At can be obtained by adding the two equations (13) and using $1 + r = t$:

$$\frac{Bt^*}{At} = \exp(2\pi i k) \frac{\sin\{\pi(k + \alpha)\}}{\sin\{\pi(k - \alpha)\}}. \qquad (35)$$

(Showing this to be equivalent to (14) is a tricky exercise, using $1 + r = t$ and the unitarity condition $r^*t + rt^* = 0$, which implies $\cos\mu = |t|$.) Thus J can be found in terms of α and k, with k one of the solutions of (31). As expected, $|B/A| = 1$, and so $J = 0$, when α is integer or half-integer.

Alternatively, an explicit formula can be found by using (31) to eliminate α, thereby obtaining J as a function of energy (proportional to k^2) and the strength K of the potential. Some algebra gives

$$J(k, K) = k \frac{\operatorname{Re}\left[\sqrt{1 - (\cos(2\pi k) + (K/2k)\sin(2\pi k))^2}\right]}{\sin(2\pi k) - (K/2k)\cos(2\pi k) + \left(K/8\pi k^2\right)\sin(4\pi k)}. \qquad (36)$$

As $k \to \infty$ and not very close to the gaps, $J \to \pm k$, which is the free-particle limit. In this situation, the geometric phase (7) differs greatly from γ_{AB}. The formula (36) also works for negative energies ($k = i\sigma$). In the tight-binding limit (K large and negative), the current is exponentially small and varies parabolically across the band:

$$J(i\sigma, -|K|) \approx 2\pi K^2 \exp(-2\pi|K|) \sqrt{1 - \left(\frac{\sigma}{|K|} - \frac{1}{2}\right)^2} \exp[2\pi|K|]. \qquad (37)$$
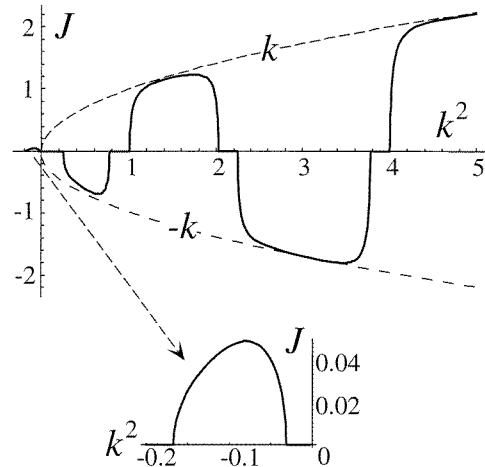
Figure 4. Deviation J of the geometric phase (7) from γ_{AB}, for the potential (28) with $K = -1$, calculated from (36).

This exemplifies the situation I envisaged before (Berry 1984b), where the box is impenetrable and $\gamma = \gamma_{AB}$. Figure 4 illustrates the transition of J between the tight-binding (AB geometric phase) and nearly-free regimes.

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