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LETTER TO THE EDITOR

Two-level systems: space curve formalism, Berry's phase and Gauss–Bonnet theorem

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Abstract. We study the projective space representation of a general two-level system introduced by Feynman *et al.* This allows a mapping onto a space curve. Geometric phases, Berry's phase and its complementary phase are calculated. The relation with the Gauss–Bonnet theorem is discussed and an inequality for the Berry phase is derived.

Two-level quantum systems are widely used in physics to model a variety of phenomena [1, 2]. The essential features of quantum mechanics can be discussed using two-level systems. The visualization, however, of the complex vector space is rather difficult, which makes the study of the geometry of quantum evolution non-trivial. On the other hand, a variety of nonlinear phenomena [3] and certain topological properties of unit vector fields [4] have been studied using a space curve formalism. This has led to new insights for some geometric properties of the phase of the wavefunction.

In the case of a two-level system, the Hilbert space is a real four-dimensional space. We will restrict ourselves here to normalized wavefunctions. In this case, the Hilbert space becomes S^3. Feynman *et al* [5] have noticed that in this case the Schrödinger equation may be written in the form of a three-dimensional vector equation:

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \boldsymbol{\xi} \wedge \boldsymbol{r} \tag{1}$$

where $\boldsymbol{r}$ is a unit three-dimensional vector with components:

$$r_1 = ab^* + ba^* \qquad r_2 = \mathrm{i}(ab^* - ba^*) \qquad r_3 = aa^* - bb^*. \tag{2}$$

This represents just the Hopf map $S^3 \to S^2$ with $\psi(t) = a(t)\psi_a + b(t)\psi_b$ and $|a|^2 + |b|^2 = 1$; ψ_a and ψ_b are the two eigenstates, corresponding to energies $\frac{1}{2}\hbar\omega_o$ and $-\frac{1}{2}\hbar\omega_o$. Here S^2 is the projective space for our system. If the Hamiltonian is given by $H = H_o + V$ and if we neglect V_{aa} and V_{bb}, then the components of $\boldsymbol{\xi}$ are given by

$$\xi_1 = (V_{ab} + V_{ba})/\hbar \qquad \xi_2 = \mathrm{i}(V_{ab} - V_{ba})/\hbar \qquad \xi_3 = \omega_o. \tag{3}$$

Let us now concentrate on equation (1) on R^3. As time evolves the tip of the unit vector $\boldsymbol{r}$ traces out a curve on the surface of a unit sphere with centre at the origin of the coordinate system. We may now introduce the unit vectors $\boldsymbol{n}$ and $\boldsymbol{b}$ such that $\boldsymbol{r}$, $\boldsymbol{n}$ and $\boldsymbol{b}$ represent an orthonormal triad, $\boldsymbol{n} = (\mathrm{d}\boldsymbol{r}/\mathrm{d}t) \cdot |\mathrm{d}\boldsymbol{r}/\mathrm{d}t|^{-1}$ and $\boldsymbol{b}$ is such that $\boldsymbol{r} = \boldsymbol{n} \wedge \boldsymbol{b}$.

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The vectors $\boldsymbol{n}$ and $\boldsymbol{b}$ are tangent to the unit sphere; $\boldsymbol{n}$ is tangent to the curve traced out by $\boldsymbol{r}$ on the unit sphere. The three vectors $\boldsymbol{r}$, $\boldsymbol{n}$ and $\boldsymbol{b}$ satisfy the following set of equations [6]:

$$\dot{\boldsymbol{r}} = k\boldsymbol{n} \qquad \dot{\boldsymbol{n}} = -k\boldsymbol{r} + \tau\boldsymbol{b} \qquad \dot{\boldsymbol{b}} = -\tau\boldsymbol{n}. \tag{4}$$

If we introduce the Darboux vector $\boldsymbol{\xi} = \tau(t)\boldsymbol{r} + k(t)\boldsymbol{b}$, equation (4) may be written in a more compact form:

$$\dot{\boldsymbol{r}} = \boldsymbol{\xi} \wedge \boldsymbol{r} \qquad \dot{\boldsymbol{n}} = \boldsymbol{\xi} \wedge \boldsymbol{n} \qquad \dot{\boldsymbol{b}} = \boldsymbol{\xi} \wedge \boldsymbol{b}.$$

Equations (4) are the Frenet–Serret equations for a space curve, where $\tau(t)$ is the torsion of the curve and $k(t)$ is its curvature; t is the length of the curve. For a cyclic evolution of our two-level system the tip of $\boldsymbol{r}$ traces out a closed curve on the top of the unit sphere. This closed curve is the spherical image [6] of the space curve whose Frenet–Serret equations are given by equation (4). It is clear that the natural frame ($\boldsymbol{n}$ and $\boldsymbol{b}$) rotates around $\boldsymbol{r}$ with an angular velocity $\tau(s)$. Thus as s increases from $s=0$ to $s=s_o$, the system develops a phase

$$\phi_1 = \int_0^{s_0} \tau(s)\,\mathrm{d}s \tag{5}$$

between ($\boldsymbol{n}, \boldsymbol{b}$) and the corresponding non-rotating frame in this plane. Such a non-rotating frame could be defined by using the usual Fermi–Walker parallel transport along the curve of a vector $\boldsymbol{A}$ [8, 9],

$$\frac{\mathrm{D}A^i}{\mathrm{d}s} = \{k\boldsymbol{b} \times \boldsymbol{A}\}^i. \tag{6}$$

Recently, Urbantke [2] has shown that a phase change of α in $|\psi\rangle$ implies the rotation of the ($\boldsymbol{n}, \boldsymbol{b}$) plane by an angle 2α. Hence from equation (5), $\phi_1 = 2\alpha$, giving

$$\alpha = \tfrac{1}{2}\int \tau(s)\,\mathrm{d}s. \tag{7}$$

From the definition of $\boldsymbol{\xi}$, we have $\tau(s) = \boldsymbol{\xi}\cdot\boldsymbol{r}$. Using expressions (2) and (3), it is easy to show that

$$\tau(s) = \frac{2}{\hbar}\langle H(s)\rangle. \tag{8}$$

Hence

$$\alpha = \frac{1}{\hbar}\int \langle H(s)\rangle\,\mathrm{d}s. \tag{9}$$

Berry has shown that under adiabatic, cyclic evolution of certain parameters (in this case a and b) an initial state $|\psi(o)\rangle$ evolves to $|\psi(T)\rangle$, where

$$|\psi(T)\rangle = \mathrm{e}^{-\mathrm{i}\alpha}|\psi(o)\rangle. \tag{14}$$

Here the accumulated phase α has a 'dynamical' as well as a 'geometric' part:

$$\alpha = +\frac{1}{\hbar}\int_o^T E(t)\,\mathrm{d}t - \gamma(c). \tag{15}$$

Comparing equations (9) and (15) we get

$$\gamma=\frac{1}{\hbar}\left\{\int_o^T \langle H(t)\rangle\,\mathrm{d}t-\int_o^T \langle H(s)\rangle\,\mathrm{d}s\right\}.$$

Using equation (8),

$$\gamma=\frac{1}{2}\left\{\int_o^T \tau(t)\,\mathrm{d}t-\int_o^T \tau(s)\,\mathrm{d}s\right\}. \tag{16}$$

The first term is an ordinary integral over time, whereas the second term is an integral along a twisted curve, whose shape depends on the form of the time-dependent Hamiltonian. By simple calculation one can show that

$$\tau(s)=\mathrm{i}\left\langle \psi(s)\,\middle|\,\frac{\mathrm{d}\psi(s)}{\mathrm{d}s}\right\rangle$$

and

$$\tau(t)=\mathrm{i}\left\langle \psi(t)\,\middle|\,\frac{\mathrm{d}\psi(t)}{\mathrm{d}t}\right\rangle$$

so that our division of the phase into 'dynamical' and 'geometrical' coincides with that in [10]. By parallel transporting the unit vectors $\boldsymbol{r}$, $\boldsymbol{n}$ and $\boldsymbol{b}$ to the origin of a cartesian coordinate system, we see that as the triad moves along the curve, their tips generate three curves on the unit sphere S^2. These are called tangent, normal and binormal indicatrices of the space curve. For cyclic evolutions, these will be closed curves.

Using the Euler angle (θ, ϕ, ψ) representation of the Frenet–Serret equations, one can show that [9]

$$\tau\,\mathrm{d}s=\cos\theta\,\mathrm{d}\phi+\mathrm{d}\psi$$

and

$$k^2\,\mathrm{d}s^2=(\mathrm{d}\theta)^2+\sin^2\theta(\mathrm{d}\phi)^2$$

so that

$$\phi_1=\int_o^T \tau(s)\,\mathrm{d}s=2\pi-\iint \sin\theta\,\mathrm{d}\theta\wedge\mathrm{d}\phi \tag{17}$$

where the last term is the area bounded by the tangent indicatrix and follows from Stokes' theorem.

The above result when used in equation (16) shows that the geometric phase γ of a two-level system is a measure of the deviation of the torsion (or twistedness) of a space curve from a constant value τ_o. In the quantum mechanical language, if the Hamiltonian H is time independent, then it implies that the mapping of the Schrödinger equation is to a space curve of constant torsion. This is because in general,

$$\frac{\mathrm{d}\tau(s)}{\mathrm{d}s}=\frac{\mathrm{d}}{\mathrm{d}s}(\boldsymbol{\xi}\cdot\boldsymbol{r})=\boldsymbol{\xi}\cdot\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}+\boldsymbol{r}\cdot\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}s}=\boldsymbol{r}\cdot\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}s}.$$

This derivative will vanish if $\boldsymbol{\xi}$ is independent of time, which happens when H is independent of time, as seen from equation (3). For this case, the two terms on the right-hand side of equation (16) become equal and the geometric phase γ *vanishes*. Note that even in the case of a constant torsion τ_o (i.e. constant-in-time Hamiltonian), cyclical evolution of the system is still possible—in this case the vector $\boldsymbol{r}$ precesses around a constant $\boldsymbol{\xi}$. This is an example of the Aharonov-Anandan phase.

From the definition of the Darboux vector, we have

$$\xi^2 = k^2(s) + \tau^2(s). \tag{18}$$

From equation (3) we can easily verify that $\xi^2 = (4/\hbar^2)\langle H\rangle^2$. Hence

$$k^2 = \frac{4}{\hbar^2}\{\langle H^2\rangle - \langle H\rangle^2\}. \tag{19}$$

Thus the above variance of the Hamiltonian is a measure of the curvature of the space curve. This is another independent geometric property, *distinct* from the torsion τ. The expression for $\boldsymbol{\xi}$ shows that by considering a non-rotating frame defined in a way similar to the Fermi–Walker transport given in equation (6), i.e. [9]

$$\frac{\mathrm{D}A^i}{\mathrm{d}s} = (\tau \boldsymbol{r} \times \boldsymbol{A})^i \tag{20}$$

the $(\boldsymbol{r}, \boldsymbol{n})$ plane rotates around $\boldsymbol{b}$ with an angular velocity $k(s)$. This leads to a phase

$$\begin{aligned}\phi_2 &= \int_o^T k\,\mathrm{d}s = \frac{2}{\hbar}\int_o^T \{\langle H^2\rangle - \langle H\rangle^2\}^{1/2}\,\mathrm{d}s \\ &= \frac{2}{\hbar}\int_o^T \Delta H\,\mathrm{d}s = \frac{2}{\hbar}\int_o^T \Delta H\,\mathrm{d}t \end{aligned}\tag{21}$$

where we have used equation (18). It is known that ϕ_2 is a measure of the length of the tangent indicatrix [6, 11]†, i.e. a curve traced out by $\boldsymbol{r}$ on the unit sphere. On the other hand $\phi_1 = \int \tau(s)\,\mathrm{d}s$, is a measure of the length of the binormal indicatrix [6]. Analogous to this latter case discussed earlier, for a cyclic evolution one can show that $\phi_2 = \int k(s)\,\mathrm{d}s$ is just the closed area bounded by the binormal indicatrix [9]. Let us consider now the tangent indicatrix of our space curve. It is generated by the tip of the radius vector $\boldsymbol{r}$. The triad $\boldsymbol{r}$, $\boldsymbol{n}$ and $\boldsymbol{b}$ may be considered as a moving triad along the tangent indicatrix—the element of length being now $\mathrm{d}s_r = k\,\mathrm{d}t$, $\boldsymbol{n}$ being the tangent and $\boldsymbol{b}$ the normal to this curve; $\boldsymbol{r}$ plays the role of a binormal to the curve and a normal to the sphere. The three vectors satisfy the Darboux–Ribaucour equations [6]:

$$\dot{\boldsymbol{r}} = \boldsymbol{n} \qquad \dot{\boldsymbol{n}} = -\boldsymbol{r} + k_g\boldsymbol{b} \qquad \dot{\boldsymbol{b}} = -k_g\boldsymbol{n} \tag{22}$$

where the overdot stands for $\mathrm{d}/\mathrm{d}s_r$ and k_g is the geodesic curvature [6], $k_g = \tau/k$. Let us now consider the following integral:

$$\oint k_g\,\mathrm{d}s_r = \int_o^T \tau\,\mathrm{d}t = \phi_1. \tag{23}$$

The integral of the geodesic curvature k_g along a closed curve is related to the area enclosed via the Gauss–Bonnet theorem [6]:

$$\oint k_g\,\mathrm{d}s_r = 2\pi - \iint_A K\,\mathrm{d}A. \tag{24}$$

† In a somewhat different context Anandan and Aharonov [11] have noticed that $(2/\hbar)\Delta H\,\mathrm{d}t$ is an element of length along the trajectory in the projective Hilbert space.

Here K is the Gaussian curvature and $\iint_A K \, \mathrm{d}A$ is the *curvatura integra* of Gauss and $\mathrm{d}A$ is an element of area on S^2. In our case $K=1$ and we get again the expression in equation (17). This is the Gauss–Bonnet theorem for a smooth closed curve. When the closed curve consists of N arcs of smooth curves making exterior angles $\theta_1, \theta_2, \ldots, \theta_N$ at the vertices where the arcs meet, equation (24) becomes:

$$\oint k_g \, \mathrm{d}s_r + \sum_{i=1}^{N} \theta_i = 2\pi - \iint_A K \, \mathrm{d}A. \tag{25}$$

This is the general Gauss–Bonnet theorem and is a generalization of equation (17).

Let us now again consider the example of a non-unitary evolution of a system which is subject to measurements [12] (a two-level system which is a subject to three measurements, which bring the system from a state $|\psi_1\rangle$ to $|\psi_2\rangle$, to $|\psi_3\rangle$ and then back to $|\psi_1\rangle$). On the unit sphere these three states are represented by points 1, 2 and 3 and these points are connected by geodesics [12]. Along a geodesic $k_g=0$ and consequently $\oint k_g \, \mathrm{d}s_r = 0$, contrary to the conclusion in [12] (taken in the context of a two-level system). For this case:

$$\sum_{i=1}^{N} \theta_i = 2\pi - \iint_A K \, \mathrm{d}A.$$

Let us now turn our attention to one inequality regarding Berry's phase. In general, the following inequality is always fulfilled: $\xi^2 \geqslant \tau^2$. Here we are considering again cyclic evolution of our system. If T is the period of the cyclic evolution the following inequality is also always fulfilled:

$$\int_o^T \xi^2 \, \mathrm{d}t \geqslant \int_o^T \tau^2 \, \mathrm{d}t. \tag{26}$$

Using the Cauchy-Schwarz inequality for the second integral in equation (26) we arrive at

$$\int_o^T \tau^2 \, \mathrm{d}t \geqslant \frac{1}{T} \left(\int_o^T \tau \, \mathrm{d}t \right)^2 \tag{27}$$

and equation (26) yields

$$\int_o^T \left(\omega_0^2 + \frac{4|V_{ab}|^2}{\hbar^2} \right) \mathrm{d}t \geqslant \frac{1}{T} \left(\int_o^T \tau \, \mathrm{d}t \right)^2. \tag{28}$$

The integral on the RHS of equation (28) may be expressed in terms of Berry's phase, equation (16). Then inequality (28) becomes:

$$\int_o^T \xi^2 \, \mathrm{d}t \geqslant \frac{1}{T} \left(\gamma + \int_o^T \frac{E(t')}{\hbar} \mathrm{d}t' \right)^2. \tag{29}$$

Using $\xi^2 = 4\langle H^2 \rangle / \hbar^2 = 4E^2(t)/\hbar^2$ we get

$$\frac{\hbar^2}{T} \int_o^T E^2(t) \, \mathrm{d}t \geqslant \frac{1}{T^2} \left(\gamma + \int_o^T \frac{E(t')}{\hbar} \mathrm{d}t' \right)^2 \tag{30}$$

and finally we arrive at the following inequality for the Berry phase:

$$(\sqrt{\langle E^2(s) \rangle} - \langle E(t) \rangle) \geqslant \hbar\gamma \tag{31}$$

where now

$$\langle E^2(s)\rangle = \frac{1}{T}\int_o^T E^2(s)\,\mathrm{d}s$$

is the time average of E^2 along the curve and $\langle E(t)\rangle$ is the time average of E.

In summary, by mapping the Schrödinger equation for a two-level quantum system to a classical vector equation for $\boldsymbol{r}$ (equation (4)), we have analysed the problem using a space curve formalism. We conclude the following. For a cyclic evolution of the quantum state, the tip of $\boldsymbol{r}$ traces out a closed curve on the unit sphere S^2. It then becomes possible to identify *two* independent geometric quantities (phases) with this closed curve. The first is 2π minus the *area* of the surface enclosed by the closed curve (which in turn depends on the *torsion* of the space curve in R^3) given by $\phi_1 = \int \tau\,\mathrm{d}s$. In the case when the closed curve consists of a sum of arcs the phase ϕ_1 is given by the integral over the torsion plus a sum of the exterior angles at the vertices where the arcs meet. Thus in general Berry's phase is given by the area enclosed by the closed curve on S^2, but the proper way to get it is via the Gauss–Bonnet theorem, rather than Stokes' theorem. Only when the curve is smooth, do both approaches give the same result. The second quantity is the *length* of this curve (which depends on the *curvature* of the space curve in R^3) given by $\phi_2 = \int k\,\mathrm{d}s$. The geometric phase derived by Berry is just the former phase, when the dynamical phase is subtracted out. Geometrically, it measures the *deviation* of torsion of the space curve from a constant value. (This deviation can be seen to arise essentially from the time dependence of the Hamiltonian.) The latter phase ϕ_2 is related to $\int_o^T \mathrm{d}s[\langle H^2\rangle - \langle H\rangle^2]^{1/2}$, measures the curvature of the underlying space curve, and appears to arise from the basic time–energy uncertainty principle of quantum mechanics. We have also established the relationship between the geometrical phases in two-level systems and the Fermi–Walker parallel transport.

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