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Time evolution, cyclic solutions and geometric phases for general spin in an arbitrarily varying magnetic field

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Abstract
A neutral particle with general spin and magnetic moment moving in an arbitrarily varying magnetic field is studied. The time evolution operator for the Schrödinger equation can be obtained if one can find a unit vector that satisfies the equation obeyed by the mean of the spin operator. There exist at least $2s + 1$ cyclic solutions in any time interval. Some particular time interval may exist in which all solutions are cyclic. The nonadiabatic geometric phase for cyclic solutions generally contains extra terms in addition to the familiar one that is proportional to the solid angle subtended by the closed trace of the spin vector.

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Since the discovery of the geometric phase [1–9], particles with spin and magnetic moment moving in time-dependent magnetic fields have received much attention [10–23], though the subject is rather old and some discussions can be found in the textbook [24]. Neutral particles are of special interest since the problem is easier and the Schrödinger equation can be solved analytically in some special cases, say, uniform magnetic fields with a fixed direction or rotating ones. Thus the model is very suitable for the study of time evolution, cyclic solutions and geometric phases etc. However, some problems in this model are still not clear. First, the Schrödinger equation for general spin, or even for spin $1/2$, in an arbitrarily varying magnetic field seems impossible to solve analytically. Second, though the existence of cyclic solutions in a given time interval may be ensured by the existence of eigenvectors for the unitary time evolution operator, it does not seem clear how many there are in the general case.

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Third, for spin $1/2$ it is well known that any cyclic solution in an arbitrary magnetic field has a nonadiabatic geometric phase proportional to the solid angle subtended by the closed trace of the spin vector. For higher spin, however, this is true only for cyclic solutions with special initial conditions [15, 16, 22]. For more general cyclic solutions in a rotating magnetic field, we have shown that the nonadiabatic geometric phase contains an extra term in addition to the one proportional to the solid angle. The extra term vanishes automatically for spin $1/2$. For higher spin, however, it depends on the initial condition [22]. It is still not clear what is the relation between the nonadiabatic geometric phase and the solid angle for general cyclic solutions in an arbitrary magnetic field. In this paper, we are going to deal with these problems, and try to solve them to some extent. Besides the theoretical interest in itself and other applications [9, 19], this subject has been recently recognized to be of great interest in the physics of quantum computation [25, 26].

Consider a neutral particle with spin s ($s = 1/2, 1, 3/2, \ldots$) and magnetic moment $\boldsymbol{\mu} = \mu\mathbf{s}/s$, where $\mathbf{s}$ is the spin operator in units of $\hbar$, satisfying $[s_i, s_j] = \mathrm{i}\epsilon_{ijk}s_k$ (for spin $1/2$, $\mathbf{s} = \boldsymbol{\sigma}/2$ and $\boldsymbol{\mu} = \mu\boldsymbol{\sigma}$). In a uniform but time-dependent magnetic field $\mathbf{B}(t) = B(t)\mathbf{n}(t)$ where $\mathbf{n}(t)$ is a unit vector, it has the Hamiltonian $H(t) = -\boldsymbol{\mu}\cdot\mathbf{B}(t) = -\hbar\omega_B(t)\mathbf{s}\cdot\mathbf{n}(t)$, where $\omega_B(t) = \mu B(t)/s\hbar$, and the Schrödinger equation $\mathrm{i}\hbar\partial_t\psi(t) = H(t)\psi(t)$ takes the form

$$\partial_t\psi(t) = \mathrm{i}\omega_B(t)\mathbf{s}\cdot\mathbf{n}(t)\psi(t). \tag{1}$$

Define the spin vector as

$$\mathbf{v}(t) = (\psi(t), \mathbf{s}\psi(t)). \tag{2}$$

Using equation (1) it is easy to show that it obeys the equation

$$\dot{\mathbf{v}}(t) = -\omega_B(t)\mathbf{n}(t)\times\mathbf{v}(t). \tag{3}$$

We are not going to solve equation (1) in the general case since this seems impossible. However, we will show that the time evolution operator for equation (1) can be obtained without any chronological product if one can find one nontrivial (nonzero) solution, say, a unit vector $\mathbf{e}(t)$, to equation (3). This is of interest since the latter is easier and more cases can be solved [14]. Actually, equation (1) involves operators while equation (3) involves only c-numbers. On the other hand, if transformed to a matrix equation, equation (1) involves $2s+1$ complex variables, while equation (3) involves only three real ones (actually two since it is easy to see that $\mathbf{v}^2(t) = \mathbf{v}^2(0)$). Using the time evolution operator and equation (3), one can discuss cyclic solutions and geometric phases in a most general way. In particular, we will show that there exist at least $2s + 1$ cyclic solutions in any time interval. A general relation between the nonadiabatic geometric phase and the solid angle subtended by the closed trace of the spin vector will be established.

To begin, we take an arbitrary unit vector $\mathbf{e}_0$, and the eigenstate of $\mathbf{s}\cdot\mathbf{e}_0$ with eigenvalue m will be denoted by χ_m. We take the initial state of the system to be $\psi(0) = \chi_m$, that is

$$\mathbf{s}\cdot\mathbf{e}_0\psi(0) = m\psi(0) \qquad m = s, s-1, \ldots, -s. \tag{4}$$

Obviously $\mathbf{v}(0) = m\mathbf{e}_0$ in this initial state. Now we define a vector $\mathbf{e}(t)$ by equation (3) with the initial condition $\mathbf{e}_0$, that is

$$\dot{\mathbf{e}}(t) = -\omega_B(t)\mathbf{n}(t)\times\mathbf{e}(t) \tag{5}$$

with $\mathbf{e}(0) = \mathbf{e}_0$. We would assume that $\mathbf{B}(t)$ varies continuously, so that any solution $\mathbf{e}(t)$ is well behaved. As pointed out above, $\mathbf{e}^2(t) = \mathbf{e}_0^2$, so $\mathbf{e}(t)$ is a unit vector at any time. We have proved in [22] that

$$\mathbf{s}\cdot\mathbf{e}(t)\psi(t) = m\psi(t) \tag{6}$$

holds at all later times. To be self-contained, we repeat here the proof by induction.

By definition, equation (6) is valid at $t = 0$. We assume that it is valid at time t, what we need to do is to show that it is also true at time $t + \Delta t$ where Δt is an infinitesimal increment of time. In fact, using equations (1) and (5) we have

$$\psi(t + \Delta t) = \psi(t) + \mathrm{i}\omega_B(t)\mathbf{s}\cdot\mathbf{n}(t)\psi(t)\Delta t \tag{7a}$$

$$\mathbf{e}(t + \Delta t) = \mathbf{e}(t) - \omega_B(t)\mathbf{n}(t)\times\mathbf{e}(t)\Delta t. \tag{7b}$$

After some simple algebra, the conclusion is achieved.

Because $\mathbf{e}(t)$ is a unit vector, we can write in some rectangular coordinates

$$\mathbf{e}(t) = (\sin\theta(t)\cos\phi(t), \sin\theta(t)\sin\phi(t), \cos\theta(t)). \tag{8}$$

Using the formula [22, 27]

$$\mathrm{e}^{\mathrm{i}\xi\mathbf{s}\cdot\mathbf{b}}\mathbf{s}\,\mathrm{e}^{-\mathrm{i}\xi\mathbf{s}\cdot\mathbf{b}} = [\mathbf{s} - (\mathbf{s}\cdot\mathbf{b})\mathbf{b}]\cos\xi + (\mathbf{b}\times\mathbf{s})\sin\xi + (\mathbf{s}\cdot\mathbf{b})\mathbf{b} \tag{9}$$

where $\mathbf{b}$ is any unit vector, it is not difficult to show that

$$\mathbf{s}\cdot\mathbf{e}(t) = \mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}s_z\,\mathrm{e}^{\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)} \tag{10}$$

where

$$\mathbf{d}(t) = (-\sin\phi(t), \cos\phi(t), 0). \tag{11}$$

Therefore, the eigenstate of $\mathbf{s}\cdot\mathbf{e}(t)$ with eigenvalue m is

$$\psi(t) = \mathrm{e}^{\mathrm{i}\alpha_m(t)}\,\mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\chi_m^0 \tag{12}$$

where χ_m^0 is the eigenstate of s_z with eigenvalue m, and $\alpha_m(t)$ is a phase that cannot be determined by the eigenvalue equation. However, $\alpha_m(t)$ is not arbitrary. To satisfy the Schrödinger equation, it should be determined by the other variables $\theta(t)$ and $\phi(t)$. In fact, the above equation yields

$$(\psi(t), \psi(t + \Delta t)) = 1 + \mathrm{i}\dot{\alpha}_m(t)\Delta t + \left(\chi_m^0, \mathrm{e}^{\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\partial_t\,\mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\chi_m^0\right)\Delta t. \tag{13}$$

Using the formula [27]

$$\mathrm{e}^{-F(t)}\partial_t\,\mathrm{e}^{F(t)} = \int_0^1 \mathrm{e}^{-\lambda F(t)}\dot{F}(t)\,\mathrm{e}^{\lambda F(t)}\,\mathrm{d}\lambda \tag{14}$$

where $F(t)$ is any operator depending on t, and then using equation (9), we obtain

$$(\psi(t), \psi(t + \Delta t)) = 1 + \mathrm{i}\dot{\alpha}_m(t)\Delta t + \mathrm{i}m[1 - \cos\theta(t)]\dot{\phi}(t)\Delta t. \tag{15}$$

On the other hand, from equation (1) we have

$$(\psi(t), \psi(t + \Delta t)) = 1 + \mathrm{i}\omega_B(t)\mathbf{v}(t)\cdot\mathbf{n}(t)\Delta t. \tag{16}$$

Note that $\mathbf{v}(t)$ and $\mathbf{e}(t)$ satisfy the same equation, and $\mathbf{v}(0) = m\mathbf{e}_0$, we have $\mathbf{v}(t) = m\mathbf{e}(t)$. Comparing the two results above and taking this relation into account, we obtain

$$\dot{\alpha}_m(t) = -m[1 - \cos\theta(t)]\dot{\phi}(t) + m\omega_B(t)\mathbf{e}(t)\cdot\mathbf{n}(t). \tag{17}$$

Therefore

$$\alpha_m(t) - \alpha_m(0) = m\alpha(t) \tag{18}$$

where

$$\alpha(t) = -\int_0^t [1 - \cos\theta(t')]\dot{\phi}(t')\,\mathrm{d}t' + \int_0^t \omega_B(t')\,\mathbf{e}(t')\cdot\mathbf{n}(t')\,\mathrm{d}t'. \tag{19}$$

Substituting into equation (12) we obtain

$$\psi(t) = \mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\,\mathrm{e}^{\mathrm{i}\alpha(t)s_z}\,\mathrm{e}^{\mathrm{i}\theta(0)\mathbf{s}\cdot\mathbf{d}(0)}\psi(0). \tag{20}$$

We denote the time evolution operator as $U(t)$, defined by the equation $\psi(t) = U(t)\psi(0)$ with an arbitrary $\psi(0)$, then the above equation is equivalent to

$$U(t)\chi_m = \mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\, \mathrm{e}^{\mathrm{i}\alpha(t)s_z}\, \mathrm{e}^{\mathrm{i}\theta(0)\mathbf{s}\cdot\mathbf{d}(0)}\chi_m. \tag{21}$$

Now an arbitrary initial state $\psi(0)$ can always be expanded as

$$\psi(0) = \sum_m c_m \chi_m. \tag{22}$$

Applying $U(t)$ to both sides of this equation, using equation (21), and noting that the operators on the right-hand side of that equation are independent of m, we immediately realize that equation (20) is in fact valid for an arbitrary initial state. Thus we arrive at the result

$$U(t) = \mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\, \mathrm{e}^{\mathrm{i}\alpha(t)s_z}\, \mathrm{e}^{\mathrm{i}\theta(0)\mathbf{s}\cdot\mathbf{d}(0)}. \tag{23a}$$

Using equation (9), it can be recast in the form

$$U(t) = \mathrm{e}^{-\mathrm{i}\theta(t)\mathbf{s}\cdot\mathbf{d}(t)}\, \mathrm{e}^{\mathrm{i}\theta(0)\mathbf{s}\cdot\mathbf{d}(0)}\, \mathrm{e}^{\mathrm{i}\alpha(t)\mathbf{s}\cdot\mathbf{e}_0}. \tag{23b}$$

Equation (23*b*) is suitable for the general discussions below while equation (23*a*) may be more convenient for practical calculations.

Let us make some remarks on the result. First, we see that once a solution of equation (5) is found, the time evolution operator for equation (1) is available and it involves no chronological product. The result depends formally on $\mathbf{e}_0$, but $\mathbf{e}_0$ is merely an auxiliary object, hence the result must be essentially independent of it, though it might be difficult to prove this explicitly. In practical calculations, one should choose a solution $\mathbf{e}(t)$ that is as simple as possible such that $U(t)$ can be easily reduced to the simplest form. When this approach is used for the simple cases such as rotating magnetic fields or ones with a fixed direction, it indeed leads to the same results as those obtained previously. Second, the operator $U(t)$ depends not only on $\mathbf{e}(t)$, but also on the history of it. This is obvious from equation (19). Third, though $\phi(t)$ is indefinite when $\theta(t) = 0$ or π, the above result $U(t)$ is in fact well behaved everywhere. That it is well defined at $\theta(t) = 0$ is obvious. If $\theta(0) = 0$, there is no problem either. The case with $\theta(0) = \pi$ can be avoided since one can always choose a coordinate system such that $\theta(0) \neq \pi$. However, for a general evolution, the case with $\theta(t) = \pi$ at some instant cannot be avoided. Thus we must show that $U(t)$ is well behaved at $\theta(t) = \pi$. Suppose that $\theta(t_0) = \pi$, then we have $\phi\big(t_0^+\big) - \phi\big(t_0^-\big) = \pm\pi$, $\mathbf{d}\big(t_0^+\big) = -\mathbf{d}\big(t_0^-\big)$ and $\alpha\big(t_0^+\big) - \alpha\big(t_0^-\big) = \mp 2\pi$. With these relations it is not difficult to show that $U\big(t_0^+\big) = U\big(t_0^-\big)$. Since both $U\big(t_0^+\big)$ and $U\big(t_0^-\big)$ are well defined, we may define $U(t_0) = \lim_{t\to t_0} U(t)$. This makes $U(t)$ well defined and continuous at $t = t_0$. Fourth, by straightforward calculations it can be shown that $\partial_t U(t) = \mathrm{i}\omega_B(t)\mathbf{s}\cdot\mathbf{n}(t)U(t)$ and $U(0) = 1$, as expected.

Now we can go further to discuss cyclic solutions in any time interval $[0, \tau]$ where τ is an arbitrarily given time. These cyclic solutions are not necessarily cyclic in subsequent time intervals with the same length, say, $[\tau, 2\tau]$.

Since equation (5) is a linear differential equation, the general solution $\mathbf{e}(t)$ must depend on the initial vector $\mathbf{e}_0$ linearly. Thus it can be written in a matrix form

$$e_i(t) = E_{ij}(t)e_{0j} \tag{24}$$

where the matrix $E(t)$ is obviously real. If both $\mathbf{e}_1(t)$ and $\mathbf{e}_2(t)$ are solutions to equation (5), it is easy to show that $\mathbf{e}_1(t)\cdot\mathbf{e}_2(t) = \mathbf{e}_1(0)\cdot\mathbf{e}_2(0)$. Therefore, the matrix $E(t)$ is an orthogonal one, and its eigenvalues at any time t have the form $\{1, \sigma(t), \sigma^*(t)\}$, where $\sigma(t)$ is a complex number with $|\sigma(t)| = 1$, and $\sigma^*(t)$ its complex conjugate.

If $\sigma(\tau) \neq 1$, one eigenvector $\boldsymbol{\eta}(\tau)$ of the matrix $E(\tau)$ with eigenvalue 1 can be found, which satisfies $E_{ij}(\tau)\eta_j(\tau) = \eta_i(\tau)$. It can be taken as real and normalized. Now if we choose

$$\mathbf{e}_0 = \boldsymbol{\eta}(\tau) \tag{25}$$

we have $e_i(\tau) = E_{ij}(\tau)e_{0j} = E_{ij}(\tau)\eta_j(\tau) = \eta_i(\tau) = e_i(0)$, that is

$$\mathbf{e}(\tau) = \mathbf{e}_0. \tag{26}$$

This means that $\theta(\tau) = \theta(0)$ and $\mathbf{d}(\tau) = \mathbf{d}(0)$, and leads to

$$U(\tau) = \mathrm{e}^{\mathrm{i}\alpha(\tau)\mathbf{s}\cdot\mathbf{e}_0}. \tag{27}$$

Now it is clear that with the initial condition $\psi(0) = \chi_m$ ($m = s, s-1, \ldots, -s$), we have a cyclic solution in the time interval $[0, \tau]$. More specifically, $\psi(\tau) = \mathrm{e}^{\mathrm{i}\delta}\psi(0)$, where the total phase change is $\delta = m\alpha(\tau)$, mod2π, with $\alpha(\tau)$ given by

$$\alpha(\tau) = -\Omega_e + \int_0^\tau \omega_B(t)\,\mathbf{e}(t)\cdot\mathbf{n}(t)\,\mathrm{d}t \tag{28}$$

where

$$\Omega_e = \int_0^\tau [1 - \cos\theta(t)]\dot{\phi}(t)\,\mathrm{d}t$$

is the solid angle subtended by the closed trace of $\mathbf{e}(t)$. Note that $\mathbf{v}(t) = m\mathbf{e}(t)$, the dynamic phase $\beta = -\hbar^{-1}\int_0^\tau \langle H(t)\rangle\,\mathrm{d}t$ turns out to be

$$\beta = m\int_0^\tau \omega_B(t)\,\mathbf{e}(t)\cdot\mathbf{n}(t)\,\mathrm{d}t. \tag{29}$$

Therefore, the nonadiabatic geometric phase is

$$\gamma = \delta - \beta = -m\Omega_e \qquad \mathrm{mod}\ 2\pi. \tag{30}$$

Since $\Omega_e = \epsilon(m)\Omega_v$, mod$\,4\pi$, where Ω_v is the solid angle subtended by the closed trace of the spin vector, we have finally

$$\gamma = -|m|\Omega_v \qquad \mathrm{mod}\ 2\pi \tag{31}$$

in accord with the results previously obtained [15, 16, 22]. Thus we see that $2s+1$ cyclic solutions are available in any time interval $[0, \tau]$, and all phases can be expressed in terms of the unit vector $\mathbf{e}(t)$.

States with initial condition other than the above ones are, in general, not cyclic ones, even those in which $\mathbf{v}(0)$ points in the direction of $\mathbf{e}_0$ such that $\mathbf{v}(\tau) = \mathbf{v}(0)$. However, if $\alpha(\tau)/\pi$ happens to be a rational number other than an even integer (the case with $\alpha(\tau)/\pi$ an even integer will be discussed below), some other cyclic solutions may be available. To be more specific, let $\alpha(\tau) = p\pi/n$, where n is a natural number and p an integer. When $n = 1$, p is an odd number, and when $n > 1$ it is prime with p. If $s \geqslant n$, we have cyclic solutions with initial condition, say (no such solution exists for $s = 1/2$),

$$\psi(0) = \sum_{j=-N_1}^{N_2} c_j \chi_{m+2nj} \tag{32}$$

where N_1 and N_2 are nonnegative integers, and

$$m - 2nN_1 \geqslant -s \qquad m + 2nN_2 \leqslant s \qquad \sum_{j=-N_1}^{N_2} |c_j|^2 = 1.$$

In this initial state

$$\mathbf{v}(0) = v_0\mathbf{e}_0 \tag{33}$$

where $v_0 = \sum_{j=-N_1}^{N_2}(m + 2nj)|c_j|^2$ may be either positive or negative. It is easy to show that $\psi(\tau) = \mathrm{e}^{\mathrm{i}\delta}\psi(0)$, where $\delta = m\alpha(\tau), \bmod 2\pi$. Because of equation (33), we have $\mathbf{v}(t) = v_0\mathbf{e}(t)$, and the dynamic phase is

$$\beta = -\hbar^{-1}\int_0^\tau \langle H(t)\rangle\,\mathrm{d}t = \int_0^\tau \omega_B(t)\mathbf{v}(t)\cdot\mathbf{n}(t)\,\mathrm{d}t = v_0\int_0^\tau \omega_B(t)\,\mathbf{e}(t)\cdot\mathbf{n}(t)\,\mathrm{d}t.$$

Using equation (28), we have

$$\beta = v_0[\alpha(\tau) + \Omega_e]. \tag{34}$$

This holds regardless of the values of v_0 and $\alpha(\tau)$, as long as equation (33) is valid. Suppose that in the process from $t = 0$ to $t = \tau$, $\mathbf{e}(t)$ encircles the polar axis K times ($K > 0$ for anticlockwise traces and $K < 0$ for clockwise ones), then we have

$$\Omega_e + \Omega_{-e} = 4\pi K. \tag{35}$$

This leads to $v_0\Omega_e = |v_0|\Omega_v + 2\pi K(v_0 - |v_0|)$. The geometric phase turns out to be

$$\gamma = -|v_0|\Omega_v + 2\pi K(|v_0| - v_0) + (m - v_0)p\pi/n \qquad \bmod 2\pi. \tag{36}$$

In this case we see that the geometric phase contains extra terms in addition to the one proportional to Ω_v, unless the sum of these extra terms happens to be an integral multiple of 2π. Note that the above relation holds for the case $v_0 = 0$ as well, though Ω_v is not well defined in this case.

If it happens that $\alpha(\tau) = 2k\pi$, then $U(\tau) = \mathrm{e}^{\mathrm{i}2\pi ks}$ becomes a c-number and all solutions are cyclic in the time interval $[0, \tau]$. However, this is true only on the premise of (26). Thus $\alpha(\tau) = 2k\pi$ alone is not a sufficient condition for all solutions to be cyclic, but it is easy to show that it is a necessary one. A sufficient condition is $\sigma(\tau) = 1$.

Now if $\sigma(\tau) = 1$, $E(\tau)$ becomes a unit matrix. In this case any vector is its eigenvector with eigenvalue 1. Therefore equations (26) and (27) hold for any unit vector $\mathbf{e}_0$. In particular, we have

$$U(\tau) = \mathrm{e}^{\mathrm{i}\alpha_1(\tau)s_x} = \mathrm{e}^{\mathrm{i}\alpha_2(\tau)s_y} = \mathrm{e}^{\mathrm{i}\alpha_3(\tau)s_z} \tag{37}$$

where $\alpha_1(\tau)$ is given by equation (28) with $\mathbf{e}_0 = \mathbf{e}_x$ and similarly for $\alpha_2(\tau)$ and $\alpha_3(\tau)$. Since s_x, s_y and s_z are independent operators, the above equation cannot hold unless $\alpha_i(\tau) = 2\pi k_i$ where k_i are integers such that $U(\tau)$ becomes a c-number. In general, with an initial unit vector $\mathbf{e}_0$, we have

$$\alpha(\tau) = 2\pi k \tag{38}$$

and

$$U(\tau) = \mathrm{e}^{\mathrm{i}\alpha(\tau)\mathbf{s}\cdot\mathbf{e}_0} = \mathrm{e}^{\mathrm{i}2\pi ks}. \tag{39}$$

Let us see what is the dependence of $\alpha(\tau)$ or k on the direction of $\mathbf{e}_0$. Consider two initial unit vectors $\mathbf{e}_0$ and $\mathbf{e}'_0$, whose difference $\delta\mathbf{e}_0 = \mathbf{e}'_0 - \mathbf{e}_0$ is infinitesimal (then $\delta\mathbf{e}_0\cdot\mathbf{e}_0 = 0$). The difference in $\alpha(\tau)$ is, according to equation (28),

$$\delta\alpha(\tau) = \alpha'(\tau) - \alpha(\tau) = -\delta\Omega_e + \int_0^\tau \omega_B(t)\delta\,\mathbf{e}(t)\cdot\mathbf{n}(t)\,\mathrm{d}t. \tag{40}$$

Since $e_i(t) = E_{ij}(t)e_{0j}$, we have $\delta e_i(t) = E_{ij}(t)\delta e_{0j}$, and the second term in the above equation is consequently infinitesimal. Moreover, the trace of $\mathbf{e}'(t)$ is very close to that of $\mathbf{e}(t)$, thus the difference in the solid angles subtended by them is infinitesimal. Therefore, both

$\delta\alpha(\tau)$ and $\delta k = \delta\alpha(\tau)/2\pi$ are infinitesimal as well. Now that k can take only integer values, an obvious consequence is that $\delta\alpha(\tau) = 0$ and $k' = k$.

A subtle case has been overlooked in the above discussions, however. This happens when $\mathbf{e}(t)$ goes by the south pole ($\theta = \pi$) on one side and $\mathbf{e}'(t)$ goes by it on the other. In other words, the closed trace of $\mathbf{e}(t)$ as a whole goes across the south pole when $\mathbf{e}_0$ varies to $\mathbf{e}'_0$. In this case $\alpha(\tau)$ will be changed by an integral multiple of 4π and k by an even integer. One can of course remove this change by rotating the coordinate system such that the trace of $\mathbf{e}(t)$ does not go across the south pole. However, this can only be done locally, and globally it is impossible in general. In other words, one cannot choose a coordinate system such that k is the same for all $\mathbf{e}_0$, except for some simple cases, say, magnetic fields with a fixed direction. The above dependence of $\alpha(\tau)$ on $\mathbf{e}_0$ has no consequence on the time evolution operator as expected. This is easily seen from equation (39): when k changes by an even integer, $U(\tau)$ remains the same.

In the special case where k is the same for all $\mathbf{e}_0$, a geometric explanation of k is available. If we take the unit vector $\mathbf{e}'_0 = -\mathbf{e}_0$ as an initial condition to equation (5), then the solution is $\mathbf{e}'(t) = -\mathbf{e}(t)$. Since $\alpha(\tau)$ corresponding to $\mathbf{e}(t)$ and $\alpha'(\tau)$ corresponding to $\mathbf{e}'(t)$ are equal as assumed, we have, according to equation (28), $2\alpha(\tau) = -(\Omega_e + \Omega_{-e})$. As before, $\Omega_e + \Omega_{-e} = 4\pi K$, and $2\alpha(\tau) = 4\pi k$, so that $k = -K$. Here K is the winding number of $\mathbf{e}(t)$ around the polar axis. Unfortunately, the geometric meaning of k in the general case is still not clear.

Now that $U(\tau)$ is a c-number, all solutions to equation (1) become cyclic in the time interval $[0, \tau]$. The total phase change is $\delta = 2\pi ks = s\alpha(\tau)$, mod 2π. Since this phase is determined only up to an integral multiple of 2π, the dependence of $\alpha(\tau)$ or k on the initial vector $\mathbf{e}_0$ does not affect the result. For convenience we take the $\alpha(\tau)$ or k that is the same as that which appears below. If in the initial state $\mathbf{v}(0) \neq 0$, we take $\mathbf{e}_0 = \mathbf{v}(0)/v_0$ where $v_0 = |\mathbf{v}(0)| > 0$. Thus $\mathbf{v}(t) = v_0\mathbf{e}(t)$ and $\Omega_e = \Omega_v$. The dynamic phase is, as shown in equation (34), $\beta = v_0[\alpha(\tau) + \Omega_v]$. It should be remarked that both $\alpha(\tau)$ and Ω_v may be different by an integral multiple of 4π in different coordinate systems. However, β has a definite value, independent of the choice of coordinate systems, which can be easily seen from the expression $\beta = v_0 \int_0^\tau \omega_B(t)\, \mathbf{e}(t) \cdot \mathbf{n}(t)\, \mathrm{d}t$. The geometric phase turns out to be

$$\gamma = -v_0\Omega_v + (s - v_0)2\pi k \qquad \text{mod } 2\pi. \tag{41}$$

Here the first term is the familiar one, but an extra term appears. If $s = 1/2$, we have $v_0 = 1/2$ for any initial state, and the above result reduces to $\gamma = -\Omega_v/2$, a well-known result. For higher spin, however, the extra term depends on the initial state, as both v_0 and k depend on it. It vanishes (mod 2π of course) when $s - v_0$ is an integer, especially when the initial state is an eigenstate of $\mathbf{s} \cdot \mathbf{e}_0$ (it cannot be an eigenstate of $\mathbf{s} \cdot \mathbf{e}'_0$ with some other unit vector $\mathbf{e}'_0$ since $\mathbf{v}(0)$ points in the direction of $\mathbf{e}_0$), as expected. If in the initial state $\mathbf{v}(0) = 0$, we have $\mathbf{v}(t) = 0$ and thus $\beta = 0$. It is easy to see that equation (41) holds in this case as well, though Ω_v is not well defined.

The general result (41) has been confirmed by practical calculations in the case of a rotating magnetic field, where both γ and Ω_v can be calculated explicitly [22]. For a magnetic field with a fixed direction, it is easier to carry out similar calculations to verify this result.

In summary, we have shown that the time evolution operator for the Schrödinger equation (1) can be obtained if one nontrivial solution to equation (5) can be found. We proved that at least $2s + 1$ cyclic solutions of the Schrödinger equation exist in any time interval. These cyclic solutions can be worked out in principle if the general solution to equation (5) is known. There may exist some particular time interval in which all solutions are cyclic. The nonadiabatic geometric phase for cyclic solutions contains in general extra terms in addition to the familiar one that is proportional to the solid angle subtended by the trace of the spin vector. For spin $1/2$ there is no such extra term.

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