EVOLUTION LOOPS AND SPIN-1/2 SYSTEMS

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Abstract

The derivation of a new family of magnetic fields inducing exactly solvable spin evolutions is presented. The conditions for which these fields generate the evolution loops (dynamical processes for which any spin state evolves cyclically) are studied. Their natural connection with geometric phases and the corresponding calculation is also elaborated.

1. INTRODUCTION

In nonrelativistic quantum mechanics, the pure states of spin-1/2 systems are usually represented by two-component ket vectors \( |\psi\rangle \equiv (\psi_1, \psi_2) \), where \( \psi_1, \psi_2 \in \mathbb{C}^1 \) are the components of \( |\psi\rangle \) along the two orthogonal eigenstates \( |+\rangle \) and \(|-\rangle \) of \( S_z \) with eigenvalues \( \hbar/2 \) and \(-\hbar/2 \) respectively. If the spin is placed in a homogeneous time-dependent magnetic field \( B(t) \), then the Hamiltonian is described by \( H(t) \equiv -\mu B(t) \cdot S \), and the Schrödinger equation governing the evolution becomes explicitly time-dependent:

\[
 i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle = -\mu B(t) \cdot S |\psi(t)\rangle . \tag{1.1}
\]
In order to solve (1.1), usually it is rewritten in terms of the time-evolution operator $U(t)$, $U(t = 0) \equiv I$. The most elementary case arises when $[H(t), H(t')] = 0$ for all $t \neq t'$ [1]. In the case when $[H(t), H(t')] \neq 0$, however, to sum up the continuous Baker-Campbell-Hausdorff exponent becomes hard [2], and thus it is not easy to construct exact solutions to (1.1). Due to this, the approximate methods (see for example [3] and references quoted therein) or direct numerical techniques [4] are the standard tools applied in the general case. Is there any optional technique leading to exactly solvable situations? The answer seems to come of the so called inverse techniques, which take full advantage of the geometrical picture involved in the spin-1/2 description [5].

Suppose that somehow one knows the time evolution of the system, i.e., the state vector $|\psi(t)\rangle$ satisfying (1.1) for all $t$, but there is no information about the external field $B(t)$ driving the system. Can one find at least one field which could in principle be created and would dynamically induce that state? This is the essence of the dynamical manipulation problem whose main ideas were developed by Lamb [6] and followed later by other authors [7, 8, 9]. In the spin-1/2 case (1.1), this technique was successfully applied to generate exactly solvable situations [5]. It would be interesting to show that this is so using the standard direct approach.

The aim of this paper is to prove explicitly that given the family of magnetic fields derived in [5], they lead to exact solutions to equation (1.1). Moreover, we shall show that those magnetic fields can induce some special dynamical processes on the system such that the evolution operator becomes the identity (modulo phase) at some $t = \tau$, i.e., $U(\tau) = e^{i\phi}I$. Such kind of processes have been widely studied under the name of evolution loops (EL). It has been also proposed that the EL can be perturbed in order to induce any unitary operator as a result of the precession of the distorted loop [8]. This proposal has been successfully realized by inducing the squeezing inside of a modified Penning trap and by rigidly displacing the wavepacket in a magnetic chamber perturbed by homogeneous time-dependent electric fields [9]. Here, the EL will mean just closed orbits on $S^2$ (independent of the initial condition) which can be either periodic or aperiodic and whose corresponding geometric phases can be simply evaluated.

The paper is organized as follows. In Section 2 we briefly sketch the derivation of the magnetic fields of [5] with a discussion of their basic properties. In section 3 we directly solve (1.1) taking for $B(t)$ the analytic expressions of these fields. Then we shall establish the conditions on the fields in order to induce the EL on the system. To conclude, we will show that these EL give place to integrable expressions for the corresponding geometric phases.

### 2. THE INVERSE METHOD

For the set of pure states of spin-1/2 systems, a geometric picture is easily found by noticing that the inner product between any two ket vectors is invariant if both are multiplied by an arbitrary unimodular complex number $\lambda \in \mathbb{C}^1$, $|\lambda| = 1$. Hence, the space of physical states corresponds to the projective space $\mathbb{C}P(2)$ which, as is well known, is usually modeled by the Riemman sphere $S^2$ with each point of the surface...
representing a pure state of the spin-1/2 system.

Now, according to Eherenfest theorem the mean value of the operator $S \equiv S_x \mathbf{i} + S_y \mathbf{j} + S_z \mathbf{k}$, where $S_k \equiv (\hbar/2) \sigma_k$ and $[S_k, S_l] = i\hbar \epsilon_{klm} S_m$, evolves as:

$$\frac{d}{dt} \langle S \rangle = -\mu \mathbf{B}(t) \times \langle S \rangle = -\mathbf{b}(t) \times \langle S \rangle,$$

where $\mathbf{b}(t) \equiv \mu \mathbf{B}(t)$. The identification $\mathbf{n} \equiv (2/\hbar) \langle S \rangle$, $\mathbf{n} \cdot \mathbf{n} = 1$ shows that (2.1) is precisely the dynamical rule governing the evolution on $S^2$. In the direct approach the initial vector $\mathbf{n}(0)$ and the field $\mathbf{b}(t)$ are given, and one looks for the solution $\mathbf{n}(t)$ to (2.1). Here we assume that the spin state $\mathbf{n}(t)$ is given and rewrite (2.1) as $\dot{\mathbf{n}}(t) = M[\mathbf{n}(t)] \mathbf{b}(t)$. An element of arbitrariness arises by noticing that the matrix $M[\mathbf{n}(t)]$ is antisymmetric, and hence its determinant is equal to zero. Thus $M^{-1}[\mathbf{n}(t)]$ does not exist, which does not allow to determine uniquely $\mathbf{b}(t)$. Let us take the third component $b_3(t)$ also as given; henceforth the other two components become:

$$b_1(t) = [b_3(t) n_1(t) + \dot{n}_2(t)]/n_3(t), \quad b_2(t) = [b_3(t) n_2(t) - \dot{n}_1(t)]/n_3(t).$$

Notice that, departing from a given point $\mathbf{n}(0) \in S^2$, any other point $\mathbf{n}(t) \in S^2$ can be achieved by a set of successive infinitesimal rotations encoded in $R(t) \in SO(3)$, i.e., $\mathbf{n}(t) = R(t) \mathbf{n}(0)$. Therefore, the field $\mathbf{b}(t)$ given by (2.2) depends on the generic motion (a generalized rotation) and the initial condition. Thus, two paths with common $R(t)$ but different $\mathbf{n}(0)$ are induced by two different fields with the same $b_3(t)$. Would it be possible that trajectories sharing the same $R(t)$ determine a unique $\mathbf{b}(t)$? In order to find the answer, let us consider the case when $\mathbf{n}(t)$ rotates simultaneously around two fixed directions with variable angular velocities. By simplicity, one of these directions is fixed along $\mathbf{k}$ and the other one along a vector $\mathbf{e}_x$ on the $x-z$ plane at an angle $\chi$ from $\mathbf{k}$, $\mathbf{e}_x = \sin \chi \mathbf{i} + \cos \chi \mathbf{k}$. The rotation matrix is:

$$R(t) = R_3(\beta(t)) R_\chi(\alpha(t)) = R_3(\beta(t)) R_2^{-1}(-\chi) R_3(-\alpha(t)) R_2(-\chi),$$

where $R_2(\omega)$ and $R_3(\omega)$ are finite rotations by $\omega$ around $\mathbf{j}$ and $\mathbf{k}$ respectively and $\alpha(0) = \beta(0) = 0$. Using (2.2), one will find $\mathbf{b}(t)$ dependent of the initial condition; the field independent of $\mathbf{n}(0)$ arises after imposing the restriction $b_3(t) + \beta(t) = \alpha(t) \cos \chi$, and then:

$$\mathbf{b}(t) = \dot{\alpha}(t) \sin \chi [\cos \beta(t) \mathbf{i} + \sin \beta(t) \mathbf{j}] + [\dot{\alpha}(t) \cos \chi - \dot{\beta}(t)] \mathbf{k}.$$
space $\mathcal{H}$ correspond to antipodal points on the sphere $S^2$. By simplicity, let us choose $e_\pm \equiv (0, 0, \pm 1)$; then the probability transition is given by:

$$P_{+\rightarrow-}(t) = \frac{1 - n_3(t)}{2} = \sin^2 \chi \sin^2[\alpha(t)/2].$$  \hspace{1cm} (2.5)

As our treatment is exact, equation (2.5) is indeed a generalization of Rabi’s formula for any $t$ and arbitrary $\alpha(t)$. It reduces to the standard Rabi expression when we take $\alpha(t) = \alpha_0 t$ for small $t$ (see e.g., Rabi et al. [10] and Shirley [4]). Therefore, by choosing specific forms for $\alpha(t)$ and $\beta(t)$ in (2.4) one is led to obtain diverse particular cases of $b(t)$ [4], some of which could have been previously discussed.

Let us finish this section by remarking that the product $b_k(t)S_k$ of (1.1) satisfy $b_k(t)b_l(t')[S_k,S_l] = i\hbar \epsilon_{k\ell m}b_k(t)b_l(t')S_m$. Hence, for arbitrary functions $\alpha(t)$ and $\beta(t)$ (see the expressions of $b_k(t)$ in (2.4)), the Hamiltonians $H(t) = -\mathbf{b}(t) \cdot \mathbf{S}$ at different times do not commute, i.e., $[H(t), H(t')] \neq 0, t \neq t'$. Then, we have arrived at a family of exactly solvable Hamiltonians which, at first sight, should be solved by approximate or numerical methods when using the direct approach.

3. THE DIRECT METHOD

In this section we are going to solve (1.1) with the magnetic field (2.4) using ordinary quantum mechanical operator methods. The key point is that, by means of the commutation rules $[\sigma_k, \sigma_\ell] = 2i\epsilon_{k\ell m}\sigma_m$, and the expression

$$e^{-i\beta(t)\sigma_3/2} \sigma_1 e^{i\beta(t)\sigma_3/2} = \cos \beta(t) \sigma_1 + \sin \beta(t) \sigma_2,$$

the Hamiltonian $H(t) = -\mathbf{b}(t) \cdot \mathbf{S}$ can be rewritten as:

$$H(t) = e^{-i\beta(t)\sigma_3/2}[H_{\text{eff}}(t) + \hbar \dot{\beta}(t)\sigma_3/2] e^{i\beta(t)\sigma_3/2},$$  \hspace{1cm} (3.1)

where $H_{\text{eff}}(t)$ is defined by

$$-(2/\hbar) H_{\text{eff}}(t) \equiv \dot{\alpha}(t)(\sin \chi \sigma_1 + \cos \chi \sigma_3).$$  \hspace{1cm} (3.2)

Now, let us introduce a new reference frame which rotates with angular velocity $\dot{\beta}(t)$ around $\mathbf{k}$. Notice that rotating frames are very useful in magnetic resonance because when successfully used, the original problem can be mapped into a static one, which simplifies the physical analysis of the problem [11]. The key transformation in this case is given by $U(t) = e^{-i\beta(t)\sigma_3/2} W(t)$, where $W(t)$ is a new unitary operator satisfying the equation:

$$i\hbar \frac{dW(t)}{dt} = H_{\text{eff}}(t)W(t).$$  \hspace{1cm} (3.3)

It is clear now that $H_{\text{eff}}(t)$ is the Hamiltonian in the rotating frame, and thus $W(t)$ represents precisely the evolution operator in that frame. Notice that $H_{\text{eff}}(t)$ satisfies
\[ H_{\text{eff}}(t), H_{\text{eff}}(t') = 0; \text{ henceforth, the solution of (3.3) is given by just integrating } H_{\text{eff}}(t): \]

\[
W(t) = e^{-i\hbar \int_0^t H_{\text{eff}}(t') \, dt'} = e^{i\alpha(t)(\sin \chi \sigma_1 + \cos \chi \sigma_3)/2} \tag{3.4}
\]

\[
= \cos(\alpha(t)/2) + i(\sin \chi \sigma_1 + \cos \chi \sigma_3) \sin(\alpha(t)/2),
\]

where we have used again the algebraic properties of \( \sigma_k \). Notice that at \( t = 0 \) equation (3.4) reads \( W(0) = I \). Hence, initially the evolution operators \( U(t) \) and \( W(t) \) coincide. At arbitrary times \( t \neq 0 \), there will be a time-dependent factor operator \( \exp(-i\beta(t)\sigma_3/2) \) making the difference between the descriptions at the lab and at the rotating frames.

Let us construct now the generic expression for the ket vectors |\( \psi(0) \rangle \). First, the normalization condition gives \( |\psi_1(0)|^2 + |\psi_2(0)|^2 = 1 \). It suggest the following representation \( \psi_1(0) = \cos(\theta_0/2) \), \( \psi_2(0) = \sin(\theta_0/2) \). Now, the normalization remains invariant if we take \( \psi_1(0) = \exp(-i\phi_1) \cos(\theta_0/2) \), \( \psi_2(0) = \exp(i\phi_2) \sin(\theta_0/2) \). As mentioned at Section 2, the multiplication of \( |\psi(0) \rangle \) by a common phase factor \( \lambda = e^{i(\phi_1-\phi_2)/2} \) does not change the representative of the corresponding physical state. Hence, we can take:

\[
|\psi(0) \rangle \equiv \begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix} = \begin{pmatrix} \cos(\theta_0/2) e^{-i\phi_0/2} \\ \sin(\theta_0/2) e^{i\phi_0/2} \end{pmatrix}, \tag{3.5}
\]

with \( \phi_0 = \phi_1 + \phi_2 \). We are using the half angle convention whose utility will be apparent below. The solutions \( |\psi(t) \rangle \) to (1.1), with the magnetic field \( \mathbf{b}(t) \) given in (2.4), arise just as time displacements induced by the evolution operator \( U(t) \) acting on the initial vector (3.3):

\[
|\psi(t) \rangle = U(t) |\psi(0) \rangle = e^{-i\beta(t)/2} e^{i\alpha(t)(\sin \chi \sigma_1 + \cos \chi \sigma_3)/2} |\psi(0) \rangle, \tag{3.6}
\]

where we have used (3.4). Let us remark that the map \( |\psi(t) \rangle \rightarrow (2/\hbar) \langle \mathbf{S} |(t) = \mathbf{n}(t) \) reproduces the results derived in Section 2, \( i.e. \), the vector \( \mathbf{n}(t) \), connected with \( |\psi(t) \rangle \) in (3.6) by this map, is the result of two simultaneous rotations performed by the vector

\[
\mathbf{n}(0) \equiv (2/\hbar) \langle \psi(0) \mathbf{S} |\psi(0) \rangle = \langle \sin \theta_0 \cos \phi_0, \sin \theta_0 \sin \phi_0, \cos \theta_0 \rangle \tag{3.7}
\]

around the two directions and with the two angular velocities characteristic of the matrix (2.3). Notice that, from a geometrical point of view, the above map corresponds to the Hopf map [11, 12], which is useful in the description of monopole magnetic charges in the fibre-bundle formulation of electrodynamics [13], and provides an interesting geometrical interpretation of the Aharonov-Bohm effect [14, 12].

### 3.1. Evolution Loops and Geometric Phases

Let us formulate now the requirements which has to be satisfied in order to induce the evolution loops. With this aim, let us rewrite the evolution operator in (3.6) as:

\[
U(t) = \left[ \cos \left( \frac{\beta(t)}{2} \right) - i\sigma_3 \sin \left( \frac{\beta(t)}{2} \right) \right] \left[ \cos \left( \frac{\alpha(t)}{2} \right) + i(\sin \chi \sigma_1 + \cos \chi \sigma_3) \sin \left( \frac{\alpha(t)}{2} \right) \right].
\]

5
It is apparent that \( \alpha(\tau) = 2\ell \pi \) and \( \beta(\tau) = 2m \pi \), with \( \ell, m \in \mathbb{Z} \), produce \( U(\tau) = \cos(m \pi) \cos(\ell \pi) = \cos(m + \ell) \pi = (-1)^{m+\ell} I \). The loop conditions are thus:

\[
\alpha(\tau) = 2\ell \pi, \quad \beta(\tau) = 2m \pi, \quad m, \ell \in \mathbb{Z}; \quad \tau > 0. \tag{3.8}
\]

Notice that there is a strong loop condition in which the evolution operator becomes the identity \textit{sensu stricto}. In our spin-1/2 case this strong loop condition consists of the restriction (3.8) and the additional requirement \( m + \ell = 2k, \quad k \in \mathbb{Z} \). Here and throughout the paper we will use the relaxed loop condition (3.8).

The conditions (3.8) have been intuitively used in the case when the magnetic field (2.4) rotates with constant angular velocity, and then the vector \( \mathbf{n}(t) \) describes a \textit{hypocycloid} on \( S^2 \) \cite{16} (similar results can be found in \cite{10} and Zhang \textit{et. al.} \cite{14}). That case is recovered here by taking \( \alpha(t) = \alpha_0 t, \quad \beta(t) = \beta_0 t \) and by forcing the loop condition (3.8). Other selection of the functions \( \alpha(t) \) and \( \beta(t) \) allows us to generate deformed versions of such a case and generalized nontrivial cases (see the specific examples of \cite{16}).

The loop condition (3.8) and equation (3.6) give \( |\psi(\tau)\rangle = (-1)^{m+\ell} |\psi(0)\rangle \). As Aharonov and Anandan have shown, any cyclic quantum state has naturally associated a geometric phase \( \gamma \) characterizing somehow the projective Hilbert space curvature (see also the general geometric treatment introduced long ago by Mielnik \cite{17}). In the spin-1/2 case, it turns out that \( \gamma = -\Delta \Omega/2 \), where \( \Delta \Omega \) is the solid angle subtended by the oriented closed curve \( \mathbf{n}(t) \):

\[
\Delta \Omega = \int_0^\tau \frac{n_1 \dot{n}_2 - n_2 \dot{n}_1}{1 + n_3} dt. \tag{3.9}
\]

Let us remark that, although the general expression (3.9) has been recurrently studied and discussed in the literature \cite{15-20}, it is not always possible to perform the involved integrals (see \cite{13} and references quoted therein). Therefore, it is interesting to look for explicit expressions for \( \gamma \). For the magnetic fields (2.4) we have gotten the generic time-evolution (3.6), and this added to the loop conditions (3.8) allow one to simplify considerably the calculation:

\[
\gamma = [\ell - m + \cos(\theta_0 - \chi)(m \cos \chi - \ell)] \pi - \frac{1}{2} \sin \chi \sin(\theta_0 - \chi) \int_0^\tau \dot{\beta}(t) \cos \alpha(t) dt, \tag{3.10}
\]

where in (3.7) we have taken \( \phi_0 = 0 \). Notice the arising of the atypical integral term in (3.10). This formula generalizes the corresponding expression for the traditional rotating magnetic field with constant amplitude and angular velocity \cite{13}.

In order to illustrate the generality of our expression (3.10), let us consider some particular cases of (2.4). The first simple case arises by taking \( b_3(t) = b_0 \) in (2.4), and thus

\[
\gamma = [\ell - m + \cos(\theta_0 - \chi)(m \cos \chi - \ell)] \pi + \frac{b_0}{2} \sin \chi \sin(\theta_0 - \chi) \int_0^\tau \cos \alpha(t) dt. \tag{3.11}
\]
The remaining integral depends just on $\alpha(t)$ and $\tau$. Notice that it vanishes for the simplest time-dependent function $\alpha(t) = \alpha_0 t$ with the loop condition $\alpha_0 \tau = 2k\pi$, which is indeed the case discussed in [15] and [16]. The first nontrivial case of (3.11) arises after taking $\alpha(t)$ quadratic in $t$, for instance, $\alpha(t) = \alpha_0 t^2$, with $\alpha_0 = 5/2\pi$, $b_0 = 3$ and $\cos \chi = 4/5$. This choice immediately satisfies the loop condition $\alpha(t = 2\pi) = 10\pi$ and $\beta(2\pi) = 2\pi$, and leads to $\int_0^{2\pi} \cos \alpha(t) dt = \pi C(2\sqrt{5})/\sqrt{5} = 0.700896 \neq 0$, where $C(x)$ is the Fresnel cosine integral.

Up to now, we have seen that the loop conditions (3.8) guarantee the cyclic time evolution of any initial state (3.5) (or equivalently (3.7)). It should be clear now that without these restrictions on $\alpha(t)$ and $\beta(t)$, an arbitrary state not necessarily will be cyclic. An interesting question arises: are the loop conditions (3.8) the only way to ensure cyclic evolutions of the involved states? In order to get an answer let us consider two special initial states of the spin-$1/2$ system. Let us make in (3.7) $\phi_0 = 0$ and $\theta_0 = \chi$, and denote the resulting vector by $\mathbf{n}_+^\chi(0)$; now let us make $\phi_0 = \pi$ and $\theta_0 = \pi - \chi$, and denote the resulting vector by $\mathbf{n}_-^\chi(0)$. The corresponding evolution (3.11) leads to $\mathbf{n}_\chi^\pm(t)$, where $\mathbf{n}_\chi^\pm(0) \equiv \pm \mathbf{e}_\chi$. Hence, if the spin state points initially along $\pm \mathbf{e}_\chi$, the rotation around that vector has no effect on it, and we have $\mathbf{n}_\chi^\pm(t) = \mathbf{n}_\chi^\pm(0)$. The subtended solid angles are $\Delta\Omega^\pm = 2n\pi(1 \mp \cos \chi)$, and so the geometric phases become:

$$\gamma^\pm = -n\pi(1 \mp \cos \chi). \quad (3.12)$$

Let us notice that $n$ represents here the number of effective turns that $\mathbf{n}_\chi^\pm(t)$ performs around the $z$-axis, and that (3.12) is a general result valid for any $\chi$, with $\alpha(t)$ and $\beta(t)$ arbitrary. In particular, when $\chi = \pi/2$ (orthogonal rotations) we get $\gamma^\pm = -n\pi$; this phase is zero (modulo $2\pi$) when $n$ is even, while it is $\pi$ (modulo $2\pi$) when $n$ is odd. On the other hand, if the number of effective turns is zero ($\chi$ arbitrary) we get $\gamma^\pm = 0$. This is indeed the trivial case discussed by Zhang et.al. with $\alpha(t) = \alpha_0 t$, $\beta(t) = \beta_0 \sin(\omega t)$ and $\chi = \pi/2$ [4].

In conclusion, we have shown that the fields (2.4), derived by using inverse techniques in [3], produce exactly solvable spin-$1/2$ Hamiltonians which, at first sight, should be solved by approximate or numerical methods. We have shown also that the time evolution induced by these Hamiltonians can produce evolution loops, which simplify the calculation of the integrals involved in the formula for the corresponding geometric phases.

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