DYNAMICAL MANIPULATION FOR SPIN-1/2 SYSTEMS

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Abstract

By means of the inverse techniques we analyse the evolution of purely spin-1/2 systems in homogeneous magnetic fields as well as the generation of exact solutions. Some evolution loops, dynamical processes for which any state evolves cyclically, are presented, and their corresponding geometric phases are evaluated.

In the direct approach to quantum dynamics, the main goal is to look for solutions $|\psi(t)\rangle \in S(H)$ to Schrödinger’s equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle,$$

provided the Hamiltonian $H(t)$ and the initial state $|\psi(0)\rangle$ are given, where $S(H) = \{|\psi\rangle \in \mathcal{H} | \langle \psi | \psi \rangle = 1\}$, $\mathcal{H}$ is the system Hilbert space [1]. The same ideology is present in the study of the ‘shadow’ motion of $|\psi(t)\rangle$ on projective Hilbert space $\mathcal{P}$, where $p \in \mathcal{P}$ represents a possible physical state. $\mathcal{P}$ is obtained through a projective map $\pi : S(H) \to \mathcal{P}$, and all $|\psi\rangle = e^{i\phi}|\psi\rangle$, $\phi \in \mathbb{R}$ (a ray of $S(H)$), are carried into the same $p \equiv \pi(|\psi\rangle) \in \mathcal{P}$. In this way, $S(H)$ is seen as a fibre bundle with base space $\mathcal{P}$ and fibre $U(1)$ [2-3].

For spin-1/2 systems in magnetic fields $B(t)$, the spin part of the Hamiltonian reads:

$$H(t) = -\mu B(t) \cdot S = -\frac{\mu \hbar}{2} B(t) \cdot \sigma,$$

where $S$ is the spin operator, $\sigma$-components are Pauli matrices, $S(H)$ is a sphere $S^3$ embedded in $\mathbb{R}^4$, $\mathcal{P}$ is a sphere $S^2$ embedded in $\mathbb{R}^3$, and $\pi(|\psi\rangle) = n \equiv \langle \psi | \sigma | \psi \rangle \in S^2$. The evolution equation for $n(t)$ is obtained from (1-2):

$$\frac{dn(t)}{dt} = -\mu B(t) \times n(t).$$

Equations (1-3) are usually solved by means of numerical integration.

It is interesting also to look for exactly solvable models where the relevant information would be found in one analytic expression. However, it is hard to find them due to the complexity to sum up the ‘continuous’ Baker-Campbell-Haussdorf exponent arising when the evolution operator is a true exponential [4]. It is well known that exact solutions to (1-3) arise when: $i$) the field has a fixed direction, $B(t) = B(t)e_B$; $ii$) $B(t)$ rotates around a fixed direction with constant angular
velocity, and \(|B(t)| = |B(0)|\). In the first case, by solving the eigenproblem for the constant matrix \(\sigma_B = \sigma \cdot e_B\) and expanding then \(|\psi(0)|\) in that basis the general solution \(|\psi(t)|\) is found. For the rotating field, the key is the ‘transition to the rotating frame’ where it arises a constant effective Hamiltonian, which can be solved as previously [5]; by coming back to the initial frame the solution is gotten.

For general \(B(t)\) one can try again the transition to the rotating frame in which the direction of \(B(t)\) would be fixed though the effective Hamiltonian won’t be constant; thus, this problem generally cannot be solved (see, e.g., [6]). This is the motivation to look for alternative techniques to circumvent these difficulties.

In this work, a method to generate solutions for (1-3) is studied. We will use inverse techniques, i.e., we are going to look for the magnetic fields inducing a given \(n(t)\). This subject, introduced by Lamb [7], has been pursued with different names (inverse problem, control theory, dynamical manipulation, etc. [8-11]). We use dynamical manipulation because somehow it has implicit our ideals: to enforce systems to evolve as we want.

Suppose that a spin state \(n(t) \in S^2\) is given. The system of equations (3) for \(b(t) \equiv \mu B(t), M(n)b(t) = \dot{n}(t)\), is such that \(\det M(n) = 0\). Thus, one \(n(t)\) does not lead to a unique \(b(t)\). If \(b_3(t)\) is left arbitrary the other components are:

\[
\begin{align*}
b_1(t) &= [b_3(t)n_1(t) + \dot{n}_2(t)]/n_3(t), \\
b_2(t) &= [b_3(t)n_2(t) - \dot{n}_1(t)]/n_3(t).
\end{align*}
\]

As \(n(t) = R(t)n(0)\), \(b(t)\) depends of the generic motion (encoded in \(R(t) \in SO(3)\)) and the initial condition. This is unsatisfactory because two different fields would be needed to induce two trajectories with common \(R(t)\) but different \(n(0)\). However, in the direct approach a constant field leads unambiguously to \(R(t)\). Would it be possible that one \(R(t)\) determines a unique \(b(t)\) when the inverse techniques are applied? This is analysed below for specific forms of \(R(t)\).

Let us suppose first that \(n(t)\) rotates with angular velocity \(\hat{\delta}(t)\) around \(z\)-axis:

\[
n(t) = \sin \theta_0 \cos(\phi_0 + \delta(t)) i + \sin \theta_0 \sin(\phi_0 + \delta(t)) j + \cos \theta_0 k,
\]

where \(i, j, k\) are unit vectors along \(x, y, z\), \(\delta(0) = 0\). The fields inducing (5) become:

\[
b(t) = \tan \theta_0 [b_3(t) + \hat{\delta}(t)][\cos(\phi_0 + \delta(t))i + \sin(\phi_0 + \delta(t))j] + b_3(t)k.
\]

It is clear that \(b(t)\) depends on \(n(0)\); to avoid this we make \(b_3(t) = -\hat{\delta}(t)\). Hence:

\[
b(t) = -\hat{\delta}(t)k.
\]

If \(\hat{\delta}(t) = \omega\), we recover the standard solution for the spin in a constant field.

Let us analyze a more general case including the standard magnetic resonance model [5]. To this aim, suppose that \(n(t)\) rotates simultaneously around two fixed directions with variable angular velocities. Let us choose one of these directions along \(k\) and the other one along a vector \(e_\chi\) on \(x - z\) plane at an angle \(\chi\) from \(k\). 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 rotation by \(\omega\) around \(j\) and \(k\). If the \(R_2(\omega)\) and \(R_3(\omega)\) of [1] are used to evaluate \(n(t) = R(t)n(0)\) and this is substituted into (4) one arrives at:

\[
\begin{align*}b_1(t) &= [-\sqrt{1 - \chi^2}N_2(t) + \lambda N_3]^{-1}\{\sin \beta(t) \{\lambda \alpha(t) - [b_3(t) + \hat{\beta}(t)]\} N_1(t) \\
&+ \cos \beta(t) \{[b_3(t) + \hat{\beta}(t)][\lambda N_2(t) + \sqrt{1 - \chi^2}N_3] - \hat{\alpha}(t)N_2(t)\}\}. \end{align*}
\]
\[
\begin{align*}
  b_2(t) &= \left[-\sqrt{1-\lambda^2}N_2(t) + \lambda N_3\right]^{-1}\left\{-\cos \beta(t) \{\lambda \dot{\alpha}(t) - [b_2(t) + \dot{\beta}(t)]\} N_1(t) + \sin \beta(t) \{[b_3(t) + \dot{\beta}(t)]\} \right\} N_2(t) \\
  &= \sin \beta(t) \{b_3(t) + \dot{\beta}(t)\} N_2(t) + \left[\lambda N_2(t) + \sqrt{1-\lambda^2}N_3\right] - \dot{\alpha}(t) N_2(t) \\
  &+ \sin \beta(t) \{[b_3(t) + \dot{\beta}(t)]\} N_2(t) \left\{\lambda N_2(t) + \sqrt{1-\lambda^2}N_3\right\} - \dot{\alpha}(t) N_2(t) \\
\end{align*}
\]

where \(\lambda \equiv \cos \chi\), \(b_n(0) \equiv (x_n, y_n, z_n)\), and:

\[
\begin{align*}
  N_1(t) &= -\lambda \sin \alpha(t) x_0 + \cos \alpha(t) y_0 + \sqrt{1-\lambda^2} \sin \alpha(t) z_0, \\
  N_2(t) &= \lambda \cos \alpha(t) x_0 + \sin \alpha(t) y_0 - \sqrt{1-\lambda^2} \cos \alpha(t) z_0, \\
  N_3 &= \sqrt{1-\lambda^2} x_0 + \lambda z_0.
\end{align*}
\]

The field independent of \(n(0)\) appears if \(b_2(t) + \dot{\beta}(t) = \lambda \dot{\alpha}(t)\):

\[
\begin{align*}
  b(t) &= \dot{\alpha}(t) \sqrt{1-\lambda^2} \left[\cos \beta(t) \hat{i} + \sin \beta(t) \hat{j}\right] + \left[\lambda \dot{\alpha}(t) - \dot{\beta}(t)\right] \hat{k}.
\end{align*}
\]  

There is a consistency condition, firstly those of the introduction. On the one hand, our solution (8-12) provides in two ways the case when \(n(t)\) rotates around \(\hat{k}\): by taking \(\chi = 0, \lambda = 1, \) and \(b(t) = \left[\dot{\alpha}(t) - \dot{\beta}(t)\right] \hat{k}\); take now \(\alpha(t) = 0\), which leads to \(b(t) = -\dot{\beta}(t) \hat{k}\). On the other hand, if the rotations of \(n(t)\) are uniform \((\alpha(t) = \alpha_0 t, \beta(t) = \beta_0 t)\), we arrive at the traditional model used to examine the magnetic resonance [5]:

\[
\begin{align*}
  b(t) &= \alpha_0 \sqrt{1-\lambda^2} \left[\cos(\beta_0 t) \hat{i} + \sin(\beta_0 t) \hat{j}\right] + (\lambda \alpha_0 - \beta_0) \hat{k}.
\end{align*}
\]

The resonance explanation runs as follows. Suppose that the spin points along \(\hat{k}\), and it is placed in a constant field \(B_0 = B_0 \hat{k} = (\lambda \alpha_0 - \beta_0) \hat{k}/\mu\). Hence, at \(t = 0\) the spin state is an eigenstate of the ‘base’ Hamiltonian \(H_0 = -(\lambda \alpha_0 - \beta_0) S_z, |\psi(0)\rangle = |+\rangle\), where \(S_z|+\rangle = (\hbar/2)|+\rangle\). On \(S^2\) we have \(n(0) = (0, 0, 1)\). Now, at \(t = 0\) we superimpose to \(B_0\) the field \(B_0 = (\alpha_0/\mu) \sqrt{1-\lambda^2} \left[\cos(\beta_0 t) \hat{i} + \sin(\beta_0 t) \hat{j}\right]\). Thus, a formally ‘perturbative Hamiltonian’ \(W = -\alpha_0 \sqrt{1-\lambda^2} \left[\cos(\beta_0 t) S_x + \sin(\beta_0 t) S_y\right]\) is gotten (permitting however the exact treatment). It could induce at \(t > 0\) a transition to the orthogonal eigenstate \(|-\rangle\) of \(H_0\), which on \(S^2\) is represented by the vector \(n_- = (0, 0, -1)\). The probability transition is:

\[
\begin{align*}
  P_{+\rightarrow -}(t) &= |\langle-|\psi(t)\rangle|^2 = \left[1 - n_3(t)\right]/2 = (1 - \lambda^2) \left[1 - \cos(\alpha_0 t)\right]/2.
\end{align*}
\]

Notice that \(P_{+\rightarrow -}(t)\) is small if \(\chi\) is small or \(\chi \approx \pi\), i.e., when the rotations axes of \(n(t)\) are aligned. The greatest value arises for \(\chi = \pi/2\) (orthogonal rotation axes):

\[
\begin{align*}
  P_{+\rightarrow -}(t) &= \left[1 - \cos(\alpha_0 t)\right]/2.
\end{align*}
\]

At \(\tau_n = (2n + 1)\pi/\alpha_0\) this probability is 1, i.e., the state certainly will be \(|-\rangle\). This resonance is understood analysing the physics in the rotating frame: the rotating observer will see that (due to a non-inertial field produced by the rotation) the level spacing between \(|+\rangle\) and \(|-\rangle\) will decrease with respect to the inertial observer. For \(\lambda = 0\) this spacing will be zero because the non-inertial field cancels \(B_0\), and the transition in the eyes of the rotating observer certainly will be induced. In terms of \(S^2\) there is an equivalent explanation: in the rotating frame it is present a constant effective field \(b_{eff} = \alpha_0 \sqrt{1-\lambda^2} \hat{i} + \lambda \hat{k}\) around which \(n(0) = (0, 0, 1)\) starts to precess. But if \(n(0)\) has to be converted into \(n_- = (0, 0, -1), b_{eff}\) should have vanishing \(z\) component (\(\lambda = 0\).
In this case, \( \mathbf{n}(t) \) will simply precess around \( \mathbf{i} \) with angular velocity \( \alpha_0 \) (period \( T = 2\pi/\alpha_0 \)), and at \( \tau_n = T/2 + nT = (2n + 1)\pi/\alpha_0 \) the spin state will be \( \mathbf{n}(\tau_n) = n_\perp = (0,0,-1) \).

Let us remind the absence of essential restrictions on the real functions \( \alpha(t) \) and \( \beta(t) \) in (8-12). This makes possible to study a lot of other interesting examples, e.g., the case when the two rotations (8) would be induced by a field with a constant third component, \( b_3(t) = b_0 \), which leads to \( \alpha(t) = [b_0t + \beta(t)]/\lambda \). Hence:

\[
\mathbf{b}(t) = \frac{\sqrt{1 - \lambda^2}}{\lambda} [b_0 + \dot{\beta}(t)][\cos \beta(t)\mathbf{i} + \sin \beta(t)\mathbf{j}] + b_0 \mathbf{k}. \tag{16}
\]

This field has a \( x - y \) projection rotating around \( \mathbf{k} \) with angular velocity \( \dot{\beta}(t) \) and amplitude \( \sqrt{b_0^2 + (\dot{\beta}(t))^2} \). It represents a new resonance model analogous to (13-15) where the zero Hamiltonian is associated to \( b_0 \mathbf{k} \) and the ‘perturbation’ corresponds to the field component orthogonal to \( \mathbf{k} \). Let us suppose that \( \mathbf{n}(0) = (0,0,1) \) and evaluate the probability that at time \( t \) the system will be in \( \mathbf{n}_\perp = (0,0,-1) \):

\[
P_{+\rightarrow -}(t) = [1 - n_3(t)]/2 = (1 - \lambda^2) [1 - \cos \alpha(t)]/2. \tag{17}
\]

Once again, the greatest probability arises for \( \lambda = 0 \):

\[
P_{+\rightarrow -}(t) = [1 - \cos \alpha(t)]/2, \tag{18}
\]

and at \( \tau_n \) such that \( \alpha(\tau_n) = (2n + 1)\pi \), \( P_{+\rightarrow -}(\tau_n) = 1 \), i.e., the system certainly will make the transition from \( |+\rangle \) to \( |-\rangle \) due to the ‘perturbation’ \( W = -[b_1(t)S_1 + b_2(t)S_2] \).

It is interesting to study the possibility that any \( \mathbf{n}(t) \in S^2 \) would be cyclic, i.e., that the evolution operator \( U(t) (|\psi(t)\rangle = U(t)|\psi(0)\rangle) \) would be the identity (modulo phase) at some \( t = \tau \). These processes, named evolution loops (EL) [8,11-12], mimic the harmonic oscillator behaviour for systems with time-dependent Hamiltonians. The EL are useful to manipulate quantum systems, e.g., to induce the squeezing of the wavepacket inside of a Penning trap variant [11]. They are helpful as well to produce the rigid displacement of the wavepacket inside of a ‘magnetic chamber’, perturbed by homogeneous time-dependent electric fields [11]. Some arguments indicate that, by applying perturbations, they can be used to induce any unitary operator as the result of the precession of the distorted loop [8].

For 1/2 spin systems, the EL provide non-trivial cyclic evolutions for which the geometric phase can be explicitly evaluated [13] (see also [12] and below). In our example (8-12), the loop condition is immediately formulated: the EL exist if there is a time \( \tau \) for which \( \mathbf{n}(t) \) simultaneously performs \( n \) effective rotations around \( \mathbf{k} \) and \( l \) around \( \mathbf{e}_\chi \), \( \alpha(\tau) = 2l\pi, \beta(\tau) = 2n\pi, \tau > 0, n \in \mathbb{Z}, l \in \mathbb{Z} \). This condition translates into some equations for the field-spin parameters and \( \tau \). It was proposed in [13] for the rotating field (13), and an example of a hypocycloid performing 1 rotation around \( \mathbf{k} \) and 5 rotations around \( \mathbf{e}_\chi \) was shown [1]. Other authors obtained interesting results for the same physical system [14]. Here, we want to show ‘deformed versions’ of the figure in [13], for a field of form (16) with \( \beta(t) = a\lambda \sin(\alpha_0 t) + (\lambda\alpha_1 - b_0)t \). Our results are drawn in figure 1 for two essentially different EL with \( \tau = 2\pi, b_0 = 3, \lambda = 4/5 \). a) first we choose \( a = 0.7, \alpha_1 = \alpha_0 = 5 \); b) now we choose \( a = 1, \alpha_1 = 5 - 1/2\pi, \alpha_0 = 9/4 \).

\[1\] There it was explored also the EL for the spin in the oscillating field \( \mathbf{b}(t) = [b_0 + b \cos(\omega t)]\mathbf{k} \).
Fig.1. Spin trajectories illustrating two EL of period $\tau = 2\pi$ induced by (16) with $\beta(t) = a\lambda \sin(\alpha_0 t) + (\lambda \alpha_1 - b_0) t$, $b_0 = 3$, $\lambda = 4/5$, $n(0) = (\sqrt{3}/2, 0, 1/2)$, and: a) $a = 0.7$, $\alpha_1 = \alpha_0 = 5$; b) $a = 1$, $\alpha_1 = 5 - 1/2\pi$, $\alpha_0 = 9/4$.

It is easy to see that case $a$ provides a periodic loop: $U(\tau = 2\pi) = 1$ and $U(m\tau) = 1$, $m \in \mathbb{N}$. This happens because the Hamiltonian, for this choice of parameters, is periodic with period $\tau = 2\pi$. For case $b$ the parameters are such that $U(\tau = 2\pi) = 1$, but this EL is not periodic, $U(2\tau) \neq 1$, because the Hamiltonian is not. Different examples of this kind of aperiodic loop, when the field oscillates along $k$, are given elsewhere [13].

Now, if an EL is produced at $t = \tau$, then any state $n(t)$ becomes cyclic, $n(\tau) = n(0)$. Thus, it makes sense to evaluate the corresponding geometric phases, which characterize some global curvature effects of $P = S^2$ [3,12-15]. For spin-1/2 systems the geometric phase turns out to be minus one half of the solid angle $\Delta \Omega$ subtended by the oriented closed curve $n(t) \in S^2$ [13], where:

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

(19)

For our case (8-12), this formula can be evaluated using the loop condition:

$$\Delta \Omega = 2n\pi[1 - \cos \chi \cos(\theta - \chi)] - 2l\pi[1 - \cos(\theta - \chi)] + \sin \chi \sin(\theta - \chi) \int_0^\tau \dot{\beta} \cos \alpha dt,$$

(20)

where we have taken $n(0) = (\sin \theta, 0, \cos \theta)$. This expression is equal to the corresponding one for the rotating field (13) but for the last term [13], which depends on the explicit form of both $\alpha(t)$ and $\beta(t)$. If $b_3(t) = b_0$ (the case discussed at (16-18)) we get:

$$\Delta \Omega = 2n\pi[1 - \cos \chi \cos(\theta - \chi)] - 2l\pi[1 - \cos(\theta - \chi)] - b_0 \sin \chi \sin(\theta - \chi) \int_0^\tau \cos \alpha dt,$$

(21)

and the integral depends just of $\alpha(t)$. Notice that this integral vanishes if $\alpha(t) = \alpha_0 t$ and $\alpha_0 \tau = 2l\pi$, which leads once again to the known result for the EL in the standard case (13). The simplest
situation leading to EL for which the integral in (21) does not vanish arises when \( \alpha(t) \) is quadratic in \( t \). With this choice, that term will involve Fresnel integrals\(^2\).

In conclusion, the manipulation techniques are appropriate to generate solvable examples for the spin evolution in homogeneous magnetic fields. When these techniques are applied to produce the EL, it arises cyclic evolutions for which the geometric phases can be explicitly evaluated. We hope that our treatment has shed as well some light on the functioning of the resonance mechanism.

The authors acknowledge the support of CONACYT (México).

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\(^2\)Take \( \alpha(t) = \alpha_0 t^2 \) with \( \alpha_0 = 5 (2\pi)^{-1} \), \( b_0 = 3, \lambda = 4/5 \), to produce an EL such that \( \alpha(\tau = 2\pi) = 10\pi \), \( \beta(2\pi) = 2\pi \). Moreover, \( \int_0^{2\pi} \cos \alpha(t) dt \equiv \pi (5)^{-1/2} C(2\sqrt{5}) = 0.700896 \neq 0 \).