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The Berry Phase and the Nuclear Magnetic Resonance

Jose M. Cerveró[1]

[1] *Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain*
cervero@usal.es

Abstract: *The celebrated Berry Phase is fully extracted from the analysis of the operator formalism without using classical equations but rather the algebra of the unitary operators acting on time dependent Hamiltonians. To illustrate the powerfulness of the method I use as an example in the rest of the paper the physical case of the Magnetic Nuclear Resonance. This formalism of dealing with the study of dynamical and geometric phases is used to find the adiabatic limit in a simple manner as well as to calculate numerical values for the Berry Phase. Two remarks in classical Wilberforce Pendulum and Coupled Harmonic Oscillators are made both at the beginning and at the end.*

Keywords: Berry Phases, Quantum Mechanics, Unitary Operators Algebra

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I. MAGNETIC SPIN RESONANCE: AN OVERVIEW

In a recent paper published in the the "Revista Espaola de Fisica" [1], a practical example of the classical Wilberforce Pendulum has been developped [2]. My purpose on this paper is to fully study1 the analogous quantum system in the framework of Quantum Mechanics. Here the vertical oscillator is now replaced for a stationary magnet B_0 and the vertical oscillator by a time dependent magnet of magnitude B_1 oscillating with a frequency given by the Larmor frequency. The magnet changes $N \Leftrightarrow S$ according with a rf of magnitude ω. Now we send to this double magnetic device a non polarized spin beam of magnetic moment $\mu_S = \mu_{\mathbf{B}} = \frac{|e|\hbar}{2mc}$ where $\mid e \mid$ is the absolute value of the electric charge and m is the bare mass of the electron. Now in the paper we shall use the time evolution picture developed by Heisenberg. In this formalism one uses a time dependent unitary operator $U(t)$ such that converts an stationary system in a time dependent one using judiciously the form of $U(t)$ as we shall see below.

Let the stationary Hamiltonian H_0 be:

$$\hat{H}_0 = \frac{\hbar\omega_0}{2}\sigma_3 \tag{1}$$

pointing in the z^+. After the disposition of the initial state we shall introduce the oscillating magnet in the $\{x, y\}$-plane in the form:

$$\begin{aligned}\hat{H}(t) &= \frac{\hbar\omega_0}{2}\sigma_3 + \frac{\hbar\omega_1}{2}[\,\sigma_1\cos\omega t + \sigma_2\sin\omega t] = \\ &= \frac{\hbar}{2}[\,\omega_1\sigma_1\cos\omega t + \omega_1\sigma_2\sin\omega t + \omega_0\sigma_3]\end{aligned} \tag{2}$$

where μ_B is the *Bohr magneton* and $\{\omega_0; \omega_1\}$ the two Larmor frequencies of the two magnetic fields: .

$$\hbar\omega_0 = \mu_S B_0, \qquad \hbar\omega_1 = \mu_S B_1 \tag{3}$$

There exist always a time dependent operator that interchanges the two Hamiltonians (Heisenberg, 1926) $\hat{H}_0$ in $\hat{H}(t)$:

$$\hat{H}(t) = U(t)\hat{H}_0 U^\dagger(t) + i\hbar\left[\partial_t U(t)\right] U^\dagger(t) \tag{4}$$

The explicit form of the operator is:

$$\begin{aligned}U(t) = \quad & \exp\left\{\frac{-i\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1 + \cos\theta\sigma_3\right]\right\} \\ & \exp\left\{i\frac{\omega_0 t}{2}\sigma_3\right\}\end{aligned} \tag{5}$$

where:

$$\sin^2\theta = \frac{\omega_1^2}{(\omega_0-\omega)^2+\omega_1^2}; \quad \cos^2\theta = \frac{(\omega_0-\omega)^2}{(\omega_0-\omega)^2+\omega_1^2} \tag{6}$$

and Ω is given by:

$$\Omega = \left[(\omega_0-\omega)^2+\omega_1^2\right]^{\frac{1}{2}} \tag{7}$$

After this previous calculation, the evolving state can now be written as:

$$\mid \mathbf{\Psi}(t)\rangle = U(t) \mid \mathbf{\Psi}_0(t)\rangle \tag{8}$$

and $\mid \mathbf{\Psi}_0(t)\rangle$ is the **Exact solution of the initial evolved state** from $\hat{H}_0$ to $\hat{H}(t)$ acquiring in the journey a trivial dynamical phase:

$$\mid \mathbf{\Psi}_0(t)\rangle = \exp\left\{-i\frac{\omega_0 t}{2}\sigma_3\right\}\begin{pmatrix}1\\0\end{pmatrix} = \exp\left\{-i\frac{\omega_0 t}{2}\right\}\begin{pmatrix}0\\1\end{pmatrix} \tag{9}$$

Looking now to the form of $U(t)$ given previously in (5), we obtain:

$$\begin{aligned}&\mid \mathbf{\Psi}(t)\rangle = U(t) \mid \mathbf{\Psi}_0(t)\rangle = \\ &= \exp\left\{-i\frac{\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1+\cos\theta\sigma_3\right]\right\}\begin{pmatrix}1\\0\end{pmatrix}\end{aligned} \tag{10}$$

After simple manipulations with Pauli matrices we finally are lead to:

$$\mid \mathbf{\Psi}(t)\rangle = \exp\left\{-i\frac{\omega t}{2}\right\}\left[\cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}1\\0\end{pmatrix}$$
$$-i\exp\left\{i\frac{\omega t}{2}\right\}\left[\sin\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}0\\1\end{pmatrix} \qquad (11)$$

This is the **general solution of the state after some arbitrary time**. The form of this general solution will be of primary importance in the next section for calculating the **Dynamical and Topological** phases that the state acquires in this journey.

The time dependent magnetic device of our experiment can be put in a mathematical form as:

$$B_1(t) = B_1\cos\omega t \qquad (12)$$
$$B_2(t) = B_1\sin\omega t \qquad (13)$$
$$B_3(t) = B_0 \qquad (14)$$

where γ is proportional to the *Bohr magnetic unit above defined*. More precisely:

$$\gamma = \frac{\mid e \mid \hbar}{mc}; \qquad \frac{\mid e \mid B_0}{mc} = \omega_0; \qquad \frac{\mid e \mid B_1}{mc} = \omega_1; \quad (15)$$

where $\mid e \mid$ is the **modulus of the electric charge** . Then:

$$\hat{H}(t) = \frac{\hbar}{2}\left[\omega_1\sigma_1\cos\omega t + \omega_1\sigma_2\sin\omega t + \omega_0\sigma_3\right] \qquad (16)$$

The Hamiltonian just written above is in the heart of the descriptions of all quantum magnetic resonance phoenomena: i.e Atomic (Rabi, 1931) an/or nuclear (Purcell, 1946).

Let us now remember how one performs a measurement at the quantum level. This is done through the **Density Matrix Formalism**. The result of the measurement is delivered by finding the trace of the Density Matrix operator: $Tr(\hat{A}\rho)$. In our case:

$$\langle\sigma_1(t)\rangle = Tr(\sigma_1\rho(t));\ \langle\sigma_2(t)\rangle = Tr(\sigma_2\rho(t));$$
$$\langle\sigma_3(t)\rangle = Tr(\sigma_3\rho(t)); \qquad (17)$$

Given the zero trace of the Pauli matrices one easily finds:

$$\langle\sigma_1(t)\rangle = \mathbf{n}_1(t);\ \langle\sigma_2(t)\rangle = \mathbf{n}_2(t);\ \langle\sigma_3(t)\rangle = \mathbf{n}_3(t) \quad (18)$$

The following result is found from this procedure without too much effort:

$$\frac{d}{dt}\mathbf{n}_j(t)\langle\frac{d\sigma_j(t)}{dt}\rangle = Tr\left(\sigma_j\frac{d\rho(t)}{dt}\right) \qquad (19)$$
$$= \frac{1}{2i}Tr\left(\sigma_j\left[\omega_1\sigma_1\cos\omega t + \omega_1\sigma_2\sin\omega t + \omega_0\sigma_3, \rho(t)\right]\right)$$

One has to made use in the last step of the *Von Neumann Equation* and the specific form of our Hamiltonian. Now we use the mathematical relationship:

$$[\mathbf{\Pi}(\mathbf{n}), \mathbf{\Pi}(\mathbf{m})] = \frac{i}{2}\epsilon^{ikl}\sigma_i\mathbf{n}_k\mathbf{m}_l \qquad (20)$$

which leads to the following system of time dependent first order differential equations for the **n's**:

$$\frac{d}{dt}\mathbf{n}_1(t) = -\left[\omega_0\mathbf{n}_2(t) - \omega_1\mathbf{n}_3(t)\sin\omega t\right] \qquad (21)$$
$$\frac{d}{dt}\mathbf{n}_2(t) = +\left[\omega_0\mathbf{n}_1(t) - \omega_1\mathbf{n}_3(t)\cos\omega t\right] \qquad (22)$$
$$\frac{d}{dt}\mathbf{n}_3(t) = \omega_1\left[\mathbf{n}_2(t)\cos\omega t - \mathbf{n}_1(t)\sin\omega t\right] \qquad (23)$$

The system can be exactly solved. Obviously it **looks quite similar to the one describing the classical precession of a vector around a moving axis**. However the parallelism stops here as we are dealing with a quantum mechanical description of the system:

$$\mathbf{n}_1(t) = \left[(\sin\Omega t)\sin\omega t + (1-\cos\Omega t)\cos\omega t\cos\theta\right]\sin\theta$$
$$\mathbf{n}_2(t) = \left[(1-\cos\Omega t)\sin\omega t\cos\theta - (\sin\Omega t)\cos\omega t\right]\sin\theta$$
$$\mathbf{n}_3(t) = \cos^2\theta + \sin^2\theta\cos\Omega t = 1 - \sin^2\theta(1-\cos\Omega t)$$
$$(24)$$

One can easily check that:

$$\mathbf{n}_1^2(t) + \mathbf{n}_2^2(t) + \mathbf{n}_3^2(t) = 1 \qquad (25)$$

Therefore we are dealing with a **pure state**. Any pure state must be written as:

$$\rho(t) = \mid \mathbf{\Psi}(t)\rangle\langle\mathbf{\Psi}(t)\mid \qquad (26)$$

where of course $\mid \mathbf{\Psi}(t)\rangle$ takes the well known form given by (11):

$$\mid \mathbf{\Psi}(t)\rangle = \exp\left\{-i\frac{\omega t}{2}\right\}\left[\cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}1\\0\end{pmatrix}$$
$$-i\exp\left\{i\frac{\omega t}{2}\right\}\left[\sin\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}0\\1\end{pmatrix} \qquad (27)$$

Consistence claims for an equivalence between the **Heisenberg and Density Matrix** formalisms. In order to check that we operate with the explicit form of $\rho(t)$ using the expression given by $\mid \mathbf{\Psi}(t)\rangle\langle\mathbf{\Psi}(t)\mid$ one obtains:

$$\rho(t) = \mid \mathbf{\Psi}(t)\rangle\langle\mathbf{\Psi}(t)\mid =$$
$$= \frac{1}{2}\begin{pmatrix}1+\mathbf{n}_3(t), & \mathbf{n}_1(t) - i\mathbf{n}_2(t)\\ \mathbf{n}_1(t) + i\mathbf{n}_2(t), & 1-\mathbf{n}_3(t)\end{pmatrix} =$$
$$= \frac{1}{2}\left(\mathbf{I}_2 + \sum_{j=1}^{3}\mathbf{n}_j(t)\sigma^j\right) \qquad (28)$$

It is easy to convince yourself that the $\mathbf{n}_1(t)$, $\mathbf{n}_2(t)$ y $\mathbf{n}_3(t)$ take the same form that the ones written above.

II. DYNAMICAL AND GEOMETRIC PHASES

In the course of the journey undergone by the state described for the **Density Matrix** analyzed above, the state generates some phases [3], [4] that we wish to analyze in the present Section. As the state $\mid \mathbf{\Psi}(t)\rangle$ is also a solution of the Schrödinger equation:

$$\hat{H}(t) \mid \mathbf{\Psi}(t)\rangle = i\hbar\frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle \tag{29}$$

it is trivial to see that:

$$-\frac{1}{\hbar}\langle\mathbf{\Psi}(t) \mid \hat{H}(t) \mid \mathbf{\Psi}(t)\rangle + i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = 0 \tag{30}$$

The general form of the state $\mid \mathbf{\Psi}_0(t)\rangle$ is again:

$$\begin{aligned} \mid \mathbf{\Psi}_0(t)\rangle &= \exp\left\{-i\frac{\omega_0 t}{2}\sigma_3\right\}\begin{pmatrix} a \\ b \end{pmatrix} \\ &= a\exp\left\{-i\frac{\omega_0 t}{2}\right\}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\exp\left\{i\frac{\omega_0 t}{2}\right\}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{31}$$

where a y b are complex numbers $\mid a \mid^2 + \mid b \mid^2 = 1$. **Without loss of generality we set $a = 1$ y $b = 0$.** Taking into account the explicit form of $\mid \mathbf{\Psi}_0(t)\rangle$ and $U(t)$ we obtain:

$$\begin{aligned} &\mid \mathbf{\Psi}(t)\rangle = U(t) \mid \mathbf{\Psi}_0(t)\rangle = \\ &= \exp\left\{-i\frac{\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1 + \cos\theta\sigma_3\right]\right\}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \exp\left\{-i\frac{\omega t}{2}\right\}\left[\cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \\ &\quad -i\exp\left\{i\frac{\omega t}{2}\right\}\left[\sin\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{32}$$

One obtains the following results for the two matrix elements:

$$\begin{aligned} &\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle \\ &= \frac{\hbar}{2}\left\{\omega_1\sin\theta\cos\theta - \omega_0\sin^2\theta\right\}\left[1 - \cos\Omega t\right] + \frac{\hbar\omega_0}{2} \\ &i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle \\ &\quad = \frac{\omega_0}{2} - \frac{\omega}{2}\sin^2\theta\left[1 - \cos\Omega t\right] \end{aligned} \tag{33}$$

The sum of these two contributions is:

$$\begin{aligned} &-\frac{1}{\hbar}\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle + \\ &+i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = \\ &= \frac{1}{2}\left[1 - \cos\Omega t\right]\left[-\omega_1\sin\theta\cos\theta + (\omega_0 - \omega)\sin^2\theta\right] \end{aligned} \tag{34}$$

and with the values of ω_1 y $\omega_0 - \omega$ as functions (6-7) of $\sin\theta$ y $\cos\theta$, one finally obtains:

$$\begin{aligned} &-\frac{1}{\hbar}\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle + \\ &+i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = \\ &= \frac{\Omega}{2}\left[1 - \cos\Omega t\right]\left[-\sin^2\theta\cos\theta + \cos\theta\sin^2\theta\right] = 0 \end{aligned} \tag{35}$$

Initially it was establised in (4) that $\hat{H}_0$ transforms under the unitary operator $U(t)$ as:

$$\hat{H}(t) = U(t)\hat{H}_0U^\dagger(t) + i\hbar\left[\partial_t U(t)\right]U^\dagger(t) \tag{36}$$

Let us now take the inverse operation:

$$U^\dagger(t)\hat{H}(t)U(t) - i\hbar U^\dagger(t)\left[\partial_t U(t)\right] = \hat{H}_0 \tag{37}$$

and as we already know that $U(t)$ has the explicit form (5):

$$\begin{aligned} U(t) = \exp\left\{-i\frac{\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1 + \cos\theta\sigma_3\right]\right\} \\ \exp\left\{i\frac{\omega_0 t}{2}\sigma_3\right\} \end{aligned} \tag{38}$$

One can ask he/her-self whether we shall obtain the initial form of $\hat{H}_0$ **just by using the form of the initial state $\mid \mathbf{\Psi}_0(t)\rangle$ and the form of the unitary operators** by performing the inverse operation.

In terms of the matrix elements we obtain:

$$U^\dagger(t)\hat{H}(t)U(t) - i\hbar U^\dagger(t)\left[\partial_t U(t)\right] = \frac{\hbar\omega_0}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{39}$$

This calculation is easy but tedious. We collect the main formulae used to tackle this lenghty operation. Firstly we define:

$$C_\pm = \cos\frac{\Omega t}{2} \pm i\cos\theta\sin\frac{\Omega t}{2} \tag{40}$$

$$C_0 = -i\sin\theta\sin\frac{\Omega t}{2} \tag{41}$$

$$\delta_\pm = (\omega_0 \pm \omega) \tag{42}$$

The following identities hold:

$$C_+C_- - C_0^2 = C_+C_- + C_0C_0^* = 1 \tag{43}$$

$$\begin{aligned} C_+C_- + C_0^2 = C_+C_- - C_0C_0^* = \\ = \cos^2\theta + \sin^2\theta\cos\Omega t \end{aligned} \tag{44}$$

Other useful identities are:

$$\begin{aligned} C_+\dot{C}_- &= -\frac{\Omega}{4}\left[\sin^2\theta\sin\Omega t + 2i\cos\theta\right] \\ C_-\dot{C}_+ &= -\frac{\Omega}{4}\left[\sin^2\theta\sin\Omega t - 2i\cos\theta\right] \\ C_0\dot{C}_+ &= -\frac{i\Omega\sin\theta}{4}\left[i\cos\theta\sin\Omega t - (1 - \cos\Omega t)\right] \\ C_+\dot{C}_0 &= -\frac{i\Omega\sin\theta}{4}\left[i\cos\theta\sin\Omega t + (1 + \cos\Omega t)\right] \\ C_0\dot{C}_- &= +\frac{i\Omega\sin\theta}{4}\left[i\cos\theta\sin\Omega t + (1 - \cos\Omega t)\right] \\ C_-\dot{C}_0 &= +\frac{i\Omega\sin\theta}{4}\left[i\cos\theta\sin\Omega t - (1 + \cos\Omega t)\right] \\ C_0\dot{C}_0 &= -\frac{\Omega}{4}\sin^2\theta\sin\Omega t \end{aligned} \tag{45}$$

also the following cuadratic identities are very useful for the calculation:

$$C_+^2 - C_0^2 = \sin^2\theta + \cos^2\theta\cos\Omega t + i\cos\theta\sin\Omega t \quad (46)$$
$$C_-^2 - C_0^2 = \sin^2\theta + \cos^2\theta\cos\Omega t - i\cos\theta\sin\Omega t \quad (47)$$

Finally the operator $U(t)$ which we have written until now in the form:

$$U(t) = \exp\left\{-i\frac{\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1 + \cos\theta\sigma_3\right]\right\} \exp\left\{i\frac{\omega_0 t}{2}\sigma_3\right\} \quad (48)$$

it shall be written henceforth in the form:

$$U(t) = \begin{pmatrix} \exp\left\{i\frac{\delta_-}{2}t\right\}C_- & \exp\left\{-i\frac{\delta_+}{2}t\right\}C_0 \\ \exp\left\{i\frac{\delta_+}{2}t\right\}C_0 & \exp\left\{-i\frac{\delta_-}{2}t\right\}C_+ \end{pmatrix} \quad (49)$$

The adjoint matrix is:

$$U^\dagger(t) = \begin{pmatrix} \exp\left\{-i\frac{\delta_-}{2}t\right\}C_+ & \exp\left\{-i\frac{\delta_+}{2}t\right\}C_0^* \\ \exp\left\{i\frac{\delta_+}{2}t\right\}C_0^* & \exp\left\{i\frac{\delta_-}{2}t\right\}C_- \end{pmatrix} \quad (50)$$

We shall be using the following quantities in our calculation:

$$\begin{pmatrix} \exp\{i\omega_0 t/2\} & 0 \\ 0 & \exp\{-i\omega_0 t/2\} \end{pmatrix} U^\dagger(t) = $$
$$= \begin{pmatrix} \exp\{+i\omega t/2\}C_+ & \exp\{-i\omega t/2\}C_0^* \\ \exp\{+i\omega t/2\}C_0^* & \exp\{-i\omega t/2\}C_- \end{pmatrix} \quad (51)$$

The analog conversion of $\hat{H}(t)$ in matrix form yields:

$$\begin{aligned} \hat{H}(t) &= \frac{\hbar}{2}\left\{\omega_1\sigma_1\cos\omega t + \omega_1\sigma_2\sin\omega t + \omega_0\sigma_3\right\} \\ &= \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\exp\{-i\omega t\} \\ \omega_1\exp\{+i\omega t\} & -\omega_0 \end{pmatrix} \end{aligned} \quad (52)$$

Indeed:

$$U(t)\begin{pmatrix} \exp\{-i\omega_0 t/2\} & 0 \\ 0 & \exp\{i\omega_0 t/2\} \end{pmatrix} = $$
$$= \begin{pmatrix} \exp\{-i\omega t/2\}C_- & \exp\{-i\omega t/2\}C_0 \\ \exp\{+i\omega t/2\}C_0 & \exp + i\omega t/2\}C_+ \end{pmatrix} \quad (53)$$

Now we are ready for the final calculation. The operator product $U^\dagger(t)\hat{H}(t)U(t)$ is:

$$U^\dagger(t)\hat{H}(t)U(t) = \frac{\hbar}{2}\begin{pmatrix} A_{[1,1]}, & A_{[1,2]} \\ A_{[2,1]}, & A_{[2,2]} \end{pmatrix} \quad (54)$$

where

$$\begin{aligned} A_{[1,1]} &= \omega_0\left[C_+C_- + C_0^2\right] + \omega_1\left[C_+ - C_-\right]C_0 \\ &= -\omega\sin^2\theta\left[1-\cos\Omega t\right] + \omega_0 \\ A_{[1,2]} &= 2\omega_0 C_+C_0 + \omega_1\left[C_+^2 - C_0^2\right] \\ &= \omega_1 + \omega\sin\theta\cos\theta\left[1-\cos\Omega t\right] - i\omega\sin\theta\sin\Omega t \\ A_{[2,1]} &= -2\omega_0 C_-C_0 + \omega_1\left[C_-^2 - C_0^2\right] \\ &= \omega_1 + \omega\sin\theta\cos\theta\left[1-\cos\Omega t\right] + i\omega\sin\theta\sin\Omega t \\ A_{[2,2]} &= -\omega_0\left[C_+C_- + C_0^2\right] - \omega_1\left[C_+ - C_-\right]C_0 \\ &= \omega\sin^2\theta\left[1-\cos\Omega t\right] - \omega_0 \end{aligned} \quad (55)$$

One needs also the derivative of the unitary operator:

$$[\partial_t U(t)] = \quad (56)$$
$$= \begin{pmatrix} e^{\frac{i\delta_-}{2}t}\left[\frac{i\delta_-}{2}C_- + \dot{C}_-\right], & e^{-\frac{i\delta_+}{2}t}\left[-\frac{i\delta_+}{2}C_0 + \dot{C}_0\right] \\ e^{\frac{i\delta_+}{2}t}\left[\frac{i\delta_+}{2}C_0 + \dot{C}_0\right], & e^{-\frac{i\delta_-}{2}t}\left[-\frac{i\delta_-}{2}C_+ + \dot{C}_+\right] \end{pmatrix}$$

We are now in a position to finish the calculation with the help of the identities already found. First:

$$[\partial_t U(t)]\begin{pmatrix} e^{-\frac{i\omega t}{2}}, & 0 \\ 0, & e^{\frac{i\omega t}{2}} \end{pmatrix} = \quad (57)$$
$$= \begin{pmatrix} e^{-\frac{i\omega t}{2}}\left[\frac{i\delta_-}{2}C_- + \dot{C}_-\right], & e^{-\frac{i\omega t}{2}}\left[-\frac{i\delta_+}{2}C_0 + \dot{C}_0\right] \\ e^{\frac{i\omega t}{2}}\left[\frac{i\delta_+}{2}C_0 + \dot{C}_0\right], & e^{\frac{i\omega t}{2}}\left[-\frac{i\delta_-}{2}C_+ + \dot{C}_+\right] \end{pmatrix}$$

and using $i\hbar U^\dagger(t)\left[\partial_t U(t)\right]$ we obtain the following result:

$$i\hbar\begin{pmatrix} e^{\frac{i\omega t}{2}} & 0 \\ 0 & e^{-\frac{i\omega t}{2}} \end{pmatrix} U^\dagger(t)\left[\partial_t U(t)\right]\begin{pmatrix} e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} =$$
$$= \frac{\hbar}{2}\begin{pmatrix} A_{[1,1]}, & A_{[1,2]} \\ A_{[2,1]}, & A_{[2,2]} \end{pmatrix} \quad (58)$$

and having carried out the calculation for the left hand side, we obtain for the right hand side:

$$\hat{H}_0 = \frac{\hbar\omega_0}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar\omega_0}{2}\sigma_3 \quad (59)$$

which reproduces the required result

$$U^\dagger(t)\hat{H}(t)U(t) - i\hbar U^\dagger(t)\left[\partial_t U(t)\right] = \hat{H}_0 \quad (60)$$

III. MAGNETIC SPIN RESONANCE: BERRY PHASE

Let us begin by considering a time dependent quantum system. The corresponding eigenstate of the system may evolve in two different ways. First: The system is defined by a **time dependent Hamiltonian** with specific rules such that any set of eigenstates (or combination of them) is forced by the **time dependent Hamiltonian** to walk along a very definite trajectory in Hilbert Space. The equation of such an evolution is called **Time Dependent Schrödinger Equation**. Second: one can take a state with or without obeying a specific Hamiltonian and **force the state to follow a given trajectory** without necessarily relying on a specific dynamics. Obviously we cannot force the state with the naked hand but we can do it by finding first the **geommetry of the Hilbert Space of States** and at a definite instant of time push the state, for instance along one of the geodesics of such a space, and forcing it to come back to the initial starting point from which the evolution took place [5].

Another question to be considered is **the speed of the travel**. For the definition of the **Berry Phase** we shall consider only **travels realized at a very slow speed**. As we shall see in the example only in such case there will be a contribution to the phase of the state as compared with the initial phase which will depend **only of the area enclosed by the trajectory in the Hilbert Space of the States** but not either of the speed nor the time spent in the journey. The physical system describing the **Spin Magnetic Resonances** are particularly suitable to describe the analysis and the calculation of the **Berry Phase**. The control of the magnetic fields involved in these experiments plus the geometric consideration of the Hilbert Space of States -which is particularly easy- makes the calculation both feasible and possible.

In **Section I**, we were picking up an **initial state** of the form.:

$$\begin{aligned} &\mid \mathbf{\Psi}_0(t)\rangle = e^{-i\frac{\omega_0 t}{2}\sigma_3}\begin{pmatrix} a \\ b \end{pmatrix} = \\ &a e^{-i\frac{\omega_0 t}{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b e^{i\frac{\omega_0 t}{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{61}$$

where a y b are complex numbers fulfilling $\mid a\mid^2 + \mid b\mid^2 = 1$. In turn the state obeys the well known **Time Dependent Schrödinger Equation**

$$\hat{H}(t) \mid \mathbf{\Psi}(t)\rangle = i\hbar\frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle \tag{62}$$

Multiplying at left by the conjugate bra $\langle\mathbf{\Psi}(t)\mid$ state:

$$-\frac{1}{\hbar}\langle\mathbf{\Psi}(t)\mid\hat{H}(t)\mid\mathbf{\Psi}(t)\rangle + i\langle\mathbf{\Psi}(t)\mid\frac{\partial}{\partial t}\mid\mathbf{\Psi}(t)\rangle = 0 \tag{63}$$

Obviously a **Temporal Evolution Operator** exists such that :

$$\mid \mathbf{\Psi}(t)\rangle = U(t)\mid\mathbf{\Psi}_0(t)\rangle \tag{64}$$

The initial state with $(a = 1, b = 0)$ yields zero when substituted in (30). This is because the parameter space does not exist. In fact one cannot manipulate the state without these parameters. So, one cannot dictate the precise trail of the state without extra parameters included in the evolution and the calculation yields no variation in the phase of the state.

Let us now suposse that: $[a = \cos\theta/2;\ b = \exp{(i\varphi)}\sin\theta/2]$, where θ is still constant in time but we allow the **phase** $\varphi = \varphi(t)$ an azimutal variation depending on time. Thus, the vector moves around the axis (**precesses**) as it is not necessarily aligned with the direction of the magnetic field in any arbitrary later time **t**:

$$\begin{aligned} &\mathbf{R}(t) = [\sin\theta\cos\varphi(t), \sin\theta\sin\varphi(t), \cos\theta] \Rightarrow \\ &\mid \mathbf{\Psi}(t)\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi(t)}\sin\frac{\theta}{2} \end{pmatrix} \end{aligned} \tag{65}$$

Therefore, the second term of the left hand side in equation (30) can easily be calculated in the form:

$$\begin{aligned} d\gamma(\mathcal{C}) &= i\langle\mathbf{\Psi}(t)\mid\frac{\partial}{\partial t}\mid\mathbf{\Psi}(t)\rangle = \\ &= i\left[\cos\frac{\theta}{2}, e^{-i\varphi(t)}\sin\frac{\theta}{2}\right]\frac{d}{dt}\begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi(t)}\sin\frac{\theta}{2} \end{pmatrix} = \\ &= i\left[\cos\frac{\theta}{2}, e^{-i\varphi(t)}\sin\frac{\theta}{2}\right]\begin{pmatrix} 0 \\ i\frac{d\varphi(t)}{dt}e^{i\varphi(t)}\sin\frac{\theta}{2} \end{pmatrix} = \\ &= -\left(\frac{d\varphi(t)}{dt}\right)\sin^2\frac{\theta}{2} \end{aligned} \tag{66}$$

One can interpret geommetrically **the Berry Phase** as the integral over a **complete closed cycle of the time evolution from the beginning to the end in the Hilbert space of quantum states**. Therefore $\varphi = \omega t$ with the **period** $T = 2\pi/\omega$. In mathematical language this is:

$$\begin{aligned} \gamma(\mathcal{C}) &= -\int_0^t (dt)\left[\frac{d\varphi(t)}{dt}\right]\sin^2\frac{\theta}{2} = \\ &= -\frac{1}{2}(1-\cos\theta)\oint d\varphi = -\pi(1-\cos\theta) \end{aligned} \tag{67}$$

The phase just depends on a *cosine* function of certain angle. **This angle can be seen as the tilting of the spin vector with respect to the rotation axis**. A more precise definition in terms of Quantum Mechanics would be: **The state of the system takes the eigenvalue of spin $+\frac{\hbar}{2}$ measured with respect to the magnetic axis rotating with cyclotron frequency** ω_0. This quantity (the angle) is proportional to a **geommetrical invariant** as we shall see henceforth.

Let us suppose the our initial system of coordinates is formed by an arbitrary tangent plane to the surface which contains the mentioned vector normal to the surface and a third vector orthogonal to both, normal and tangent vector in such a way that they form a triplet (*dreibein*) acting as a system of coordinates fixed at the point P, for example on a sphere of radius **R**, although the whole thing can easily be generalized to any manifold.

Then let us proceed to move ourselves riding with the system of coordinates. For any point we can easily identify the normal vector in each point as it is unambiguously determined as the normal to the tangent plane in each point. What happens however with the tangent vector?. In principle although it can takes any direction must be forced to lay in the tangent plane. However we impose an additional condition: **If we were going backwards in the excursion, the tangent plane has**

to coincide always with the tangent vector in the initial point $\mathcal{P}$. This is called **Parallel Transport**.

The last thing we have to remember is that the state is represented by a **complex vector**. Therefore it must have **a phase** attached to it. At the end of the **parallel transported excursion** the phase of the initial vector **might be different of the returned vector**. The difference of phases form an angle $\alpha(\mathcal{C})$. This angle depends just of C and in spite of this semiclassical consideration is the first step to a complete definition of the **Berry Phase**.

The last details in this description are related to pure quantum mechanics. Let us consider a cone of apex A touching the sphere at the latitude defined by its polar angle latitude θ, taking $\theta = 0$ as the latitude at the pole and at the equatorial latitude a value of $\theta = \frac{\pi}{2}$. After the journey we cut the cone along one generatrix and extend the cone in a flat surface (remember that this can be done as the cylinder and the cone have zero curvature). The trajectory $\mathcal{C}$ corresponds obviously to the length of the journey. The condition of parallel transport is seen as if the vector $\tilde{\mathbf{v}}(\mathbf{t})$ would keep its direction constant and parallel to $\tilde{\mathbf{v}(\mathbf{0})}$: it points in the same direction as $\tilde{\mathbf{v}(\mathbf{0})}$ in each point. At the end of the excursion both vectors form an angle $\alpha(\mathcal{C})$. What really counts is to measure the angle difference between the angle measured with respect to the latitude. **In other words is the angle between the transported $\tilde{\mathbf{v}}$ with the tangent vector in the final position** (See **Fig. 1**). This is exacy the interpretation of $\alpha(\mathcal{C})$ previously calculated. Elementary euclidean geommetry shows that the arc of length $\mathcal{C}$ equals $2\pi\mathbf{R}\sin\theta$. The radius of the cone at a given latitude is $\mathbf{a} = \mathbf{R}\tan\theta$. Therefore $\alpha(\mathcal{C})$ equals the angle of the *cheese portion* stolen to the circle in **Fig. 1**.

After all these considerations we obtain:

$$\alpha(\mathcal{C}) = 2\pi(1-\cos\theta) \implies \gamma(\mathcal{C}) = -\frac{1}{2}\alpha(\mathcal{C}) \qquad (68)$$

The quantity $\alpha(\mathcal{C})$ is **the solid angle subtended by the cone $\mathcal{C}$ from the center of the sphere**. For $\mathcal{C}$ being at the equatorial line thus $\theta = \pi/2$ and then $\alpha(\mathcal{C}) = 2\pi$. Therefore the **Berry Phase** $\gamma(\mathcal{C})$ in this quantum system, equals to **minus sign the half of the subtended surface of the sphere with borderline $\mathcal{C}$. In other words a pure geometric quantity.**

It is extremely worthwhile to keep in mind that the **Berry Phase does not depend on the form of the curve fixed by the excursion but only depends upon the area enclosed**. This topological property allows a quantum time dependent system to generate the same Berry Phase with different evolution operators by keeping the property of **equal area enclosed in different pathways**. Besides no mention whatsoever appears to be of physical interest in the **Time Employed in the Journey (TEJ) : The Berry Phase is then a truly topological invariant.** One must keep in mind always that the effect takes place by looking at the geometry of **the Space of States as opposed to Ordinary**

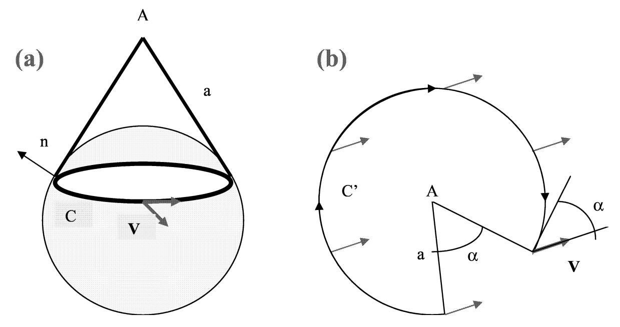

FIG. 1: Parallel Transport on the Sphere and Berry Phase

$\{x, y, z\}$ space.

We would like to explicitly calculate the Berry Phase in our system of Magnetic Nuclear Resonance which has been fully developed in previous Sections. Without loss of generality we use the exact states (9) and (11) together with the unitary operator given by (5). The operation we want to do obviously is:

$$\begin{aligned}
&\mid \mathbf{\Psi}(t)\rangle = U(t) \mid \mathbf{\Psi}_0(t)\rangle = \\
&= \exp\left\{-i\frac{\omega t}{2}\sigma_3\right\}\exp\left\{-i\frac{\Omega t}{2}\left[\sin\theta\sigma_1 + \cos\theta\sigma_3\right]\right\}\begin{pmatrix}1\\0\end{pmatrix} = \\
&= e^{\frac{-i\omega t}{2}}\left[\cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}1\\0\end{pmatrix} - \\
&-ie^{\frac{i\omega t}{2}}\left[\sin\theta\sin\frac{\Omega t}{2}\right]\begin{pmatrix}0\\1\end{pmatrix} \qquad (69)
\end{aligned}$$

An operation which yields the following result:

$$\begin{aligned}
&\frac{1}{\hbar}\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle = \\
&= \frac{\omega_0}{2} + \frac{(1-\cos\Omega t)}{2}\left[\omega_1\sin\theta\cos\theta - \omega_0\sin^2\theta\right] (70)
\end{aligned}$$

$$i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = \frac{\omega_0}{2} - \frac{\omega}{2}\sin^2\theta\left[1-\cos\Omega t\right] \quad (71)$$

Adding up the two contributions as in (30):

$$\begin{aligned}
&\frac{1}{\hbar}\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle + i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = \\
&= -\frac{1}{2}(1-\cos\Omega t)\left[-\omega_1\sin\theta\cos\theta + (\omega_0-\omega)\sin^2\theta\right] \quad (72)
\end{aligned}$$

Inserting ω_1 y $\omega_0 - \omega$ as functions of $\sin\theta$ and $\cos\theta$ [See (7)], we finally obtain:

$$\begin{aligned}
&\frac{1}{\hbar}\langle\mathbf{\Psi}_0(t) \mid U^\dagger(t)\hat{H}(t)U(t) \mid \mathbf{\Psi}_0(t)\rangle + i\langle\mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t)\rangle = \\
&= -\frac{\Omega}{2}(\ 1-\cos\Omega t)\left[-\sin^2\theta\cos\theta + \cos\theta\sin^2\theta\right] = 0 \quad (73)
\end{aligned}$$

in agreement with (35). **The pure geometric phase** is given by (67) through the line integral where the circuit is drawn by the extreme of the vector Ω precessing with the a very slow rfc ω around the axis of the main B_0

magnetic field: $T \to \{0, \frac{2\pi}{\omega}\}$. This operation yields the following result:

$$i \oint dt \langle \mathbf{\Psi}(t) \mid \frac{\partial}{\partial t} \mid \mathbf{\Psi}(t) \rangle \tag{74}$$

This the **exact nonadiabatic geometric phase**. The adiabatic limit of it (very slow motion) is the geometric exact phase: The topological phase (independent of the velocity of the journey) that we want to calculate. The condition is $\{\omega << \Omega\}$. Expanding the function $\Omega(\omega)$ [See (7)] in powers of ω we obtain the effective very slow frequency of the rotation $\omega \Rightarrow T = 2\pi$ with respect to the vertical-axis (the ω_0-axis). See **Fig. 1**.

$$\begin{aligned} \Omega_{ef} = \quad & \Omega_{\{\omega \to 0\}} - \frac{\omega}{1!} \cos\theta_{\{\omega \to 0\}} + ... \\ & + \mathcal{O}\left(\frac{d^n \Omega}{d\omega^n}_{\{\omega \to 0\}} \frac{\omega^n}{n!}; n \geq 2 \right) \end{aligned} \tag{75}$$

After one slow circuit like this, the reckoned phase $\omega T = 2\pi$ takes the form:

$$\begin{aligned} \Phi^{reckoned} &= \Phi + 2\pi = \Omega_{\{\omega \to 0\}} T + 2\pi \left(1 - \cos\theta_{\{\omega \to 0\}}\right) = \\ &= \left[\omega_0^2 + \omega_1^2\right]^{\frac{1}{2}} T + 2\pi \left(1 - \frac{\omega_0}{\left[\omega_0^2 + \omega_1^2\right]^{\frac{1}{2}}} \right) = \\ &= \left[\omega_0^2 + \omega_1^2\right]^{\frac{1}{2}} T + \alpha(\mathcal{C}) \end{aligned} \tag{76}$$

where:

$$\alpha(\mathcal{C}) = 2\pi(1 - \cos\theta) = 2\pi \left(1 - \frac{\omega_0}{\left[\omega_0^2 + \omega_1^2\right]^{\frac{1}{2}}} \right) \tag{77}$$

To be compared with (67) and (68). The first and second term of the adiabatic expansion (84) represent respectively the **abiabatic approximation** of the **dynamical** and **geometric** phases of the total phase acquired by the state as a consequence of its the closed journey. One can easily compare the geometry of the Berry phase with **Fig.1** and references [6] and [7].

The properly educated reader has probably already noticed that the only quantity of interest for the Phase is the ratio of the two main magnetic fields involved $\{\omega_0\}$ and $\{\omega_1\}$. In terms of this ratio, the Berry Phase can trivially be written as:

$$\gamma(\mathcal{C}) = -\frac{1}{2}\alpha(\mathcal{C}) = -\pi \left(1 - \frac{1}{\left[1 + \mathbf{R^2}\right]^{\frac{1}{2}}} \right) \tag{78}$$

with

$$\mathbf{R} = \frac{\omega_\mathbf{1}}{\omega_\mathbf{0}}. \tag{79}$$

This ratio plays here the semi-classical role of Lissajous rational resonant ratios in the motion of two Coupled Harmonic Oscillators. Whether or not this property plays a significant role at the experimental level remains to be seen as far as the author's knowledge is concerned.

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