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NONADIABATIC GEOMETRIC ANGLE IN NUCLEAR MAGNETIC RESONANCE CONNECTION

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Abstract. By using the Grassmannian invariant-angle coherents states approach, the classical analogue of the Aharonov-Anandan nonadiabatic geometrical phase is found for a spin one-half in Nuclear Magnetic Resonance (NMR). In the adiabatic limit, the semi-classical relation between the adiabatic Berry's phase and Hannay's angle gives exactly the experimental result observed by Suter *et al* [12].

1. Introduction

The adiabatic **Berry's phase** and its classical counterpart (adiabatic **Hannay's angle**) are one of the most finding in the quantum and classical dynamics these recent years. Their extension to the nonadiabatic case has attracted great interest. Indeed, removing the nonadiabatic hypothesis, Aharonov and Anandan [1] have generalized Berry's result. They have considered a cyclic evolution of states which return to itself after some time up to a phase. A way to get such a basis of cyclic states is to consider the eigenvectors of a Hermetian periodic invariant $I(t)$ defined by

$$\frac{\partial \hat{I}}{\partial t} = \mathrm{i}\left[\hat{I}, \hat{H}\right]. \tag{1}$$

Indeed, any eigenstate $|n, 0\rangle$ (relative to the time-independent eigenvalue λ_n) of the invariant operator $I(0)$ at time zero evolves into the corresponding eigenstate $|n, t\rangle$ of the invariant operators $I(t)$ at time t exactly as an eigenstate of the Hamiltonian does when the evolution is adiabatic [8].

Since the **invariant action** due to Lewis and Riesenfield exists, a geometrical angle can be defined on constant-action surface for a cyclic evolution [2, 4] and the angle thus obtained is the classical counterpart of the **geometrical phase** due to Aharonov and Anandan.

In the literature, the nonadiabatic geometric phase is studied in various ways. A special cyclic state of the Gaussian wave packet's form were found for a generalized harmonic oscillator. The nonadiabatic geometric phase is explicitly calculated and found to be one-half of the classical nonadiabatic Hannay's angle. It was also discussed for the case of the cyclic states of a generalized Harmonic oscillator with nonadiabatic time-periodic parameters in the framework of **squeezed states** [9]. The nonadiabatic implementation of the conditional geometric phase shift with NMR were also explored [13]. Also a non perturbative method which is different from that of Aharonov and Anandan, was presented in order to determine the nonadiabatic corrections to Berry's phase [6].

In our recent papers [5] we have determined the nonadiabatic Hannay's angle of a spin one-half in a varying magnetic field in the framework of the Grassmannian invariant-angle coherent states approach.

Our aim is to develop the ideas of references [4] and [5] in more detail, for the well known example of spin one-half particle in the presence of an external magnetic field in Nuclear Magnetic Resonance experiment.

2. Spin One-Half Model in the NMR

We consider a spin $1/2$ coupled to a time-dependent magnetic field which precess around the z-axis, at a fixed angle θ with constant angular velocity $\dot{\varphi} = \omega$ and with constant modulus $|\vec{B}(t)| = B$ (θ and φ are the polar and azimuthal angle, respectively)

$$\vec{B}(t) = B(\sin\theta\cos(\omega t)\vec{e}_x + \sin\theta\sin(\omega t)\vec{e}_y + \cos\theta\vec{e}_z) \tag{2}$$

where B is the modulus of the magnetic field.

According to the reference [4], the classical Hamiltonian in Grassmannian version of our system is given by

$$H = -\frac{\mathrm{i}}{2}\varepsilon_{kij}B_k(t)\xi_i\xi_j \tag{3}$$

or

$$H(t) = -\mathrm{i}(B_1\xi_2\xi_3 + B_2\xi_3\xi_1 + B_3\xi_1\xi_2) \tag{4}$$

where the components ξ_i, $i = 1, 2, 3$, of the vectors $\vec{\xi}$ are real **Grassmann variables** which satisfy the **Grassmann algebra** relations $\xi_m\xi_l + \xi_l\xi_m = 0$.

When we quantize the variables ξ_i with the rules given in the Appendix, we get the quantum Hamiltonian as

$$\widehat{H}(t) = \frac{1}{2}\vec{B}(t).\vec{\sigma}. \tag{5}$$

Substituting the components B_i, $i = 1, 2, 3$, of the magnetic field into the Hamiltonian, we get

$$\hat{H}(t) = \frac{B}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta \end{pmatrix}. \tag{6}$$

Here we have taken $\hbar = 1$, $g\mu_B = 1$, g is the **Landé's factor** and μ_B is the **Bohr magneton**.

The eigenstates $|\Psi_\pm(t)\rangle$ of $\hat{H}(t)$ are given by

$$|\Psi_+(t)\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{i\omega t}|\downarrow\rangle$$
$$|\Psi_-(t)\rangle = \sin\frac{\theta}{2}|\uparrow\rangle - \cos\frac{\theta}{2}e^{i\omega t}|\downarrow\rangle$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the z-component of the spin.

As we have mentioned in the introduction, the eigenvectors of the invariant in the nonadiabatic case, play the same basic role as the eigenvectors of the Hamiltonian in the adiabatic case, for this reason we introduce a time dependent invariant $I(t)$ associated to the Hamiltonian (4)

$$I(t) = -i(R_1\xi_2\xi_3 + R_2\xi_3\xi_1 + R_3\xi_1\xi_2) \tag{7}$$

which satisfies the relation

$$\frac{\partial I(t)}{\partial t} = -\{H, I\}_{P.B} = -i\sum_m H\overleftarrow{\partial}_i.\overrightarrow{\partial}_i I \tag{8}$$

where R_i, $i = 1, 2, 3$, are 3 time-dependent parameters space and $\overleftarrow{\partial}_i$ and $\overrightarrow{\partial}_i$ are right and left derivatives with respect to ξ_i.

According to (8) the parameters R_1, R_2 and R_3 satisfy the system of coupled differential equations

$$\dot{\overrightarrow{R}} = \overrightarrow{B} \wedge \overrightarrow{R}. \tag{9}$$

By setting $B_\pm = B_1 \pm iB_2$, $R_\pm = R_1 \pm iR_2$ equations (9) are equivalent to

$$\begin{aligned} \dot{R}_+ &= i(R_+B_3 - R_3B_+) \\ \dot{R}_- &= i(R_3B_- - R_-B_3) \\ \dot{R}_3 &= \frac{i}{2}(R_-B_+ - R_+B_-). \end{aligned} \tag{10}$$

Note that equations (9) may be regarded as the classical equations of motion in the parameter space $\overrightarrow{R}$. By solving them, we obtain a curve in the parameter space and hence the nonadiabatic geometrical angle. When this curve is closed the evolution is cyclic. For this reason we will determine the solutions of the equations (9) which are cyclic.

The equations (10) can be simplified by making a change of the variable R_+

$$R_+ = \frac{r^2(t)}{2}.$$

With the new variable $r(t)$, this system of coupled differential equations reduces to the following differential equation

$$\frac{\mathrm{d}^2 r}{\mathrm{d}t^2} - \mathrm{i}\omega\frac{\mathrm{d}r}{\mathrm{d}t} + \frac{(B^2 - 2\omega B\cos\theta)}{4} r = \frac{B^2\sin^2\theta\exp(2\mathrm{i}\omega t)}{r^3}. \qquad (11)$$

The cyclic solution of this equation is given by

$$r(t) = \frac{\sqrt{2\sin\theta}}{(1-2x\cos\theta+x^2)^{\frac{1}{4}}}\exp\left(\mathrm{i}\frac{\omega t}{2}\right) \qquad (12)$$

with $x = \omega/B$.

From this expression for $r(t)$, we deduce the solutions of equations (10)

$$R_+(t) = \Gamma(x)\sin\theta\exp(\mathrm{i}\omega t) \qquad (13)$$

$$R_-(t) = \frac{[r^*(t)]^2}{2} = \Gamma(x)\sin\theta\exp(-\mathrm{i}\omega t) \qquad (14)$$

where $r^*(t)$ denotes the complex conjugate of $r(t)$ and

$$R_3 = (\cos\theta - x)\Gamma(x). \qquad (15)$$

Here $\Gamma(x)$ is equal to

$$\Gamma(x) = \frac{1}{\sqrt{1-2x\cos\theta+x^2}} \qquad (16)$$

and one can see that R_+ and R_- precess around the z-axis with the same angular velocity ω, and make with this axis an angle α given by

$$\cos\alpha = (\cos\theta - x)\Gamma(x). \qquad (17)$$

The invariant (7) can be written explicitly in the form

$$I(t) = -\frac{\mathrm{i}}{2}\{(R_+ + R_-)\xi_2\xi_3 - \mathrm{i}(R_+ - R_-)\xi_3\xi_1 + 2R_3\xi_1\xi_2\}. \qquad (18)$$

The quantum invariant $\hat{I}(t)$ corresponding to the classical one is

$$\hat{I}(t) = \frac{1}{2}\overrightarrow{R}(t).\overrightarrow{\sigma} \qquad (19)$$

or in matrix form

$$\hat{I}(t) = \frac{1}{2}\begin{pmatrix} R_3 & R_-(t) \\ R_+(t) & -R_3 \end{pmatrix}. \qquad (20)$$

The instantaneous eigenstates $|1,t\rangle$ and $|0,t\rangle$ of $\hat{I}(t)$ are

$$|1,t\rangle = \frac{\sqrt{1+R_3}}{\sqrt{2}}\exp(-\mathrm{i}\frac{\omega t}{2})|\uparrow\rangle + \frac{\sqrt{1-R_3}}{\sqrt{2}}\exp(\mathrm{i}\frac{\omega t}{2})|\downarrow\rangle \tag{21}$$

$$|0,t\rangle = \frac{\sqrt{1-R_3}}{\sqrt{2}}\exp(-\mathrm{i}\frac{\omega t}{2})|\uparrow\rangle - \frac{\sqrt{1+R_3}}{\sqrt{2}}\exp(\mathrm{i}\frac{\omega t}{2})|\downarrow\rangle \tag{22}$$

$|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates the z-component of the spin.

This eigenstates of $\hat{I}(t)$ are related to those of $\hat{H}(t)$ by

$$|1,t\rangle = \Omega_1(t)|\Psi_+(t)\rangle + \Omega_2(t)|\Psi_-(t)\rangle \tag{23}$$

$$|0,t\rangle = -\Omega_2(t)|\Psi_+(t)\rangle + \Omega_1(t)|\Psi_-(t)\rangle \tag{24}$$

with

$$\Omega_1(t) = (\sqrt{1+R_3}\cos\frac{\theta}{2} + \sqrt{1-R_3}\sin\frac{\theta}{2})\exp(-\mathrm{i}\frac{\omega t}{2})$$

and

$$\Omega_2(t) = (\sqrt{1+R_3}\sin\frac{\theta}{2} - \sqrt{1-R_3}\cos\frac{\theta}{2})\exp(-\mathrm{i}\frac{\omega t}{2}).$$

Explicited the instantaneous eigenstates of $\hat{I}(t)$, we can embark on the calculation of the nonadiabatic geometric angle which is the subject of the next section.

3. The Nonadiabatic Geometric Angle

A simple way to provide a quantum description of the evolution of a classical system and to derive the geometrical angle from the geometrical phase, is to study the evolution of the Grassmannian invariant-angle coherent states [5].

According to the reference [4], the Grassmannian invariant-angle coherent states in the (NMR) are given by

$$|\xi(t),t\rangle = \exp\left[-\frac{1}{2}\xi^*(t)\xi(t)\right](|0,t\rangle - \xi(t)|1,t\rangle) \tag{25}$$

where

$$\xi(t) = \xi(0)\mathrm{e}^{-\mathrm{i}\theta(t)} \tag{26}$$

is Grassmannian complex variable and $|1,t\rangle$ and $|0,t\rangle$ are the instantaneous eigenstates of $\hat{I}(t)$ given in equation (20).

Let us show how this angle appears in evolution of the Grassmannian invariant-angle coherent states.

Indeed, the evolution of the phase of the eigenstates of the quantum invariant $\hat{I}(t)$

$$|0,0\rangle \rightarrow \mathrm{e}^{\mathrm{i}\phi_0}|0,t\rangle \qquad |1,0\rangle \rightarrow \mathrm{e}^{\mathrm{i}\phi_1}|1,t\rangle \tag{27}$$

induces the evolution of the Grassmannian invariant-angle coherent states

$$|\xi(0),0\rangle \rightarrow \mathrm{e}^{\mathrm{i}\phi_0(t)}|\xi(t),t\rangle \tag{28}$$

where the angle

$$\theta(t) = \phi_1(t) - \phi_0(t) \tag{29}$$

is the difference of the to global phases ϕ_n, $n = 0, 1$.

As it is well known [2] $\theta(t)$ contains a dynamical part

$$\theta^D(t) = \phi_1^D(t) - \phi_0^D(t) \tag{30}$$

and a geometrical part

$$\theta^G(t) = \phi_1^G(t) - \phi_0^G(t) \tag{31}$$

where

$$\phi_n^D(t) = -\int_0^t \mathrm{d}t' \, \langle n, t'|\hat{H}(t)|n, t'\rangle \qquad n = 0, 1 \tag{32}$$

and

$$\phi_n^G = \mathrm{i} \int_0^t \mathrm{d}t' \, \langle n, t'|\frac{\partial}{\partial t'}|n, t'\rangle \qquad n = 0, 1. \tag{33}$$

This geometrical part $\theta^G(t)$ is nothing but (minus) the nonadiabatic geometric angle in a cyclic evolution [10].

Let us embark on the calculation of this angle.

From equations (31) and (33) above and for a cyclic evolution of duration T in the parameter space $\overrightarrow{R}$, where $\overrightarrow{R}(T + t) = \overrightarrow{R}(t)$

$$\theta^G = \mathrm{i} \int_0^T \mathrm{d}t \, \left(\langle 0, t|\frac{\partial}{\partial t}|0, t\rangle - \langle 1, t|\frac{\partial}{\partial t}|1, t\rangle \right). \tag{34}$$

Finally, substituting $|1, t\rangle$ and $|0, t\rangle$ from equations (21) and (22) we get explicitly the nonadiabatic geometric angle

$$\theta^G = 2\pi \left(1 - \frac{\cos\theta - x}{\sqrt{1 - 2x\cos\theta + x^2}} \right). \tag{35}$$

4. Adiabatic and Weak Nonadiabatic Approximations

We have explicitly calculated the nonadiabatic geometric angle in NMR and we are now interesting on the adiabatic and the weak nonadiabatic approximations.

As it is well known [3] in the model of the spin 1/2, the Berry's phase is one-half of the Hannay's angle. In the adiabatic limits: $x = \omega/B \to 0 \Rightarrow T \to \infty$.

The Taylor development up to the second order in x of equation (35) gives

$$\theta^G = 2\pi \left(1 - \cos\theta + x\sin^2\theta + O(x^2) \right). \tag{36}$$

The first two terms of θ^G in this last equation correspond exactly to the experimental result observed by Suter *et al* [12] for the adiabatic Berry's phase and the third term in this equation is the first order correction in the weak nonadiabatic approximation.

5. Concluding Remarks

In this paper, the nonadiabatic geometrical angle is calculated for a spin one-half in Nuclear Magnetic Resonance experiment by using the invariant theory and in the framework of the Grassmannian invariant-angle coherent states. In the adiabatic approximation we have found the experimental result observed by Suter *et al* [12].

Finally it will be interesting to investigate experimentally the weak Nonadiabatic correction found in this paper.

Appendix

We recall in this Appendix the quantization rules for Grassmannian system. For this, the quantization rules say that we should replace the Poisson brackets by the anticommutator (instead of the commutator)

$$\{xi_i, \xi_j\}_{PB} \to \mathrm{i}\left[\widehat{\xi}_i, \widehat{\xi}_j\right]_+ \qquad \hbar = 1. \tag{37}$$

The operators $\widehat{\xi}_i$ are shown to generate the structure of Clifford algebra

$$\left[\widehat{\xi}_i, \widehat{\xi}_j\right] = \delta_{ij} \tag{38}$$

and therefore they can be represented irreducibly by the Pauli matrices as $\widehat{\xi}_i \to \sigma_i/\sqrt{2}$.

When we quantize the variables ξ_i with the rules just given above, we get for the classical Hamiltonian the quantum one

$$\hat{H} = -\frac{\mathrm{i}}{2}\varepsilon_{kij} B_k \widehat{\xi}_i \widehat{\xi}_j \tag{39}$$

and using the Pauli matrix representation for $\widehat{\xi}_i$, we obtain

$$\hat{H} = -\frac{\mathrm{i}}{4}\varepsilon_{kij} B_k \sigma_i \sigma_j = \frac{1}{2}\overrightarrow{B}(t).\overrightarrow{\sigma}. \tag{40}$$

This is the quantum mechanical Hamiltonian for a one-half spin in the magnetic field $\overrightarrow{B}$.

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