

DISSIPATIVE TWO-LEVEL SPIN SYSTEM AND GEOMETRICAL PHASE

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Abstract. We propose to extend the concept of geometric phase to quantum dissipative systems, in the case of meta-stable spin states in magnetic resonance. We use the generalized version of Lewis–Riensenfeld invariant theory to study the dissipative systems described by non-hermitian time-dependent Hamiltonian.

1. Introduction

Two decades ago, Berry [2] has discovered the geometrical phase associated to adiabatic cyclic evolution of non-degenerates eigenstates of quantum Hermitian Hamiltonian. Later, the growing investigations were devoted to the generalization of Berry's result to several contexts. Indeed, Wilzek and Zee [13] extend this result to adiabatic evolution of degenerates eigenstates. Removing the adiabatic hypothesis, Aharonov and Anandan [1] have generalized Berry's result to the non-adiabatic case. Samuel and Bhandari [12] and Pati [11] established the Berry's phase analogue in the case of non-cyclic evolutions. All this works deal with quantum Hermitian Hamiltonians.

In the last decade, there has been substantial interest in the complex geometric phase acquired by the eigenstates of the dissipative quantum systems described by non-hermitian Hamiltonians.

Garrison and Wright [5] have shown that the geometrical phase associated with cyclic unitary time evolutions are replaced by the geometrical multipliers in the case of dissipative evolution equations, phenomenologically described by non-hermitian Hamiltonian. Latter Dattoli *et al* [4] studied the geometric phase for the optical supermode propagation in a free electron laser, which is a classical system described by a Schrödinger-like equation with non-hermitian Hamiltonian. The complex geometric phase is also studied by Nenciu and Rasche [10] and by

Kvitsinsky and Putterman [7]. Maamache *et al* [3] have also worked on this issue by using Floquet decomposition of the evolution operators.

The Lewis–Riensenfeld invariant theory was generalized by Xiao-Chun *et al* [14] for the systems with non-hermitian time-dependent Hamiltonians.

In this paper we propose a derivation of the geometric phase for meta-stable spin $\frac{1}{2}$ states in the Nuclear Magnetic Resonance Experiment.

The paper is organized as follows: In Section 2 we present a brief review of closed two-levels spin states. In Section 3 we study the dynamics of two-level spin system with damping. We investigate in Section 4 the geometrical phase for our system, both in adiabatic and non-adiabatic evolutions.

2. Review of the Closed Spin 1/2 in Nuclear Magnetic Resonance Experiment

In Nuclear Magnetic Resonance (NMR) Experiment $\mathbf{B}(t)$ precesses around the z -axis, at fixed angle θ with constant angular velocity ω , and with constant modulus $|\mathbf{B}(t)| = B$

$$\mathbf{B}(t) = B(\sin \theta \cos(\omega t)\mathbf{e}_x + \sin \theta \sin(\omega t)\mathbf{e}_y + \cos \theta \mathbf{e}_z). \quad (1)$$

$\mathbf{B}(t)$ is a superposition of a static magnetic \mathbf{B}_0 field in z -direction, and a rotating in the X - Y plane with frequency ω field $\mathbf{B}_1(t)$ (radio frequency field), i.e.,

$$\mathbf{B}(t) = \mathbf{B}_0 + \mathbf{B}_1(t) \quad (2)$$

where

$$\mathbf{B}_0 = B \cos \theta \mathbf{e}_z \quad (3)$$

and

$$\mathbf{B}_1(t) = B \sin \theta (\cos(\omega t)\mathbf{e}_x + \sin(\omega t)\mathbf{e}_y). \quad (4)$$

The spin $\frac{1}{2}$ particle coupled to a time-dependent magnetic field $\mathbf{B}(t)$ is described by the Hamiltonian

$$\hat{H}(t) = \frac{1}{2} \mathbf{B}(t) \boldsymbol{\sigma} \quad (5)$$

in which $\hbar = 1$ and where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (6)$$

The matrix form of $\hat{H}(t)$ is

$$\hat{H}(t) = \frac{B}{2} \begin{bmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{bmatrix}. \quad (7)$$

Other standard notations here are $\omega_0 = B \cos \theta$ – the **Larmor frequency** and $\omega_1 = B \sin \theta$ – the **Rabi frequency**.

If the frequency ω coincide with the Larmor frequency ω_0 , one observe the phenomena of magnetic resonance.

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

$$|\Psi_+(t)\rangle = \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{bmatrix} \quad \text{and} \quad |\Psi_-(t)\rangle = \begin{bmatrix} -\sin \frac{\theta}{2} e^{-i\omega t} \\ \cos \frac{\theta}{2} \end{bmatrix}. \quad (8)$$

The evolution of the spin states vectors $|\Psi(t)\rangle$ is given by the time-dependent Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle. \quad (9)$$

The decomposition of $|\Psi(t)\rangle$

$$|\Psi(t)\rangle = C_a(t) |+\rangle + C_b(t) |-\rangle \quad (10)$$

leads to the following system of equations

$$\begin{aligned} i \frac{d}{dt} C_a(t) &= \frac{B}{2} \cos \theta C_a(t) + \frac{B}{2} \sin \theta e^{-i\omega t} C_b(t) \\ i \frac{d}{dt} C_b(t) &= \frac{B}{2} \sin \theta e^{i\omega t} C_a(t) - \frac{B}{2} \cos \theta C_b(t) \end{aligned} \quad (11)$$

where $|+\rangle$ and $|-\rangle$ are the eigenstates of σ_z , $C_a(t)$ and $C_b(t)$ are the amplitudes that have to be found for the spin $\frac{1}{2}$ particle with its spin up or down along the z -axis.

Introducing the rotating coordinates frame

$$\tilde{C}_a(t) = e^{i\frac{\omega}{2}t} C_a(t), \quad \tilde{C}_b(t) = e^{-i\frac{\omega}{2}t} C_b(t) \quad (12)$$

we obtain

$$\begin{aligned} i \frac{d}{dt} \tilde{C}_a(t) &= \frac{\Delta}{2} \tilde{C}_a(t) + \frac{B}{2} \sin \theta \tilde{C}_b(t) \\ i \frac{d}{dt} \tilde{C}_b(t) &= \frac{B}{2} \sin \theta \tilde{C}_a(t) - \frac{\Delta}{2} \tilde{C}_b(t) \end{aligned} \quad (13)$$

where $\Delta = B \cos \theta - \omega$.

With the initial condition $|\Psi(0)\rangle = |+\rangle$ the solutions of (11) are given by

$$C_a(t) = \left(\cos \frac{\Omega}{2} t - i \frac{B \cos \theta - \omega}{\Omega} \sin \frac{\Omega}{2} t \right) e^{-i\frac{\omega}{2}t} \quad (14)$$

$$C_b(t) = - \left(i \frac{B \sin \theta}{\Omega} \sin \frac{\Omega}{2} t \right) e^{i\frac{\omega}{2}t} \quad (15)$$

with $\Omega = \sqrt{B^2 \sin^2 \theta + (B \cos \theta - \omega)^2}$, which is the generalized Rabi frequency.

3. Dynamic of Two-level Spin System with Damping

In this paper we are interested in the interactions which cause the reduction of lifetime of the spin states.

According to [6] one class of the lifetime reduction interactions may be described phenomenologically by adding decay terms to the usual equations of motion of the isolated spin $\frac{1}{2}$ in time-dependent magnetic field as follows

$$\begin{aligned} i\frac{d}{dt}C_a(t) &= \frac{B}{2}\cos\theta C_a(t) + \frac{B}{2}\sin\theta e^{-i\omega t}C_b(t) - \frac{\gamma_a}{2}C_a(t) \\ i\frac{d}{dt}C_b(t) &= \frac{B}{2}\sin\theta e^{i\omega t}C_a(t) - \frac{B}{2}\cos\theta C_b(t) - \frac{\gamma_b}{2}C_b(t) \end{aligned} \quad (16)$$

where γ_a and γ_b are the decay rates for the upper and lower level, respectively. In matrix form they look like

$$i\frac{d}{dt}\begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix} = \frac{1}{2}\begin{bmatrix} B\cos\theta - i\gamma_a & B\sin\theta e^{-i\omega t} \\ B\sin\theta e^{i\omega t} & -B\cos\theta - i\gamma_b \end{bmatrix}\begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix}.$$

Then the Schrödinger equation

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \quad (17)$$

with

$$H(t) = \frac{1}{2}\begin{bmatrix} B\cos\theta - i\gamma_a & B\sin\theta e^{-i\omega t} \\ B\sin\theta e^{i\omega t} & -B\cos\theta - i\gamma_b \end{bmatrix} \quad (18)$$

which is obviously a non-hermitian Hamiltonian, describes the dissipative evolutions equations (16).

We note that here we work in a complex parametric space and $H(t)$ is 2×2 matrix in the two-dimensional complex Hilbert space.

Let us introduce the following change of the coordinates

$$\tilde{C}_a(t) = e^{\frac{1}{2}\Gamma t}C_a(t), \quad \tilde{C}_b(t) = e^{\frac{1}{2}\Gamma t}C_b(t) \quad (19)$$

with $\Gamma = \frac{\gamma_a + \gamma_b}{2}$.

In matrix form this reads

$$\begin{bmatrix} \tilde{C}_a(t) \\ \tilde{C}_b(t) \end{bmatrix} = \begin{bmatrix} e^{\frac{1}{2}\Gamma t} & 0 \\ 0 & e^{\frac{1}{2}\Gamma t} \end{bmatrix}\begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix}.$$

Thus, we have constructed a non-unitary transformation $U(t)$ given by

$$U(t) = \begin{bmatrix} e^{\frac{1}{2}\Gamma t} & 0 \\ 0 & e^{\frac{1}{2}\Gamma t} \end{bmatrix}$$

that allows us to define a new state vector $|\tilde{\Psi}(t)\rangle = \begin{bmatrix} \tilde{C}_a(t) \\ \tilde{C}_b(t) \end{bmatrix}$ which is related to $|\Psi(t)\rangle = \begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix}$ by the equation

$$|\tilde{\Psi}(t)\rangle = U(t)|\Psi(t)\rangle. \quad (20)$$

The equations of motion (16) are transformed to

$$\begin{aligned} i\frac{d}{dt}\tilde{C}_a(t) &= \frac{B}{2}\left(\cos\theta - i\frac{k}{B}\right)\tilde{C}_a(t) + \frac{B}{2}\sin\theta e^{-i\omega t}\tilde{C}_b(t) \\ i\frac{d}{dt}\tilde{C}_b(t) &= \frac{B}{2}\sin\theta e^{i\omega t}\tilde{C}_a(t) - \frac{B}{2}\left(\cos\theta - i\frac{k}{B}\right)\tilde{C}_b(t). \end{aligned} \quad (21)$$

Therefore the system is described by the following Schrödinger equation

$$i\frac{d}{dt}\begin{bmatrix} \tilde{C}_a(t) \\ \tilde{C}_b(t) \end{bmatrix} = \frac{B}{2}\begin{bmatrix} \cos\theta - i\frac{k}{B} & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta + i\frac{k}{B} \end{bmatrix}\begin{bmatrix} \tilde{C}_a(t) \\ \tilde{C}_b(t) \end{bmatrix} \quad (22)$$

where $k = \frac{1}{2}(\gamma_a - \gamma_b)$ and the non-hermitian Hamiltonian

$$\tilde{H}(t) = \frac{B}{2}\begin{bmatrix} \cos\theta - i\frac{k}{B} & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta + i\frac{k}{B} \end{bmatrix}. \quad (23)$$

We remark that by replacing $\cos\theta$ by $\cos\theta - i\frac{k}{B}$ in the Hamiltonian given in equation (7), which describe the isolated system we obtain the non-hermitian Hamiltonian $\tilde{H}(t)$ given above. Hence we can obtain easily the solution of our system.

Taking again the initial condition to be $|\Psi(0)\rangle = |+\rangle$, we get

$$\begin{aligned} C_a(t) &= \left(\cos\frac{\bar{\Omega}}{2}t - \frac{i(\Delta - ik)}{\bar{\Omega}}\sin\frac{\bar{\Omega}}{2}t\right)e^{-i\frac{\omega}{2}t}e^{-\frac{1}{2}\Gamma t} \\ C_b(t) &= -i\left(\frac{B\sin\theta}{\bar{\Omega}}\sin\frac{\bar{\Omega}}{2}t\right)e^{i\frac{\omega}{2}t}e^{-\frac{1}{2}\Gamma t} \end{aligned} \quad (24)$$

where $\bar{\Omega} = \sqrt{B^2\sin^2\theta + (B\cos\theta - \omega - ik)^2}$ is the generalized complex Rabi frequency.

We note also that the term $e^{-\frac{1}{2}\Gamma t}$ which appears in the two last equations, contribute to the attenuations of $C_a(t)$ and $C_b(t)$.

This confirm the dissipative character of the dynamics.

4. Geometrical Phase for Damped Two-Level Spin System

In this section we investigate the geometrical phase for our system of damped two-level spin system defined in Section 3.

The system is described by the non-hermitian Hamiltonian (23)

$$\tilde{H}(t) = \frac{B}{2} \begin{bmatrix} \cos \theta - i\frac{k}{B} & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta + i\frac{k}{B} \end{bmatrix} \quad (25)$$

where $k = \frac{\gamma_a - \gamma_b}{2}$.

We can write $\tilde{H}(t)$ in function of Pauli matrices as follows

$$\tilde{H}(t) = \frac{1}{2} \tilde{\mathbf{B}}(t) \boldsymbol{\sigma} \quad (26)$$

where $\tilde{\mathbf{B}}(t)$ is new magnetic field given by

$$\tilde{\mathbf{B}}(t) = B \begin{bmatrix} \sin \theta \cos(\omega t) \\ \sin \theta \sin(\omega t) \\ \cos \theta - i\frac{k}{B} \end{bmatrix}. \quad (27)$$

$\tilde{\mathbf{B}}(t)$ makes an angle $\bar{\theta}$ with the z -axis given by

$$\cos \bar{\theta} = \frac{\cos \theta - i\frac{k}{B}}{\sqrt{\sin^2 \theta + \left(\cos \theta - i\frac{k}{B}\right)^2}}, \quad \sin \bar{\theta} = \frac{\sin \theta}{\sqrt{\sin^2 \theta + \left(\cos \theta - i\frac{k}{B}\right)^2}}.$$

The eigenvalues of $\tilde{H}(t)$ are given by

$$\bar{E}_{\pm} = \pm \frac{1}{2} B \sqrt{\sin^2 \theta + \left(\cos \theta - i\frac{k}{B}\right)^2}.$$

The instantaneous eigenstates $|\varphi_{\pm}(t)\rangle$ of $\tilde{H}(t)$ are

$$|\varphi_{+}(t)\rangle = \begin{bmatrix} \cos \frac{\bar{\theta}}{2} \\ \sin \frac{\bar{\theta}}{2} e^{i\omega t} \end{bmatrix} \quad \text{and} \quad |\varphi_{-}(t)\rangle = \begin{bmatrix} -\sin \frac{\bar{\theta}}{2} e^{-i\omega t} \\ \cos \frac{\bar{\theta}}{2} \end{bmatrix}. \quad (28)$$

Here $\tilde{H}^{+}(t)$ is given by

$$\tilde{H}^{+}(t) = \frac{B}{2} \begin{bmatrix} \cos \theta + i\frac{k}{B} & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta - i\frac{k}{B} \end{bmatrix}. \quad (29)$$

The eigenvalues of $\tilde{H}^{+}(t)$ are given by

$$\bar{E}_{\pm}^{*} = \pm \frac{1}{2} B \sqrt{\sin^2 \theta + \left(\cos \theta - i\frac{k}{B}\right)^2}$$

where $*$ denotes the complex conjugate.

The instantaneous eigenstates $\langle \Phi_{\pm}(t) |$ of $\tilde{H}^{+}(t)$ are

$$\langle \Phi_{+}(t) | = \left(\cos \frac{\bar{\theta}}{2}, \sin \frac{\bar{\theta}}{2} e^{-i\omega t} \right), \quad \langle \Phi_{-}(t) | = \left(-\sin \frac{\bar{\theta}}{2} e^{i\omega t}, \cos \frac{\bar{\theta}}{2} \right). \quad (30)$$

According to [5] the complex adiabatic Berry phase for a cyclic evolution ($T = 2\pi/\omega$) are defined by

$$\gamma_{\pm}^G = i \int_0^T \langle \Phi_{\pm}(t) | \frac{\partial}{\partial t} | \varphi_{\pm}(t) \rangle dt. \quad (31)$$

By substituting the instantaneous eigenstates given above one obtain the complex adiabatic geometrical phase for our system

$$\gamma_{\pm}^G = \mp \pi (1 - \cos \bar{\theta}) = \mp \pi \left(1 - \frac{\cos \theta - i \frac{k}{B}}{\sqrt{\sin^2 \theta + \left(\cos \theta - i \frac{k}{B} \right)^2}} \right). \quad (32)$$

For the non-adiabatic evolutions we use the Lewis–Riensenfeld invariant theory [8] generalized by Gao *et al* to non-hermitian systems [14].

According to Lewis–Riensenfeld theory the non-hermitian invariant $I(t)$ associated to the Hamiltonian $\tilde{H}(t)$ given in equation (23) can be expressed as linear combinations of Pauli matrices, i.e.,

$$I(t) = \frac{1}{2} (r_1(t) \sigma_+ + r_2(t) \sigma_- + r_3(t) \sigma_3)$$

or

$$I(t) = \frac{1}{2} \begin{bmatrix} r_3(t) & r_1(t) \\ r_2(t) & -r_3(t) \end{bmatrix} \quad (33)$$

where $r_1(t)$, $r_2(t)$ and $r_3(t)$ are three time-dependent complex parameters.

$I(t)$ satisfies the **Liouville–von Neumann equation**

$$\frac{d}{dt} I(t) = \frac{\partial}{\partial t} I(t) - i [I(t), \tilde{H}(t)] = 0. \quad (34)$$

The substitution of expressions of $I(t)$ and $\tilde{H}(t)$ in equation (34) leads to the system of coupled differential equations

$$\frac{dr_1}{dt} = i [B \sin \theta e^{-i\omega t} r_3 - (B \cos \theta - ik) r_1] \quad (35)$$

$$\frac{dr_2}{dt} = i [(B \cos \theta - ik) r_2 - B \sin \theta e^{i\omega t} r_3] \quad (36)$$

$$\frac{dr_3}{dt} = \frac{i}{2} [B \sin \theta e^{i\omega t} r_1 - B \sin \theta e^{-i\omega t} r_2]. \quad (37)$$

The solution of these equations which satisfies the cyclicity of $I(t)$, i.e. $I(T) = I(0)$ with

$$T = \frac{2\pi}{\omega} \quad (38)$$

are given by

$$r_1(t) = \frac{B \sin \theta}{\sqrt{B^2 \sin^2 \theta + (B \cos \theta - ik - \omega)^2}} \exp(-i\omega t) \quad (39)$$

$$r_2(t) = \frac{B \sin \theta}{\sqrt{B^2 \sin^2 \theta + (B \cos \theta - ik - \omega)^2}} \exp(i\omega t) \quad (40)$$

$$r_3 = \frac{B \cos \theta - ik - \omega}{\sqrt{B^2 \sin^2 \theta + (B \cos \theta - ik - \omega)^2}}. \quad (41)$$

It is obvious that the vector $\mathbf{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \\ r_3 \end{bmatrix}$ precesses around the z -axis with the angular velocity ω , and makes with this axis an angle α given by

$$\cos \alpha = \frac{B \cos \theta - ik - \omega}{\sqrt{B^2 \sin^2 \theta + (B \cos \theta - ik - \omega)^2}} \quad (42)$$

$$\sin \alpha = \frac{B \sin \theta}{\sqrt{B^2 \sin^2 \theta + (B \cos \theta - ik - \omega)^2}}.$$

Thus, the final expressions of $r_1(t)$, $r_2(t)$, $r_3(t)$ are

$$r_1(t) = \sin \alpha \exp(-i\omega t) \quad (43)$$

$$r_2(t) = \sin \alpha \exp(i\omega t) \quad (44)$$

$$r_3 = \cos \alpha \quad (45)$$

and the invariant is

$$I(t) = \frac{1}{2} \begin{bmatrix} \cos \alpha & \sin \alpha \exp(-i\omega t) \\ \sin \alpha \exp(i\omega t) & -\cos \alpha \end{bmatrix}.$$

The eigenvalues of $I(t)$ are given by

$$\lambda_{\pm} = \pm \frac{1}{2} \quad (46)$$

which are time-independent.

The instantaneous eigenstates $|\lambda_+, t\rangle$ and $|\lambda_-, t\rangle$ are

$$|\lambda_+, t\rangle = \begin{bmatrix} \cos \frac{\alpha}{2} \\ \sin \frac{\alpha}{2} e^{i\omega t} \end{bmatrix}, \quad |\lambda_-, t\rangle = \begin{bmatrix} -\sin \frac{\alpha}{2} e^{-i\omega t} \\ \cos \frac{\alpha}{2} \end{bmatrix}. \quad (47)$$

The instantaneous eigenstates $\langle \mu_+, t|$ and $\langle \mu_-, t|$ of $I^+(t)$ are given by

$$\langle \mu_+, t| = \left(\cos \frac{\alpha}{2}, \sin \frac{\alpha}{2} e^{-i\omega t} \right), \quad \langle \mu_-, t| = \left(-\sin \frac{\alpha}{2} e^{i\omega t}, \cos \frac{\alpha}{2} \right). \quad (48)$$

Following [14] the complex geometrical non-adiabatic phase for a cyclic evolution ($T = \frac{2\pi}{\omega}$) is defined by

$$\beta_{\pm}^G(t) = i \int_0^T \langle \mu_{\pm}, t | \frac{\partial}{\partial t} | \lambda_{\pm}, t \rangle dt. \quad (49)$$

By substituting the instantaneous eigenstates given above, one obtain finally the complex geometrical non-adiabatic phase for our system

$$\beta_{\pm}^G = \mp \pi (1 - \cos \alpha) = \mp \pi \left(1 - \frac{\cos \theta - i \frac{k}{B} - \frac{\omega}{B}}{\sqrt{\sin^2 \theta + \left(\cos \theta - i \frac{k}{B} - \frac{\omega}{B} \right)^2}} \right). \quad (50)$$

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