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Non-integrable quantum phase in the evolution of a spin-1 system : a physical consequence of the non-trivial topology of the quantum state-space

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Résumé. — Quand un système quantique évolue de façon à décrire un chemin fermé dans l'espace des matrices densités, il doit acquérir, comme conséquence de la topologie non triviale de cet espace, une phase dépendante du chemin. Pour une évolution du vecteur d'état $|\psi\rangle$ telle que $\langle\psi|d/dt|\psi\rangle = 0$, la phase résultante est celle introduite par Aharonov et Anandan (appelée par la suite la phase A.A.). Mathématiquement, cette condition correspond à un transport parallèle de $|\psi\rangle$ associé à une connection sur un espace fibré. Ce travail contient une discussion élémentaire, ne nécessitant aucune connaissance préalable des concepts mathématiques mis en jeu, de la phase A.A. pour un système de spin 1. Cette phase apparaît alors comme l'holonomie de la connection naturelle définie sur l'espace complexe projectif $P_2(\mathbb{C})$. Une vérification expérimentale de ces idées requiert les expressions, d'une part de la phase, par une intégrale de contour, d'autre part d'un hamiltonien qui réalise le transport parallèle du vecteur d'état. Ces expressions sont données en termes de quatre quantités directement mesurables, qui paramétrisent la matrice densité d'un spin 1 dans un état pur. Il n'est pas possible de mesurer directement la phase A.A. sur un système isolé. On doit opérer une séparation, puis une réunion, de deux sous-systèmes qui subissent des évolutions différentes. Nous suggérons deux types de méthode qui, en principe, pourraient conduire à une détermination expérimentale de la phase A.A.

Abstract. — When a quantum state evolves in such a way as to describe a closed loop in the space of pure state density matrices, it must, as a consequence of the non trivial topology of this space acquire a path-dependent phase. When the state vector $|\psi\rangle$ evolution is such that $\langle\psi|d/dt|\psi\rangle = 0$, the resulting phase is that introduced by Aharonov and Anandan (thereafter called the A.A. phase). Mathematically this condition corresponds to a parallel transport of $|\psi\rangle$ by a connection defined on a fiber bundle. This paper contains an elementary and self-contained discussion of the A.A. phase for a spin-1 system. In this case, the phase appears as the holonomy of the natural connection over the complex projective space $P_2(\mathbb{C})$. Experimental verification of these ideas requires expressions for both the phase in terms of the path and a Hamiltonian which will parallelly transports the state vector along the path. They are given in terms of four directly measurable quantities which parametrize the pure state spin-1 density matrices. It is not possible to measure directly the A.A. phase on an isolated system ; it requires the separating and subsequent bringing together of two subsystems which undergo different evolutions. We suggest two ways in which, in principle, the A.A. phase might be measured in the laboratory.

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Introduction.

One of the most fundamental tenets of Quantum Mechanics is the Superposition Principle. Superficially this would seem to imply that the theory is basically a linear one. However, by virtue of the equally fundamental assumption that two wave func-

tions related by multiplication by a non-vanishing complex number define the same physical state, Quantum Mechanics contains some essentially non-linear features which lie at the heart of two phenomena which have received some attention recently. The first of these is the so-called « Berry phase » [1, 2] which is a contribution to the phase acquired by the wave function when some external parameters defining the system undergo an adiabatic cyclic change. The second and in many ways more fundamental phenomenon is what we shall call the « Aharonov-Anandan » or A.A. phase [3]. This is a contribution to the phase which results when the state itself, represented by a pure state density matrix $\rho = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$, undergoes a cyclic change which need not necessarily be adiabatic.

The Berry phase is a consequence of the geometry and topology of the space of parameters. The A.A. phase is a consequence of the fact that the space of quantum mechanical states, $E(\rho)$, is itself a non-linear space with a non-trivial topology, carrying non trivial geometric structures. Our purpose in this present paper is to provide a simple discussion for the spin-1 case which relates the A.A. phase to physically measurable quantities and to explain how, in principle, it may be measured in the laboratory. We have tried to write the paper in such a way as to make it self-contained and accessible to someone knowing no-more than elementary Quantum Mechanics ; as such, we hope that it may serve as a physicist's introduction to those concepts from fiber bundle theory which are useful for Quantum Mechanics [4].

We begin, in section 1, by expressing the differential of the A.A. phase along an arbitrary path in state-space, $E(\rho)$, in terms of 4 angular variables which parametrize the set of pure state 3×3 density matrices. This is done using an elementary operator technique. Mathematically $E(\rho)$ coincides with the complex projective plane, $P_2(\mathbb{C})$ (it would be $P_n(\mathbb{C})$ for a spin $n/2$ system). The A.A. phase may be understood mathematically in terms of a natural connection which allows one to parallelly transport the phase along an arbitrary curve in $P_2(\mathbb{C})$. We shall make contact with the standard mathematical machinery of connections on line bundles in section 2 where our 4 physically motivated parameters will be shown to provide an especially convenient set of coordinates for $P_2(\mathbb{C})$ and in particular to provide a remarkably simple form for its natural metric and connection.

To study the A.A. phase experimentally it is necessary to construct a time-dependent Hamiltonian which will take the pure state around an arbitrarily chosen closed loop in the pure state density matrix space $E(\rho)$ and at the same time parallelly transport the phase. We shall show in

section 3 that there are infinitely many Hamiltonians corresponding to a given closed loop in $E(\rho)$, all related by a kind of non-Abelian gauge transformation associated with the group $U(2) \times U(1)$. This is connected with the fact that $P_2(\mathbb{C})$ may be regarded as the coset space $U(3)/U(2) \times U(1)$. This freedom will be made use of to construct a particularly simple Hamiltonian which also parallelly transports the phase.

Since the density matrix contains all possible information about an isolated system the A.A. phase cannot be measured on an isolated system. This is in contrast with the Berry phase, differences of which may be measured on an isolated system provided it does not start out in an energy eigenstate. This will be explained in more detail in the conclusion where we shall give two suggestions as to how, in principle, the A.A. phase might be measured in the laboratory.

1. The A.A. phase and closed circuits in the space of pure state density matrices.

Let us consider a quantum system described by a Hilbert space state vector $|\psi(t)\rangle$ which performs a cyclic evolution generated by some Hamiltonian $H(t)$ during the time interval $0 \leq t \leq T$. By cyclic evolution we mean that $|\psi(T)\rangle = \exp i\phi |\psi(0)\rangle$. (We assume here that the states $|\psi(t)\rangle$ are of unit norm). At a given time t , the results of physical measurements performed upon the system described by $|\psi(t)\rangle$ remain unchanged if we transform $|\psi(t)\rangle$ by the $U(1)$ transformation :

$$|\psi(t)\rangle \xrightarrow{U(1)} |\psi'(t)\rangle = \exp(i f(t)) |\psi(t)\rangle. \quad (1)$$

The density matrix associated with $|\psi(t)\rangle$, $|\psi(t)\rangle\langle\psi(t)|$ is obviously invariant under the above Abelian gauge transformation. The A.A. quantum phase β is the gauge invariant quantity given by :

$$\beta = \phi + i \int_0^T \langle\psi(t)| \frac{d}{dt} |\psi(t)\rangle dt \quad (2)$$

where $|\psi(t)\rangle$ is any quantum state associated with a closed curve in the manifold $E(\rho)$ of pure state density matrices i.e. such that $\rho^2 = \rho$ and $\text{Tr } \rho = 1$ ⁽¹⁾.

⁽¹⁾ It is easily seen that any Hermitian positive definite matrix such that $\rho^2 = \rho$ and $\text{Tr } \rho = 1$ can be written as $|\psi(t)\rangle\langle\psi(t)|$ (with $\langle\psi(t)|\psi(t)\rangle = 1$). Let us consider a basis which diagonalizes ρ , $\lambda_1 \dots \lambda_i \dots \lambda_n$ being eigenvalues with $\lambda_i \geq 0$. The normalization condition $\text{Tr } \rho = 1$ reads $\sum \lambda_i = 1$, while the condition $\rho^2 = \rho$ implies $\lambda_i^2 = \lambda_i$, i.e. $\lambda_i = 0$ or 1. The two conditions can be realized simultaneously if and only if $\lambda_i = 1$ for $i = i_0$ and $\lambda_i = 0$ for $i \neq i_0$. It follows immediately that $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$.

Let us first briefly consider the simple case of the spin 1/2. The pure state density matrix ρ has the form :

$$\rho = 1/2 (1 + \mathbf{p}(t) \cdot \boldsymbol{\sigma})$$

with $\mathbf{p}(t) = \langle \boldsymbol{\sigma}(t) \rangle$ ($\mathbf{p}^2 = 1$).

A quantum cycle in the space $E(\rho)$ can be associated with a closed curve drawn by the tip of the vector \mathbf{p} on the unit sphere. In reference [5] we considered the Hamiltonian $H_{\parallel} = \mathbf{s} \cdot \mathbf{p} \wedge \dot{\mathbf{p}}$, which, for a given $\rho(t)$, satisfies the two equations :

$$i\hbar \frac{\partial}{\partial t} \rho(t) = [H_{\parallel}(t), \rho(t)]$$

$$\text{Tr}(\rho H_{\parallel}(t)) = \langle \psi(t) | H_{\parallel}(t) | \psi(t) \rangle. \quad (3)$$

β was obtained by solving the Schrödinger equation associated with $H_{\parallel}(t)$. As we shall explain in more detail later on for the spin-1 case, $H_{\parallel}(t)$ generates the parallel transport of an element of a $U(1)$ fiber bundle constructed over the complex $n = 1$ projective space $P_1(\mathbb{C})$ ($P_1(\mathbb{C})$ is isomorphic to the S_2 sphere).

The spin-1 case is much more involved and we shall proceed step by step. In this section we shall first study the density matrix for pure spin-1 state in order to get a convenient parametrization of the $E(\rho)$ manifold. An arbitrary spin state (not necessarily a pure state) is completely described by the *polarisation vector* $\mathbf{p} = \hbar^{-1} \langle \mathbf{S} \rangle$, and the *alignment tensor* $A_{ij} = (2\hbar^2)^{-1} \langle \{S_i, S_j\} \rangle$ where \mathbf{S} is the spin-1 operator. The normalized 3×3 density matrix ρ can be written as a linear combination of the unit matrix $\mathbb{1}$, and the eight traceless matrices S_i and $1/2 \{S_i, S_j\} - 1/3 \mathbf{S}^2 \delta_{ij}$. The normalization condition $\text{Tr} \rho = 1$ implies the coefficients of the unit matrix be $1/3$, while the other coefficients are simple linear functions of the components of the polarization vector \mathbf{p} and the alignment tensor A_{ij} . It is convenient to introduce the quadric surface

$$A_{ij} x_i x_j - 1 = 0.$$

The matrix A_{ij} being positive definite the surface is in general an ellipsoid. To specify completely the ellipsoid we shall use the following 5 real parameters : the three Euler angles which give the space orientation of the principal axis and the two extra parameters to define the shape, taking into account the trace relation $A_{ii} = 2$. Together with the components of the polarization vector, we need eight real parameters to describe an arbitrary spin-1 state. Let us show that these eight parameters reduce to four in the case of a pure state $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$: $|\psi(t)\rangle$ is a normalized complex 3-vectors, so it involves 5 real parameters but since $\rho(t)$ is invariant by an arbitrary phase multiplication of $|\psi(t)\rangle$ we are left with 4 parameters.

To establish the geometrical relations between the polarization vector \mathbf{p} and the alignment tensor A_{ij} for pure states it is convenient to apply a rotation to the spin system in order to bring \mathbf{p} along the z axis :

$$\mathbf{p} \rightarrow \hat{z}p = R^{-1}(\theta, \varphi) \mathbf{p} \quad (4)$$

with

$$R(\theta, \varphi) = R(\hat{z}, \varphi) R(\hat{y}, \theta).$$

$R(\mathbf{n}, \alpha)$ stands for a rotation of angle α around the axis defined by the unit vector \mathbf{n} , the angles θ ($0 \leq \theta \leq \pi$), φ ($0 \leq \varphi < 2\pi$) and the positive number p ($0 \leq p \leq 1$) are the spherical coordinates of \mathbf{p} .

We define

$$|\hat{\psi}(t)\rangle = R^{-1}(\theta, \varphi) |\psi(t)\rangle.$$

By construction we have :

$$\langle \hat{\mathbf{S}} \rangle = \langle \hat{\psi}(t) | \mathbf{S} | \hat{\psi}(t) \rangle = p \hat{z}.$$

Let $\hat{C}(m)$ be the components of $|\hat{\psi}(t)\rangle$ upon the eigenstates $|1 m\rangle$ of S_z with eigenvalues $m\hbar$: Introducing the operators $S_{\pm} = S_x \pm S_y$, the conditions $\langle S_x \rangle = \langle S_y \rangle = 0$ are equivalent to :

$$\langle \hat{\psi} | S_+ | \hat{\psi} \rangle = (\langle \hat{\psi} | S_- | \hat{\psi} \rangle)^* = 0.$$

Using the relations :

$$\begin{aligned} S_+ |1 1\rangle &= 0; & S_+ |1 0\rangle &= \hbar \sqrt{2} |1 1\rangle \\ S_+ |1 -1\rangle &= \hbar \sqrt{2} |1 0\rangle \end{aligned} \quad (5)$$

we get the conditions to be satisfied by the $\hat{C}(i)$:

$$Z = \hat{C}^*(1) \hat{C}(0) + \hat{C}^*(0) \hat{C}(-1) = 0.$$

We deduce a relation involving \mathbf{p} and $\hat{C}(0)$:

$$\begin{aligned} Z \hat{C}(1) - Z^* \hat{C}(-1) &= 0 \\ = (|\hat{C}(1)|^2 - |\hat{C}(-1)|^2) \hat{C}(0) &= p \hat{C}(0). \end{aligned} \quad (6)$$

If we assume that \mathbf{p} is non-zero, the relations

$$\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = 0 \quad \text{imply} \quad \hat{C}(0) = 0.$$

From the above conditions it follows immediately that

$$\hat{A}_{zx} = \hat{A}_{zy} = 0; \quad \hat{A}_{zz} = \langle S_z^2 \rangle = 1.$$

Let us choose the following parametrization for $\hat{C}(\pm 1)$:

$$\begin{aligned} \hat{C}(1) &= \cos \chi e^{-i\alpha}; \\ \hat{C}(-1) &= \sin \chi e^{i\alpha}. \end{aligned} \quad (6)$$

We have

$$\begin{aligned} \langle (\hat{S}_+)^2 \rangle &= 2 \sin \chi \cos \chi \\ &= \langle (\hat{S}_-)^2 \rangle. \end{aligned}$$

Using the relation

$$(S_+)^2 = (S_-)^2 \dagger = S_x^2 - S_y^2 + i \{S_x, S_y\}$$

we get :

$$\begin{aligned} \hat{A}_{xx} - \hat{A}_{yy} &= \sin 2 \chi \cos 2 \alpha \\ \hat{A}_{xy} &= (\sin 2 \chi \sin 2 \alpha) / 2. \end{aligned}$$

By applying to the state $|\hat{\psi}(t)\rangle$ the rotation

$$R(\hat{z}, -\alpha) : |\hat{\psi}(t)\rangle \rightarrow |\tilde{\psi}(t)\rangle = R(\hat{z}, -\alpha) |\hat{\psi}(t)\rangle,$$

the alignment tensor is put in diagonal form. Using the trace relation $A_{ii} = 2$, we get :

$$\tilde{A}_{xx} = (1 + \sin(2\chi))/2 \quad (7a)$$

$$\tilde{A}_{yy} = (1 - \sin(2\chi))/2 \quad (7b)$$

$$\tilde{A}_{zz} = 1; \quad \tilde{A}_{ij} = 0 \quad \text{if } i \neq j. \quad (7c)$$

The geometrical interpretation of this result is the following : for pure states the alignment ellipsoid has its major axis along the polarization \mathbf{p} . There is a single quadratic relation between the length of the polarization vector p and the anisotropy of the alignment tensor $e = \tilde{A}_{xx} - \tilde{A}_{yy}$

$$e^2 + p^2 = 1.$$

To put the results of the above analysis in a convenient form we introduce the rotation $R(t)$ given by :

$$R(t) = R(\hat{z}, \varphi(t)) R(\hat{y}, \theta(t)) R(\hat{z}, \alpha(t)) \quad (8)$$

and the orthonormal set of unit vectors $\mathbf{e}_i(t) = R(t) \hat{x}_i$ where \hat{x}_i for $i = 1, 2, 3$ stand for the unit vectors along the x, y, z axis, respectively. The polarization vector \mathbf{p} and the alignment tensor \mathbf{A} for a pure state can be written as :

$$\mathbf{p} = \sin \delta \mathbf{e}_3(t) \quad (9)$$

$$\begin{aligned} \mathbf{A} &= \mathbf{e}_3(t) \otimes \mathbf{e}_3(t) + \cos^2 \delta / 2 \mathbf{e}_1(t) \otimes \mathbf{e}_1(t) + \\ &+ \sin^2 \delta / 2 \mathbf{e}_2(t) \otimes \mathbf{e}_2(t) \quad (10) \end{aligned}$$

where $\delta(t)$ is given in terms of the angle $\chi(t)$ by $\delta(t) = \pi/2 - 2\chi(t)$ with $0 < \delta < \pi/2$.

A closed circuit is drawn in the manifold $E(\rho)$ of pure state density matrices in the time interval $0 \leq t \leq T$ if the following conditions are satisfied

$$\begin{aligned} \theta(T) &= \theta(0) (0 \leq \theta(t) \leq \pi) \\ \varphi(T) &= \varphi(0) + 2n\pi \\ \alpha(T) &= \alpha(0) + k\pi \\ \delta(T) &= \delta(0) (0 < \delta(t) < \pi/2) \end{aligned} \quad (11)$$

where n and k are arbitrary integers.

Starting from the eigenstate of S_z , $|11\rangle$, we now proceed to the construction — up to an arbitrary phase — of the state $|\psi(t)\rangle$ corresponding to a given polarization vector $\mathbf{p}(t)$, and alignment tensor $A_{ij}(t)$, compatible with the pure state condition $\rho^2 = \rho$.

It is convenient to introduce the set of four 3×3 matrices (with $i = 1, 2, 3$) satisfying the relations :

$$\tau_i \tau_j = i \varepsilon_{ijk} \tau_k + \delta_{ij} \tau_0$$

$$\tau_0 = S_z^2 / \hbar^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (12a)$$

$$\tau_3 = S_z / \hbar = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (12b)$$

$$\begin{aligned} \tau_1 &= ((S_+)^2 + (S_-)^2) / 2 \hbar^2 = (S_x^2 - S_y^2) / \hbar^2 \\ &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad (12c) \end{aligned}$$

$$\begin{aligned} \tau_2 &= ((S_+)^2 - (S_-)^2) / 2 \hbar^2 = \{S_x, S_y\} / \hbar^2 \\ &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad (12d) \end{aligned}$$

The state $|\tilde{\psi}(t)\rangle = \cos \chi |11\rangle + \sin \chi |1-1\rangle$ is built from the state $|11\rangle$ by applying the unitary operator $V(\chi(t))$ defined as :

$$\begin{aligned} V(\chi(t)) &= \exp(-i\tau_2 \chi(t)) \\ &= 1 + (\cos \chi(t) - 1) \tau_0 - i \sin \chi(t) \tau_2. \end{aligned} \quad (13)$$

The state $|\psi(t)\rangle$ is obtained from $|\tilde{\psi}(t)\rangle$ by application of the unitary operator associated with the rotation $R(t)$ given in equation (8). We get finally the following expression giving $|\psi(t)\rangle$ in term of the state $|11\rangle$:

$$|\psi(t)\rangle = U(R(t)) V(\chi(t)) |11\rangle. \quad (14)$$

We are now in a position to compute the A.A. phase relative to a given closed circuit in the manifold $E(\rho)$.

Using the conditions (11), we have :

$$\begin{aligned} V(\chi(T)) &= V(\chi(0)) \\ U(R(T)) &= \exp(-ik\pi) U(R(0)). \end{aligned}$$

We deduce that $\phi = -k\pi \pmod{2\pi}$.

Let us now compute $\langle \psi(t) | \dot{\psi}(t) \rangle$. We have :

$$\begin{aligned} |\dot{\psi}(t)\rangle &= (\dot{U}(R(t)) \cdot V(\chi(t)) + \\ &+ U(R(t)) \cdot \dot{V}(\chi(t))) |11\rangle. \end{aligned}$$

Using :

$$\langle \psi(t) | = \langle 11 | V^{-1}(\chi(t)) \cdot U^{-1}(R(t))$$

we get :

$$\langle \psi(t) | \dot{\psi}(t) \rangle = \langle 11 | (P(t) + Q(t)) | 11 \rangle$$

with :

$$\begin{aligned} P(t) &= V^{-1}(\chi(t)) \cdot \dot{V}(\chi(t)) \\ Q(t) &= V^{-1}(\chi(t)) \cdot U^{-1}(R(t)) \times \\ &\quad \times \dot{U}(R(t)) \cdot V(\chi(t)). \end{aligned}$$

Using the definition of $V(\chi(t))$ given by equation (13) one gets :

$$P(t) = -i \dot{\chi}(t) \tau_2 = -i \hbar^{-2} \{S_x, S_y\} \dot{\chi}(t).$$

One immediately sees that $\langle 11 | P(t) | 11 \rangle = 0$.

To get $Q(t)$, we write the action of the infinitesimal rotation $R^{-1}(t) dR(t)$ on an arbitrary vector \mathbf{x} as :

$$R^{-1}(t) dR(t) \mathbf{x} = (\boldsymbol{\omega}(t) \wedge \mathbf{x}) dt. \quad (15)$$

Then it follows (see the appendix) :

$$U^{-1}(R(t)) \cdot \dot{U}(R(t)) = -i/\hbar \boldsymbol{\omega}(t) \cdot \mathbf{S}.$$

The computation of $\boldsymbol{\omega}(t)$ is given in the appendix. Remembering that $|\tilde{\psi}(t)\rangle = V(\chi(t))|11\rangle$ one can write $\langle 11 | Q(t) | 11 \rangle$ as :

$$\langle 11 | Q(t) | 11 \rangle = -i/\hbar \boldsymbol{\omega}(t) \cdot \langle \tilde{\psi}(t) | \mathbf{S} | \tilde{\psi}(t) \rangle.$$

By construction the polarization of the state $|\tilde{\psi}(t)\rangle$ is along the z axis so that :

$$\langle 11 | Q(t) | 11 \rangle = -i \boldsymbol{\omega}(t) \cdot \hat{z} \cdot p.$$

Using the results of the appendix one finally arrives at the following result for $i \langle \psi(t) | \dot{\psi}(t) \rangle$:

$$i \langle \psi(t) | \dot{\psi}(t) \rangle = \omega_z(t) p = \sin \delta (\dot{\varphi} \cos \theta + \dot{\alpha}).$$

The A.A. phase is then given by the following expression :

$$\begin{aligned} \beta &= k\pi + \int_0^T \sin \delta (\cos \theta \dot{\varphi} + \dot{\alpha}) dt \text{ mod } (2\pi) \\ &= \oint_C (\sin \delta \cos \theta d\varphi + (\sin \delta - 1) d\alpha) \end{aligned} \quad (16)$$

where

$$\delta = \pi/2 - 2\chi.$$

The above derivation is strictly valid only if $0 < \delta < \pi/2$. We would like to indicate that the above formula remains valid when the two limits $\delta \rightarrow \pi/2$ and $\delta \rightarrow 0$ are taken. When $\delta = \pi/2$, the state $|\tilde{\psi}(t)\rangle$ previously introduced reduces to $\exp(i\alpha)|11\rangle$ ($\cos \chi = 1$). The state is invariant upon any rotation around the \mathbf{p} axis, so that the alignment ellipsoid is axially symmetric and the

angle α has no physical content. β should reduce to the Berry phase for $m_s = \hbar$. Indeed we have :

$$\begin{aligned} \beta &= \oint_C \cos \theta d\varphi \\ &= -\Omega(C) \text{ mod } (2\pi). \end{aligned} \quad (17)$$

The limit $\delta \rightarrow 0$ is more subtle since there is no longer any polarization axis, and the method developed in this section is no longer valid. We shall give a detailed discussion of these break-downs of our parametrization in section 2. We will show that the result obtained by taking $\delta = 0$ in (16) is the correct one.

2. The A.A. phase as the holonomy factor in the parallel transport of a line bundle element ⁽²⁾.

In this section we give a derivation of the A.A. non integrable quantum phase, based upon the concept of line bundle over the projective space $P_2(\mathbb{C})$. Then we shall choose a parametrization which involves the physical parameters $\theta, \varphi, \alpha, \delta$ introduced in section 1.

We first introduce the concept of ray. We say that two vector states $|\psi\rangle$ and $|\psi'\rangle$ belong to the same ray, if there exists a complex number ξ such that $|\psi'\rangle = \xi|\psi\rangle$. To a given ray corresponds the normalized density matrix ρ :

$$\rho = \frac{|\psi\rangle \langle \psi|}{\langle \psi | \psi \rangle} \quad (18)$$

ρ is clearly identical for all the vectors $|\psi\rangle$ belonging to the same ray. In each ray we choose a representative $|Z\rangle$. It will be convenient to choose $|Z\rangle$ in such a way that when the density matrix follows a closed path during the time interval $0 \leq t \leq T$, $\rho(T) = \rho(0)$, the representative vector $|Z\rangle$ behaves in the same way, i.e. $|Z(T)\rangle = |Z(0)\rangle$. The set of rays associated with a $2S+1$ dimension Hilbert space constitutes a $2S = n$ dimensional projective space $P_n(\mathbb{C})$. The $2S+1$ dimension Hilbert space can be endowed with a line bundle structure : the set of rays is the base space of the bundle. The one-dimensional vector space of all state vectors belonging to a given ray $|\xi Z\rangle = \xi|Z\rangle$ constitutes a fiber of the bundle.

Since $P_n(\mathbb{C})$ is by definition the set of lines through the origin of \mathbb{C}_{n+1} , this line bundle is sometimes called the « tautological » line bundle over $P_n(\mathbb{C})$. Another term which is often used is the Hopf bundle.

Calling for a moment $|\psi\rangle = |\xi Z\rangle = \xi|Z\rangle$ an

⁽²⁾ The mathematical interpretation of the Berry phase in terms of the holonomy of a $U(1)$ bundle connection is due to B. Simon [2].

element of the fiber bundle, let us split its variation $d|\psi\rangle$ into two parts :

$$d|\psi\rangle = d_V|\psi\rangle + d_H|\psi\rangle. \quad (19)$$

The vertical variation $d_V|\psi\rangle$ is along the fiber, i.e. proportional to $|Z\rangle$. So we can write $d_V|\psi\rangle$ as :

$$d_V|\psi\rangle = \omega^{(1)}|Z\rangle \quad (20)$$

where $\omega^{(1)}$ is a 1-differential form.

The horizontal variation is orthogonal to the fiber, i.e. :

$$\langle\psi|d_H|\psi\rangle = 0.$$

Writing $d_H|\psi\rangle$ as :

$$d_H|\psi\rangle = d\xi|Z\rangle + \xi d|Z\rangle - \omega^{(1)}|Z\rangle$$

we obtained the 1-form $\omega^{(1)}$ from the orthogonality condition $\langle\psi|d_H|\psi\rangle = \langle Z|d_H|\psi\rangle = 0$:

$$\omega^{(1)} = d\xi + \Theta^{(1)}\xi$$

with

$$\Theta^{(1)} = \langle Z|d|Z\rangle / \langle Z|Z\rangle. \quad (21)$$

The vanishing of the one-form $\omega^{(1)}$ i.e. of the vertical component $d_V|\psi\rangle$ defines the parallel transport of $|\psi\rangle$. Let us consider the trivial fiber bundle associated with \mathbb{R}_3 , the base space being the plane xy , and the fiber the lines parallel to the z axis. The above definition coincides with the displacement parallel to the xy plane, base of the bundle. The metric of the bundle being defined as $k = \langle\psi|\psi\rangle = |\xi|^2\langle Z|Z\rangle$, one verifies that the bundle connection associated with the one-form $\omega^{(1)}$ is compatible with the metric in the sense that $dk = 0$ when the vector is parallel transported [4]

$$\begin{aligned} \frac{dk}{k} &= \frac{\langle\psi|d|\psi\rangle}{\langle\psi|\psi\rangle} + \text{c.c.} \\ &= \frac{d\xi}{\xi} + \frac{\langle Z|d|Z\rangle}{\langle Z|Z\rangle} + \text{c.c.} \\ &= \xi^{-1}\omega^{(1)} + \text{c.c.} \end{aligned}$$

Let us first consider the simple case of a spin 1/2. We take, as a ray representative $|Z\rangle$, the following state-vector :

$$|Z\rangle = U(R(\theta, \varphi))|1/2\ 1/2\rangle \exp(i\varphi/2)$$

$R(\theta, \varphi)$ is the rotation $R(\hat{z}, \varphi) \cdot R(\hat{y}, \theta)$, where θ and φ are the polar coordinates of the polarization vector \mathbf{p} :

$$\mathbf{p} = \langle Z|\boldsymbol{\sigma}|Z\rangle = R(\theta, \varphi)\hat{z}.$$

The components Z_1, Z_2 of $|Z\rangle$ upon the eigenstates of S_z read :

$$Z_1 = \cos \theta/2, \quad Z_2 = \sin \theta/2 e^{i\varphi}. \quad (22)$$

Then :

$$\begin{aligned} \Theta^{(1)} &= Z_1^* dZ_1 + Z_2^* dZ_2 \\ &= i d\varphi \sin^2(\theta/2) = i d\varphi (1 - \cos \theta)/2. \quad (23) \end{aligned}$$

When the ray (or equivalently the polarization \mathbf{p}) describes a closed loop, let us parallel transport the vector $|\xi Z\rangle$ in the bundle. The variation of the coordinate ξ in the bundle is given by :

$$\oint_C \frac{d\xi}{\xi} = - \oint_C \Theta^{(1)} = - \frac{i}{2} \oint_C d\varphi (1 - \cos \varphi)$$

or :

$$\log(\xi(T)/\xi(0)) = -i/2 \Omega(C). \quad (24)$$

The norm of $|\xi Z\rangle$ is conserved in the parallel transport and since $\langle Z|Z\rangle = 1$, we have $|\xi(T)| = |\xi(0)|$. We write : $\xi(T) = \exp i\phi \xi(0)$. Remembering that $|Z\rangle$ has been defined in such a way that its phase remains unchanged when the tip of \mathbf{p} describes a close curve (C) on the unit sphere we have

$$\beta = \phi = -\frac{1}{2} \Omega(C) \quad (25)$$

where $\Omega(C)$ is the solid angle defined by (C) on the unit sphere. In this simple example, we see that $\exp(i\beta)$ is the holonomy 1×1 matrix for the vector in the fiber associated with a closed loop in the base space $E(\rho)$.

After these preliminaries, we turn to the spin-1 case. The ray space is now the complex projective 2 dimensional space $P_2(\mathbb{C})$ which is also a real 4 dimensional Riemannian manifold. As it was shown in references [6] and [7] it constitutes a solution of Einstein equations with a cosmological term Λ in an Euclidian curved space. The total action being finite $P_2(\mathbb{C})$ can be considered as a gravitational instanton in close analogy with the Yang-Mills instantons. It is quite remarkable that such a mathematical structure turns out to be relevant to describe the physics of a system as simple as a spin-1 particle at rest.

In order to construct a ray representative $|Z\rangle$ whose parameters are closely related to the physical observables, one may directly use the result of the previous section. However, as we have already pointed out, the whole construction breaks down when $\mathbf{p} = 0$.

To construct $|Z\rangle$ it is convenient to introduce the set of state vectors $|x\rangle, |y\rangle, |z\rangle$ defined as :

$$\begin{aligned} |1\ 1\rangle &= -(|x\rangle + i|y\rangle)/\sqrt{2}; \\ |1\ -1\rangle &= (|x\rangle - i|y\rangle)/\sqrt{2} \\ |1\ 0\rangle &= |z\rangle. \end{aligned} \quad (26)$$

(We shall also use the notation $|x_1\rangle = |x\rangle, |x_2\rangle = |y\rangle, |x_3\rangle = |z\rangle$.)

We write :

$$|Z\rangle = \sum A_i |x_i\rangle. \quad (27)$$

Under a rotation R , the A_i transform like the components of a complex 3-vector \mathbf{A} . It is useful to write \mathbf{A} as the sum of two real vectors :

$$\mathbf{A} = \mathbf{a} + i\mathbf{b} . \tag{28}$$

Under the gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A}' = \exp(i\zeta) \mathbf{A}$$

the real vectors \mathbf{a} , \mathbf{b} transform as :

$$\begin{aligned} \mathbf{a} &\rightarrow \mathbf{a}' = \cos \zeta \mathbf{a} - \sin \zeta \mathbf{b} \\ \mathbf{b} &\rightarrow \mathbf{b}' = \sin \zeta \mathbf{a} + \cos \zeta \mathbf{b} . \end{aligned} \tag{29}$$

By a suitable gauge transformation the vectors \mathbf{a} , \mathbf{b} can be taken as orthogonal $\mathbf{a} \cdot \mathbf{b} = 0$. Taking into account the normalization condition $\langle Z | Z \rangle = \mathbf{A}^* \cdot \mathbf{A} = \mathbf{a}^2 + \mathbf{b}^2 = 1$, we can write \mathbf{A} in terms of two arbitrary real orthogonal vectors of unit length :

$$\mathbf{A} = \cos \eta \mathbf{u} + i \sin \eta \mathbf{v}$$

\mathbf{A} depends upon the angle η and the three Euler angles necessary to specify the unit vectors triad \mathbf{u} , \mathbf{v} , $\mathbf{w} = \mathbf{u} \wedge \mathbf{v}$. In order to get a parametrization of \mathbf{A} which is the closest possible one to that of the physical observables, we have to compute the polarization vector \mathbf{p} and the alignment tensor in terms of \mathbf{A} . The basic tools are the formulas giving the action of S_i on a vector $|x_j\rangle$:

$$S_i |x_j\rangle = i\hbar \varepsilon_{ijk} |x_k\rangle . \tag{30}$$

The simplest way to derive the above equations is to represent the spin-1 operator by the orbital momentum operator acting on the space of $\ell = 1$ wave functions $x_i f(r)$.

On immediately gets for the polarization vector \mathbf{p} ,

$$\begin{aligned} \mathbf{p} &= \hbar^{-1} \langle Z | \mathbf{S} | Z \rangle = i\mathbf{A} \wedge \mathbf{A}^* \\ &= 2 \mathbf{a} \wedge \mathbf{b} . \end{aligned} \tag{31}$$

The calculation of A_{ij} is a bit longer but straightforward :

$$\begin{aligned} A_{ij} &= (2\hbar^2)^{-1} \langle Z | \{S_i, S_j\} | Z \rangle \\ &= \delta_{ij} - (A_i A_j^* + A_i^* A_j) / 2 \\ &= \delta_{ij} - a_i a_j - b_i b_j . \end{aligned} \tag{32}$$

By comparing with the equations (9) and (10) in 1 giving \mathbf{p} and A_{ij} we are led to the parametrization :

$$\mathbf{A} = (\sin(\delta/2) \mathbf{e}_1(t) + i \cos(\delta/2) \mathbf{e}_2(t)) e^{i\alpha} . \tag{33}$$

We recall that $\mathbf{e}_i(t)$ were obtained from the unit vectors \hat{x}_i by applying the rotation $R(t)$ given by equation (8). The role of the phase factor $e^{i\alpha}$ is to guarantee that $\mathbf{A}(T) = \mathbf{A}(0)$, when the density $\rho(t)$ is varied along a closed circuit in the time interval $0 \leq t \leq T$, according to equation (11).

The 1-form $\omega^{(1)}$ associated with parallel transport is given in terms of $\mathbf{A}(t)$ by :

$$\omega^{(1)} = d\xi + (\mathbf{A}^* \cdot d\mathbf{A}) \xi .$$

To compute the differential $d\mathbf{A}$ it is convenient to write $\mathbf{A}(t)$ as $R(t) \cdot \mathbf{A}_0(t) \exp(i\alpha)$ with

$$\mathbf{A}_0(t) = \sin(\delta/2) \hat{x} + \cos(\delta/2) \hat{y} :$$

$$d\mathbf{A} = dR(t) \cdot \mathbf{A}_0 e^{i\alpha} + i d\alpha \mathbf{A}(t) + R(t) d\mathbf{A}_0 e^{i\alpha} .$$

The scalar product $\mathbf{A}^* \cdot d\mathbf{A}$ reads as follows :

$$\begin{aligned} \mathbf{A}^* \cdot d\mathbf{A} &= \mathbf{A}_0^* (R^{-1}(t) dR(t) \mathbf{A}_0) + \\ &\quad + i d\alpha + \mathbf{A}_0^* \cdot d\mathbf{A}_0 . \end{aligned}$$

One verifies immediately that $\mathbf{A}_0^* \cdot d\mathbf{A}_0 = 0$. Using the results of the appendix for $R^{-1}(t) dR$ one gets :

$$\begin{aligned} \mathbf{A}^* \cdot d\mathbf{A} &= \mathbf{A}_0^* \cdot (\boldsymbol{\omega}(t) \wedge \mathbf{A}_0) dt + i d\alpha \\ &= -i \sin \delta \omega_z(t) dt + i d\alpha \\ &= -i \sin \delta (\cos \theta d\varphi + d\alpha) + i d\alpha . \end{aligned}$$

The connection 1-form $\omega^{(1)}$ reads :

$$\omega^{(1)} = d\xi - i (\sin \delta \cos \theta d\varphi + (\sin \delta - 1) d\alpha) \xi . \tag{34}$$

The change of ξ when the vector $|\xi Z\rangle$ is parallel transported is :

$$\oint_C \frac{d\xi}{\xi} = i \oint_C (\sin \delta \cos \theta d\varphi + (\sin \delta - 1) d\alpha) .$$

The norm of $|\xi Z\rangle$ remains unchanged in the transport so that the phase shift is given by :

$$\beta = \oint_C (\sin \delta \cos \theta d\varphi + (\sin \delta - 1) d\alpha) .$$

One recovers the formula (16) obtained in section 1 using an operator formalism.

To complete this section we would like to relate the parametrization used above to the discussion in [7]. The main point is that in both this paper and in reference [7] Euler angles are used but these correspond to 2 entirely different actions of two distinct subgroups of $SU(3)$. In this paper we used the real $SO(3)$ subgroup of $SU(3)$ with respect to which \mathbf{A} is a complex 3-vector. In [7] use was made of the $SU(2)$ subgroup of $SU(3)$ which acts only on the states $|1 1\rangle$ and $|1 - 1\rangle$ for example but leaves the state $|1 0\rangle$ invariant. With respect to this $SU(2)$ subgroup the quantities $\zeta^1 = C(1)/C(0)$, $\zeta^2 = C(-1)/C(0)$ behave as a spinor of $SU(2)$. For physical purposes, regarding $P_2(\mathbb{C})$ as a spin-1 system, it is the diagonal $SO(3)$ action which is important. In both cases the orbits of the group action on $P_2(\mathbb{C})$ are generically 3-dimensional so we can parametrize points in $P_2(\mathbb{C})$ by 3 Euler angles, one further quantity labelling the orbits. In [7] the coordinate is r , in this paper it is χ (or equivalently δ).

Since topologically $P_2(\mathbb{C})$ is not a product of $SU(2)$ or $SO(3)$ with a line on a circle, the parametrization must break down somewhere. It does so when

the orbits collapse either to points (called « NUT's » in [7]) or 2-spheres (called « Bolts » in [7]).

It should be emphasized that these are merely coordinate singularities. In the case of the parametrization used in this paper the points $\chi = 0$ and $\chi = \pi/2$ are both bolts. As mentioned above $\chi = 0$, i.e. $\delta = \pi/2$ corresponds to the case when the alignment ellipsoid is axially symmetric so to specify it we need give only the direction of the polarization vector \mathbf{p} which is its principal axis. The angle α then ceases to have any significance. The states for which $\chi = \pi/2$, $\delta = 0$ are those for which the polarization vector \mathbf{p} vanishes or equivalently those for which the real 3-vectors \mathbf{a} and \mathbf{b} are parallel. By a suitable choice of phase \mathbf{b} may be set to zero and given the normalization conditions we see that the set of such states is in 1-1 correspondence with points on a unit sphere. In the coordinates used in [7] we have a NUT at $\zeta^1 = \zeta^2 = 0$, corresponding to the single state $|10\rangle$ and a bolt at $\zeta^1 = \zeta^2 = \infty$ corresponding to the 2-spheres associated with states having $C(0) = 0$.

It is of some interest to compute the Fubini-Study metric on $P_2(\mathbb{C})$ using the parametrization defined in section 1. Using the decomposition $d|\psi\rangle = d_H|\psi\rangle + d_V|\psi\rangle$ introduced before, we can write :

$$ds^2 = (d\langle\psi|)d|\psi\rangle = (d_V\langle\psi|)d_V|\psi\rangle + (d_H\langle\psi|)d_H|\psi\rangle.$$

(If $|\psi\rangle$ is normalized, ds^2 can be considered as the metric of a S_5 sphere). The first term represents the metric associated with a displacement along the fiber while the second one is the Fubini-Study metric on the base space. If the ray representative is normalized $\langle Z|Z\rangle = 1$ and if we limit ourselves to $U(1)$ fiber bundle $\xi = e^{i\phi}$, we have :

$$(d_V\langle\psi|)d_V|\psi\rangle = |\omega^{(1)}|^2 = |i d\phi + \langle Z|d|Z\rangle|^2.$$

As we have seen before the vanishing of the 1-form $\omega^{(1)}$ defines the parallel transport of the vector $|\psi\rangle$ in the fiber.

The Fubini-Study metric on $P_2(\mathbb{C})$ is given by :

$$ds^2 = (d_H\langle\psi|)d_H|\psi\rangle = (d\langle Z|)d|Z\rangle - \langle Z|d|Z\rangle(d\langle Z|)|Z\rangle. \quad (35)$$

We have shown previously that a convenient ray representative involving the parameter introduced in section 1, is the complex 3-vector :

$$\mathbf{A} = e^{i\alpha} R(t) \mathbf{A}_0$$

with

$$\mathbf{A}_0 = (\hat{x} \sin \delta/2 + i \hat{y} \cos \delta/2).$$

The quantity $\langle Z|d|Z\rangle$ has been already computed :

$$\langle Z|d|Z\rangle = \mathbf{A}^* \cdot d\mathbf{A} = i dt \sin \delta \omega_z(t) + i d\alpha.$$

The computation of $(d\langle Z|)d|Z\rangle = d\mathbf{A}^* \cdot d\mathbf{A}$ relies upon simple rotation group properties and uses the results given in the appendix. The result reads as follows :

$$(d\langle Z|)d|Z\rangle = d\alpha^2 + (d\delta/2)^2 - 2 d\alpha dt \sin \delta \omega_z + (dt)^2 \left[\omega_z^2 + \frac{1 + \cos \delta}{2} \omega_x^2 + \frac{1 - \cos \delta}{2} \omega_y^2 \right].$$

Combining the above results as in equation (35) we get :

$$ds^2 = (d\delta/2)^2 + \cos^2 \delta \lambda_3^2 + \frac{1 + \cos \delta}{2} \lambda_1^2 + \frac{1 - \cos \delta}{2} \lambda_2^2 \quad (36)$$

where $\lambda_i = \omega_i dt$ are the left invariant 1-forms on $SO(3)$ defined in the appendix. This expression should be contrasted with the result obtained in reference [7] :

$$\frac{dr^2}{(1+r^2)^2} + \frac{r^2}{4(1+r^2)^2} \sigma_3^2 + \frac{r^2}{4(1+r^2)} (\sigma_1^2 + \sigma_2^2)$$

where $\sigma_1, \sigma_2, \sigma_3$ are left invariant 1-forms on $SU(2)$. The metric given by equation (36) is of general triaxial Bianchi IX form. It is remarkable that the physically motivated $SO(3)$ parametrization leads to such a simple expression for the metric components. This is especially so because the general triaxial Bianchi IX Einstein metric is not known and those special cases that are known can usually only be expressed in terms of elliptic functions.

3. Construction of the Hamiltonian which generates the parallel transport in the fiber bundle over $P_2(\mathbb{C})$.

An arbitrary state time-dependent states $|\psi(t)\rangle$ can be written as $|\psi(t)\rangle = |\xi(t)Z(t)\rangle = \xi(t)|Z(t)\rangle$. Let us first show that the 1-form $\langle\psi(t)|d|\psi(t)\rangle$ is proportional to the connection 1-form $\omega^{(1)}$ introduced in 2 :

$$\begin{aligned} \langle\psi(t)|d|\psi(t)\rangle &= \xi^*(t) d\xi \langle Z(t)|Z(t)\rangle + |\xi|^2 \langle Z(t)|d|Z(t)\rangle \\ &= (d\xi + \Theta^{(1)}\xi) / (\xi^* \langle Z(t)|Z(t)\rangle) \\ &= \omega^{(1)} / (\xi^* \langle Z(t)|Z(t)\rangle). \end{aligned}$$

For the physical situation where the time evolution of is governed by a Hamiltonian, $|\psi(t)\rangle$ and $|Z(t)\rangle$ have constant norms so that $\omega^{(1)} = 0$ and $\langle\psi(t)|d|\psi(t)\rangle = 0$ are equivalent statements.

In order to allow for an experimental verification of the theoretical ideas developed in this paper, it is necessary to construct a time-dependent Hamiltonian $H_{\parallel}(t)$ which satisfies the two following conditions :

i) for a given density matrix $\rho(t)$ which goes around a closed circuit in the manifold $E(\rho)$, $H_{\parallel}(t)$ must satisfy the quantum Liouville equation :

$$i\hbar \frac{\partial}{\partial t} \rho(t) = [H_{\parallel}(t), \rho(t)] \quad (37)$$

ii) the time evolution governed by $H_{\parallel}(t)$ corresponds to a parallel transport :

$$i\hbar \langle \psi(t) | \dot{\psi}(t) \rangle = \langle \psi(t) | H_{\parallel}(t) | \psi(t) \rangle$$

or in terms of the density matrix :

$$\text{Tr}(\rho(t) H_{\parallel}(t)) = 0. \quad (38)$$

As a first step we shall solve (37) considered as an equation for $H(t)$. As we shall see, there exists an infinite set of solutions, which can be related by transformations which bear a close resemblance with non-Abelian gauge transformations.

Let us perform upon the system described by $\rho(t)$ a time-dependent unitary transformation

$$|\psi(t)\rangle = X(t) |\psi_0(t)\rangle$$

where

$$X(t) = U(R(t)) \cdot V(\chi(t)) \quad (39)$$

is the unitary operator introduced in section 1.

The transformed density matrix ρ_0 , such that $\rho(t) = X(t) \rho_0 X^{-1}(t)$ is nothing but :

$$\rho_0 = |11\rangle \langle 11| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (40)$$

The evolution of the state $|\psi_0(t)\rangle = X^{-1}(t) |\psi(t)\rangle$ is governed by the Hamiltonian $H_0(t)$ which is related to $H(t)$ by the equation :

$$H(t) = i\hbar \dot{X}(t) X^{-1}(t) + X(t) H_0(t) X^{-1}(t). \quad (41)$$

By definition of H_0 we have

$$i\hbar \frac{\partial}{\partial t} \rho_0 = [H_0(t), \rho_0] = 0 \quad (42)$$

since $\rho_0 = |11\rangle \langle 11|$ is time-independent. It follows that $H_0(t)$ can be represented by the most general Hermitian 3×3 matrix which commutes with ρ_0 . It is easily seen that H_0 has to be of the following form :

$$H_0(t) = \begin{pmatrix} \hbar\omega_0(t) & 0 & 0 \\ 0 & \sqrt{h_0(t)} & \\ 0 & & h_0(t) \end{pmatrix} \quad (43)$$

where $h_0(t)$ is an arbitrary 2×2 Hermitian matrix.

To get an explicit expression for $H(t)$ as given by (41) and (43), we have to evaluate $i\hbar \dot{X}(t) X^{-1}(t)$:

$$\begin{aligned} i\hbar \dot{X}(t) \cdot X^{-1}(t) &= i\hbar \dot{U}(R(t)) \times \\ &\times U^{-1}(R(t)) + U(R(t)) \\ &\times (i\hbar \dot{V}(\chi(t)) \cdot V^{-1}(\chi(t))) \cdot U^{-1}(R(t)). \end{aligned}$$

The first term $i\hbar \dot{U}(R(t)) \cdot U^{-1}(R(t))$ is computed in the appendix and found to be :

$$i\hbar \dot{U}(R(t)) U^{-1}(R(t)) = \mathbf{\Omega} \cdot \mathbf{S} \quad (44)$$

where the component of $\mathbf{\Omega}$ along the x , y , z axes are given explicitly.

The Hermitian operator $i\hbar \dot{V}(\chi(t)) \cdot V^{-1}(\chi(t))$ is readily obtained from equation (13) :

$$i\hbar \dot{V}(\chi(t)) \cdot V^{-1}(\chi(t)) = \dot{\chi}(t) \{S_x, S_y\} / \hbar. \quad (45)$$

Using the transformation law :

$$U(R(t)) \mathbf{S} \cdot \mathbf{a} U^{-1}(R(t)) = \mathbf{S} \cdot (R(t) \mathbf{a}) \quad (46)$$

we obtain :

$$\begin{aligned} H(t) &= \hbar^{-1} \dot{\chi} \{ \mathbf{S} \cdot \mathbf{e}_1(t), \mathbf{S} \cdot \mathbf{e}_2(t) \} + \mathbf{\Omega} \cdot \mathbf{S} \\ &+ X(t) H_0 X^{-1}(t) \end{aligned} \quad (47)$$

where $\mathbf{e}_i(t) = R(t) \hat{x}_i$ and H_0 is given by (43). In order to get $H_{\parallel}(t)$ we have to impose the condition $\text{Tr}(\rho(t) H_{\parallel}) = 0$.

The first term in the r.h.s. of (47) can be easily shown to give no contribution to the trace by going to the rotated frame where

$$\tilde{\rho}(t) = U^{-1}(R(t)) \rho(t) U(R(t))$$

is given by :

$$\tilde{\rho}(t) = \frac{1}{2} (\tau_0 + \tau_3 \cos 2\chi + \tau_1 \sin 2\chi).$$

The other two contributions are readily obtained and the parallel transport condition reads :

$$\text{Tr}(\rho(t) H_{\parallel}(t)) = \hbar \mathbf{\Omega} \cdot \mathbf{p} + \hbar \omega_0(t).$$

In the appendix we show that $\mathbf{\Omega} = R(t) \boldsymbol{\omega}$. Remembering that $\hat{p} = R(t) \hat{z}$, we have :

$$\mathbf{\Omega} \cdot \mathbf{p} = p \omega_z(t).$$

The parallel transport condition determines the real parameter $\omega_0(t)$:

$$\omega_0(t) = -p \omega_z(t) = -p (\cos \theta \dot{\phi} + \dot{\alpha}) \quad (48)$$

but leaves the 2×2 matrix $h_0(t)$ undetermined. If we exclude, for H_0 , a form proportional to the unit operator, the simplest choice for $H_0(t)$, compatible with the parallel transport condition, turns out to be :

$$H_0(t) = -\hbar \omega_z(t) p \tau_0 = -\omega_z(t) p S_z^2 / \hbar.$$

The quantity $X(t) H_0 X^{-1}(t)$ is readily evaluated by noting that H_0 commutes with $V(\chi(t))$ and by using the transformation law (46). We arrive in this way to the following expression for $H_{\parallel}(t)$:

$$\begin{aligned} H_{\parallel}(t) &= \hbar^{-1} \dot{\chi} \{ \mathbf{S} \cdot \mathbf{e}_1(t), \mathbf{S} \cdot \mathbf{e}_2(t) \} + \mathbf{\Omega} \cdot \mathbf{S} - \\ &- \hbar^{-1} \mathbf{\Omega} \cdot \mathbf{p} (\mathbf{S} \cdot \hat{p})^2. \end{aligned} \quad (49)$$

It is of some interest to rewrite $H_{\parallel}(t)$ in terms of the derivative of $\hat{p}(t) = \mathbf{e}_3(t)$. We have :

$$\begin{aligned}\dot{\hat{p}}(t) &= (d/dt R(t)) \cdot \hat{z} \\ &= (d/dt R(t)) \cdot R^{-1}(t) \cdot \hat{p}(t) \\ &= \boldsymbol{\Omega}(t) \wedge \hat{p}(t).\end{aligned}$$

Using the identity :

$$\hat{p}(t) \wedge (\boldsymbol{\Omega}(t) \wedge \hat{p}(t)) = \boldsymbol{\Omega}(t) - (\boldsymbol{\Omega}(t) \cdot \hat{p}(t)) \hat{p}(t)$$

we obtain an alternative form for $H_{\parallel}(t)$:

$$\begin{aligned}H_{\parallel}(t) &= \hbar^{-1} \chi \{ \mathbf{S} \cdot \mathbf{e}_1(t), \mathbf{S} \cdot \mathbf{e}_2(t) \} \times \\ &\quad + \mathbf{S} \cdot \hat{p}(t) \wedge \hat{p}(t) \\ &\quad + \boldsymbol{\Omega} \cdot \hat{p} (\mathbf{S} \cdot \hat{p} - \hbar^{-1} p (\mathbf{S} \cdot \hat{p})^2). \quad (50)\end{aligned}$$

If we limit ourselves to the quantum cycles which can be generated by Hamiltonians linear in \mathbf{S} , the length of \mathbf{p} remain constant so that the term proportional to χ is absent. By making the further assumption that $|\mathbf{p}| = 1$, the third term can also be ignored : the state $|\psi(t)\rangle$ being of the form $U(R(t))|11\rangle$, we have :

$$\begin{aligned}(\mathbf{S} \cdot \hat{p} - \hbar^{-1} (\mathbf{S} \cdot \hat{p})^2) |\psi(t)\rangle &= \\ &= U(R(t)) (S_z - \hbar^{-1} S_z^2) |11\rangle = 0.\end{aligned}$$

When $|\mathbf{p}| = 1$, the parallel transport Hamiltonian then reduces to :

$$H_{\parallel}(t) = \left(\mathbf{p}(t) \wedge \frac{d}{dt} \mathbf{p}(t) \right) \cdot \mathbf{S}. \quad (51)$$

One recovers an expression identical to the one obtained in the spin-1/2 case [5].

We would like now to show that the Hamiltonians $H(t)$ corresponding to different choices of $H_0(t)$ having the form specified by equation (43) are connected by transformations having a close resemblance with non-Abelian gauge transformations. For a given $\rho(t)$, we construct the set of unitary transformations $W(t)$ which leave $\rho(t)$ invariant. As before we write :

$$\rho(t) = X(t) \rho_0 X^{-1}(t); \quad |\psi(t)\rangle = X(t) |\psi_0(t)\rangle.$$

The unitary transformations

$$|\psi_0(t)\rangle \rightarrow |\psi'_0(t)\rangle = W_0(t) |\psi_0(t)\rangle$$

which leave ρ_0 invariant, i.e. such that $[\rho_0, W_0(t)] = 0$, are easily seen to be of the form :

$$W_0(t) = \begin{pmatrix} \exp i \gamma(t) & 0 & 0 \\ 0 & \sqrt{w_0(t)} & \\ 0 & & \end{pmatrix} \quad (52)$$

where w_0 is a 2×2 unitary matrix. The transformations which leave $\rho(t)$ invariant are then given in terms of W_0 by :

$$W(t) = X(t) W_0 X^{-1}(t).$$

The evolution of the transformed state

$$|\psi'(t)\rangle = W(t) |\psi(t)\rangle$$

is governed by the Hamiltonian $H'(t)$ given by

$$H'(t) = W(t) H(t) W^{-1}(t) + i \hbar \dot{W}(t) W^{-1}(t). \quad (53)$$

Since $\rho'(t) = W(t) \rho(t) W^{-1}(t) = \rho(t)$, $H'(t)$ is another solution of the Liouville equation for a given $\rho(t)$. One can verify that $H'(t)$ can also be obtained from equation (41) by replacing $H_0(t)$ by :

$$H'_0(t) = W_0(t) H_0(t) W_0^{-1}(t) + i \hbar \dot{W}_0(t) W_0^{-1}(t).$$

When $W_0(t)$ is given by equation (52), $H_0(t)$ can be written in a form similar to the right hand side of equation (43).

The Hamiltonian $H(t)$ is an element of the SU_3 Lie algebra. The transformation $H(t) \rightarrow H'(t)$ given by equation (53) is that of the time component of a $U(3)$ gauge field, but with gauge matrices belonging to a subgroup $U(1) \otimes U(2)$ of $U(3)$.

The parallel transport Hamiltonian given by (49) appears as the result of a particular choice of gauge.

As a final remark, let us point out that the fact the unitary transformations $W(t)$ which leave $\rho(t)$ invariant belong to a subgroup $U(1) \otimes U(2)$ of $U(3)$, constitutes an illustration of the isomorphy property of $P_2(\mathbb{C})$ with respect to the group quotient $U(3)/(U(1) \otimes U(2))$.

4. Conclusion.

In conclusion, we would like to add a few remarks concerning the possibility of measuring the non-integrable phase β associated with a quantum cycle in the time interval $0 \leq t \leq T$. In the case of the Berry phases one deals with cycles in the external parameter space. The density matrix for $t = T$ does not coincide with the initial one if the system is initially a coherent mixture of states with different energies. By performing a measurement of the system at time T , one can get the differences of Berry phases relative to the eigenstates involved in the mixture, and consequently some information on the history of the system during the time interval $0 \leq t \leq T$ is obtained [5, 8, 9, 10]. In contrast, in the case of the A.A. phase, one considers cycles in density matrix space, which means that $\rho(0) = \rho(T)$. For an isolated system, all the measurable physical information is contained in the density matrix, so that complete sets of measurements performed at $t = 0$ and $t = T$ will give identical results and nothing can be learnt about the history of the system during the quantum cycle by performing measurement at the end of the cycle. In other words, the A.A. phase cannot be measured on an isolated system.

We are going to discuss briefly two types of methods which may lead to an empirical determination of the A.A. phase β . Instead of describing the methods in general terms, we shall illustrate the basic ideas by specific examples.

i) In the first class of methods one assumes that the density matrix $\rho(t)$, which undergoes a quantum closed circuit, describes only part of the physical degrees of freedom of the system. Writing $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$, the state vector of the system $|\Psi(t)\rangle$ is of the form :

$$|\Psi(t)\rangle = |\phi(t)\rangle \otimes |\psi(t)\rangle .$$

As a concrete example, one may take a non relativistic neutral particle of spin S , $|\phi(t)\rangle$ and $|\psi(t)\rangle$ being respectively associated with the orbital and spin degrees of freedom. An initial beam is split into two, one of the beams travels freely — as far as the spin degrees of freedom are concerned — while the second beam is subjected to the action of a spin-dependent interaction $H(t)$ in such a way that $|\psi(t)\rangle$ is parallel transported along a closed circuit during the time interval $0 \leq t \leq T$. By measuring the interference of the two beams for $t \geq T$ one can get the A.A. phase, in the same way as the Berry phase has been recently measured by a neutron interferometry experiment [11]. Cooled beams of neutral atoms are becoming available ; it is conceivable that interferometry experiments involving light neutral atoms could be performed in a not too distant future, offering an opportunity of measuring the A.A. phase for $S \geq 1$.

ii) In the second type of methods, the Hilbert space \mathcal{K} of the physical states is written as a direct sum of two subspaces \mathcal{K}_0 and \mathcal{K}_1 : $\mathcal{K} = \mathcal{K}_0 \oplus \mathcal{K}_1$. As a typical example of \mathcal{K} , one may consider the space built from the hyperfine states $|FM\rangle$ of the ground state of atomic hydrogen [5]. \mathcal{K}_0 and \mathcal{K}_1 correspond to the states with $F = 0$ and $F = 1$, respectively. Introducing the projectors P_0 and P_1 onto the subspaces \mathcal{K}_0 and \mathcal{K}_1 the total density matrix $\rho(t)$ can be decomposed as follows :

$$\rho(t) = \rho_{00}(t) + \rho_{10}(t) + \rho_{10}(t) + \rho_{11}(t)$$

with

$$\rho_{ij} = P_i \rho(t) P_j .$$

One assumes that the subdensity matrix $\rho_{11}(t)$ (which in the present example describes a spin-1 system) is parallel transported along a closed path while $\rho_{00}(t)$ remains unchanged during the time interval $0 \leq t \leq T$. In practice, for the particular class of closed circuits discussed in the end of section 3, this can be achieved by applying a magnetic field of the form given by equation (51) and having an intensity low enough for its effect on the state $F = 0$ to be neglected.

After the cycle the coherence matrix $\rho_{10}(t)$ will be multiplied by the extra phase factor $e^{i\beta}$. A phase sensitive detection of this coherence will lead to an empirical determination of β . In the case of ground state hydrogen, the coherence $\rho_{10}(t)$ gives rise to an oscillating magnetic dipole. By measuring the beat of the field radiated by this dipole with that of a reference hydrogen maser, the A.A. phase could be obtained.

Similar procedures can be used in nuclear magnetic resonance experiments as suggested by D. Suter *et al.* [12]. According to A. Pines [13], experimental results obtained by this group could already be interpreted as a manifestation of the A.A. phase.

Appendix

Let us define the rotation $R(\varphi, \theta, \alpha)$ by :

$$R(\varphi, \theta, \alpha) = R_1(\varphi) \cdot R_2(\theta) \cdot R_3(\alpha) \quad (\text{A.1})$$

with

$$R_1(\varphi) = R(\hat{z}, \varphi), R_2(\theta) = R(\hat{y}, \theta),$$

$$R_3(\alpha) = R(\hat{z}, \alpha) \quad (\text{A.2})$$

where $R(\mathbf{n}, \alpha)$ is the rotation matrix associated with a space rotation of angle α around the axis defined by the unitary vector \mathbf{n} . The purpose of this appendix is to compute the infinitesimal rotation matrix $R^{-1}(\varphi, \theta, \alpha) \cdot dR$ where dR is the variation of the matrix $R(\varphi, \theta, \alpha)$ associated with infinitesimal variation of the angles φ, θ, α , the axes remaining fixed. To first order in $d\varphi, d\theta, d\alpha$ we have :

$$R^{-1} \cdot dR = (R_2 R_3)^{-1} (R_1^{-1} dR_1) (R_2 R_3) + R_3^{-1} (R_2^{-1} dR_2) R_3 + R_3^{-1} dR_3 .$$

When the rotation $R(\mathbf{n}, \alpha)$ is subjected to an infinitesimal variation of the angle α , we have :

$$\begin{aligned} R^{-1}(\mathbf{n}, \alpha) \cdot dR \mathbf{x} &= R^{-1}(\mathbf{n}, \alpha) (R(\mathbf{n}, \alpha + d\alpha) - R(\mathbf{n}, \alpha)) \mathbf{x} \\ &= (R(\mathbf{n}, d\alpha) - \mathbb{1}) \mathbf{x} \\ &= d\alpha \mathbf{n} \wedge \mathbf{x} \end{aligned}$$

R' being an arbitrary rotation, the following identity holds :

$$R'^{-1} \cdot R(\mathbf{n}, \alpha) \cdot R' = R(R'^{-1} \mathbf{n}, \alpha) . \quad (\text{A.3})$$

Here we shall need it for an infinitesimal rotation. The proof is straightforward in this case and goes as follows :

$$\begin{aligned} R'^{-1} \cdot R(\mathbf{n}, d\alpha) \cdot R' \mathbf{x} &= R'^{-1} \cdot (R' \mathbf{x} + d\alpha \mathbf{n} \wedge \mathbf{x}) \\ &= \mathbf{x} + d\alpha R'^{-1} \mathbf{n} \wedge \mathbf{x} . \end{aligned}$$

Using the above result, we can write $R^{-1} dR$ as :

$$\begin{aligned} R^{-1} dR &= R((R_2 R_3)^{-1} \hat{z}, d\varphi) \\ &\quad + R(R_3^{-1} \hat{y}, d\theta) \\ &\quad + R(\hat{z}, d\alpha) . \end{aligned}$$

We calculate next the components of the rotated axes :

$$\begin{aligned} (R_2 R_3)^{-1} \hat{z} &= R(\hat{z}, -\alpha) \cdot R(\hat{y}, -\theta) \hat{z} \\ &= \hat{z} \cos \theta - \sin \theta (\hat{x} \cos \alpha - \hat{y} \sin \alpha) \\ R_3^{-1} \hat{y} &= R(\hat{z}, -\alpha) \hat{y} \\ &= \hat{x} \sin \alpha + \hat{y} \cos \alpha . \end{aligned}$$

We are now in a position to write down the final formula for $R^{-1} dR$. Considering φ, θ, α , as time-dependent functions, the action of $R(\varphi, \theta, \alpha) dR$ upon an arbitrary vector x reads :

$$R^{-1}(\varphi, \theta, \alpha) dR \mathbf{x} = (\boldsymbol{\omega}(t) \wedge \mathbf{x}) dt \quad (\text{A.4})$$

with

$$\begin{aligned} \omega_x &= -\sin \theta \cdot \cos \alpha \dot{\varphi} + \sin \alpha \dot{\theta} \\ \omega_y &= \sin \theta \cdot \sin \alpha \dot{\varphi} + \cos \alpha \dot{\theta} \\ \omega_z &= \cos \theta \dot{\varphi} + \dot{\alpha} . \end{aligned} \quad (\text{A.5})$$

We also need the infinitesimal rotation $dR(t) R^{-1}(t)$, which can be obtained readily from the above result. We first note that a differentiation of $R(t) \cdot R^{-1}(t)$ gives an equivalent expression :

$$\begin{aligned} dR(t) R^{-1}(t) &= -R(t) d(R^{-1}(t)) \\ &= -R'(t)^{-1} dR'(t) \end{aligned}$$

with

$$R'(t) = R^{-1}(t) = R(\hat{z}, -\alpha) R(\hat{y}, -\theta) R(\hat{z}, -\varphi) .$$

As before we write the action of $dR(t) \cdot R^{-1}(t)$ upon an arbitrary vector \mathbf{x} as :

$$dR(t) R^{-1}(t) \mathbf{x} = \boldsymbol{\Omega}(t) \wedge \mathbf{x} dt . \quad (\text{A.6})$$

Noting the simple relation between $R'(t)$ and $R(t) = R(\varphi, \theta, \alpha)$, $\boldsymbol{\Omega}(t)$ is obtained from $\boldsymbol{\omega}(t)$ by performing the following set of transformations :

$$\begin{aligned} \varphi(t) &\rightarrow -\alpha(t), \quad \alpha(t) \rightarrow -\varphi(t), \quad \theta(t) \rightarrow -\theta(t) \\ \boldsymbol{\omega}(t) &\rightarrow \boldsymbol{\Omega}(t) = -\boldsymbol{\omega}(t) . \end{aligned}$$

Using them one gets the components of $\boldsymbol{\Omega}$ from those of $\boldsymbol{\omega}$:

$$\begin{aligned} \Omega_x &= \sin \theta \cdot \cos \varphi \dot{\alpha} - \sin \varphi \dot{\theta} \\ \Omega_y &= \sin \theta \cdot \sin \varphi \dot{\alpha} + \cos \varphi \dot{\theta} \\ \Omega_z &= \cos \theta \dot{\alpha} + \dot{\varphi} . \end{aligned} \quad (\text{A.7})$$

Finally we would like to prove the relation $\boldsymbol{\Omega}(t) = R(t) \boldsymbol{\omega}(t)$ which is not apparent in the

above derivation. To do that we write $dR \mathbf{x}$ in two different ways :

$$\begin{aligned} \text{i) } dR(t) \mathbf{x} &= R(t)(R^{-1}(t) dR(t)) \mathbf{x} = \\ &= R(t) \cdot (\boldsymbol{\omega}(t) \wedge \mathbf{x}) \\ \text{ii) } dR(t) \mathbf{x} &= dR(t) R^{-1}(t) \cdot (R(t) \mathbf{x}) = \\ &= \boldsymbol{\Omega}(t) \wedge (R(t) \mathbf{x}) . \end{aligned}$$

The sought-for relation is obtained by simple inspection.

The quantities $\lambda_i = \omega_i dt$, $\rho_i = \Omega_i dt$ are left (respectively right) invariant one-forms on the group SO(3), sometimes called Maurer-Cartan forms.

Their exterior derivatives satisfy the following relations :

$$\begin{aligned} d\lambda_i &= -\varepsilon_{ijk} \lambda_j \wedge \lambda_k \\ d\rho_i &= \varepsilon_{ijk} \rho_j \wedge \rho_k . \end{aligned}$$

The above results allow an explicit evaluation of the Hermitian operators $i\hbar U^{-1}(R(t)) \dot{U}(R(t))$ and $i\hbar \dot{U}(R(t)) U^{-1}(R(t))$, in terms of the spin operator \mathbf{S} and the vectors $\boldsymbol{\omega}, \boldsymbol{\Omega}$. One first writes

$$\begin{aligned} U^{-1}(R(t)) \dot{U}(R(t)) &= \\ &= U^{-1}(R(t)) U(R(t+dt)) - U(R(t)) / dt \\ &= (U(R^{-1}(t) R(t+dt)) - \mathbb{1}) / dt . \end{aligned}$$

Noting that

$$R^{-1}(t) \cdot R(t+dt) = \mathbb{1} + R^{-1}(t) \cdot dR(t)$$

and using the standard relation between infinitesimal rotation and angular momentum operator, one gets the sought for relation :

$$i\hbar U^{-1}(R(t)) \cdot \dot{U}(R(t)) = \boldsymbol{\omega}(t) \cdot \mathbf{S} . \quad (\text{A.8})$$

Following a similar procedure, one arrives easily at the second relation :

$$i\hbar \dot{U}(R(t)) \cdot U^{-1}(R(t)) = \boldsymbol{\Omega}(t) \cdot \mathbf{S} . \quad (\text{A.9})$$

Note added in proof: In a recent work of D. Suter, K. Muller and A. Pines [13], the A-A phase was measured in three-level N.M.R. interferometry experiment, which corresponds to a particular example of the methods of type (ii) described above. This work contains an explicit experimental proof of the topological invariance of the A-A phase. We thank Prof. A. Pines for communicating his results before publication.

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