BERRY'S PHASE AND T-INVARIANCE*

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The structure of Berrry's phase for time-reversal invariant systems is reviewed. The method of constructing general "spin" Hamiltonians with quaternionic Berry's a holonomy is presented.

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1. Introduction

Since its discovery [1] Berry's phase has attracted much attention. Many physical applications have been found which make this notion very fruitful and deserving more detailed studies. In particular, the question has been raised about the structure of Berry's phase for time-reversal invariant systems. The basic example given by Berry, spin in an external magnetic field, is not invariant under time reversal. The simplest system which is time-reversal invariant is the spin in a quadrupole electric field proposed by Mead [2]. This system was studied in detail in [3] and [4]. In particular, in their very nice paper Avron *et al.* [4] revealed some very interesting general features of Berry's phase for time-reversal invariant families of Hamiltonians. It appears that the bosonic case is not very interesting. The time-reversal invariance implies essentially the reality of the space of states. Therefore, for a generic Hamiltonian, which is non-degenerate, no Berry's phase can

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appear. On the contrary, in the fermionic case we find a very interesting structure. It is well known [5] that the space of states carries in this case the quaternionic structure. The generic Hamiltonian, being quaternionically simple, has a double degeneracy in the complex sense (Kramer's degeneracy). Therefore the typical Berry's holonomy will be given by 2×2 complex matrix or, more elegantly, by unit quaternion.

In this paper we point out how one can find many examples of finitedimensional Hamiltonians with quaternionic Berry's phases/matrices which are calculable in terms of geometry of coset spaces G/H where G is any compact simple Lie group. To this end we use a general geometric approach to Berry's phase developed in [6] applicable to a wide class of Hamiltonians generated by the actions of Lie groups.

The paper is organized as follows. In Sec. 2 we give a simple discussion of the structure of Hilbert space for time-reversal invariant Hamiltonians. All results given there are known and contained in [4] but we wanted to summarize relevant properties and give very simple arguments in favor of them. In Sec. 3 we apply the formalism of [6] to time-reversal invariant systems. In particular, we discuss the example of Mead system [2]. Using again the results of [4] we point out advantages and disadvantages of our method. Finally, in Sec. 4 we sketch the general construction of "spin" Hamiltonians giving rise to quaternionic Berry's phase.

2. Physical systems invariant under time reversal

It is well known that the physical systems invariant under time reversal operation are characterized by the existence of the operator T acting in the space of states and sharing the following properties:

(i) T is antilinear,

$$T(\alpha\Psi + \beta\Phi) = \bar{\alpha}T\Psi + \bar{\beta}T\Phi\,;$$

(ii) T is antiunitary,

$$(T\Psi, T\Phi) = (\Phi, \Psi)\,;$$

(iii) T commutes with the Hamiltonian

$$TH = HT\,;$$

(iv) if s is a total spin of the system, then

$$T^2 = (-1)^{2s} I\,.$$

Let us consider first the bosonic case, $T^2 = I$. Let $\mathcal{H}_{\mathbb{R}} \subset \mathcal{H}$ be defined as follows

$$\mathcal{H}_{\mathbb{R}} = \left\{ \left(\frac{1+T}{2}\right)\Psi \mid \Psi \in \mathcal{H} \right\}.$$

$\mathcal{H}_{\mathbb{R}}$ is a real Hilbert space. $\mathbb{R}$-linearity is obvious whereas

$$\left(\left(\frac{1+T}{2}\right)\Phi,\ \left(\frac{1+T}{2}\right)\Psi\right) \in \mathbb{R}$$

follows from $T^2 = I$ and the antiunitarity of T. For any $\Psi \in \mathcal{H}_{\mathbb{R}}$ we have $T\Psi = \Psi$, so T acts as identity in $\mathcal{H}_{\mathbb{R}}$. Let $\{\Phi_n\}$ be an orthonormal basis in $\mathcal{H}_{\mathbb{R}}$; $\{\Phi_n\}$ is also a basis in $\mathcal{H}$. To see this let us write any $\Psi \in \mathcal{H}$ in the form

$$\Psi = \left(\frac{1+T}{2}\right)\Psi + i\left(\frac{1+T}{2}\right)(-i\Psi)$$

and put

$$\left(\frac{1+T}{2}\right)\Psi = \sum_n a_n\Phi_n, \quad \left(\frac{1+T}{2}\right)(-i\Psi) = \sum_n b_n\Phi_n\,.$$

Then

$$\Psi = \sum_n (a_n + ib_n)\Phi_n,$$
$$T\Psi = \sum_n (a_n - ib_n)\Phi_n\,,$$

i.e. T acts in this basis as the complex conjugation. Finally, let us consider the matrix elements of the Hamiltonian. We have

$$(\Phi_n, H\Phi_m) = (T\Phi_n, HT\Phi_m) = (T\Phi_n, TH\Phi_m) = (H\Phi_m, \Phi_n)\,.$$

Therefore H is a real operator acting in the real Hilbert space $\mathcal{H}_{\mathbb{R}}$.

The fermionic case, $T^2 = -I$, is much more interesting. Let Φ_1 be any unit vector in $\mathcal{H}$. We put $\Phi_2 = T\Phi_1$; then $\Phi_2 \neq 0$ and

$$(\Phi_1, \Phi_2) = (\Phi_1, T\Phi_1) = (T^2\Phi_1, T\Phi_1) = -(\Phi_1, T\Phi_1) = -(\Phi_1, \Phi_2)\,,$$

so that $\Phi_1 \perp \Phi_2$ and, obviously, $||\Phi_2|| = 1$. Now take Φ_3 to be any unit vector orthogonal to Φ_1 and Φ_2. We put $\Phi_4 \equiv T\Phi_3$; again $\Phi_4 \perp \Phi_3$, $||\Phi_4|| = 1$ and

$$(\Phi_4, \Phi_1) = (T\Phi_3, \Phi_1) = -(T\Phi_1, \Phi_3) = -(\Phi_2, \Phi_3) = 0$$

and the same holds true for Φ_2. Continuing this process we obtain an orthogonal basis $\Phi_1, \Phi_2, \ldots$ (note that this implies $\mathcal{H}$ to be either even- or infinitedimensional). The action of T can be easily described. Any subspace spanned by Φ_{2k-1}, Φ_{2k} is invariant under T:

$$T(a\Phi_{2k-1} + b\Phi_{2k}) = -\bar{b}\Phi_{2k-1} + \bar{a}\Phi_{2k}\,. \tag{1}$$

In any such subspace T has the form

$$T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K = -i\sigma_2 K\,, \tag{2}$$

where K is the operation of complex conjugation. Let now A be a linear operator commuting with T, $TA = AT$. Let $[A_{ij}^{(kl)}]$ be 2×2 matrix defined as follows

$$A_{ij}^{(kl)} \equiv (\Phi_{2k-2+i}, A\Phi_{2l-2+j}), \qquad i,j = 1,2\,. \tag{3}$$

Then, by virtue of Eqs (2), (3), we get

$$(-i\sigma_2)\overline{A^{(kl)}} = A^{(kl)}(-i\sigma_2)\,. \tag{4}$$

This implies

$$A^{(kl)} = a_0\sigma_0 - ia_k\sigma_k, \qquad a_0, a_k \in \mathbb{R}\,. \tag{5}$$

But this is just the matrix representation of the quaternion $q = a_0 + a_k e_k$. Therefore the matrix representing A can be considered as quaternionic matrix obtained from the original one by replacing any 2×2 block by a corresponding quaternion.

Let H be a Hamiltonian commuting with T. Then we can start the above construction with Φ_1 being an eigenvector of H; Φ_2 is then an eigenvector corresponding to the same eigenvalue. In this way we obtain the basis $\Phi_1, \Phi_2, \ldots$, in which H takes the form

$$H^{(kl)} = \delta_{kl} E_k \sigma_0\,. \tag{6}$$

This is the celebrated Kramers degeneracy. The above construction can be formalized by using the notion of quaternionic vector space. Let $\mathbb{H}$ denote the field of quaternions. The quaternionic vector space V is defined by the following properties [4] ($v, w \in V$, $x, y \in \mathbb{H}$).

$$\begin{aligned} (v+w)x &= vx + wx\,, \\ v(x+y) &= vx + vy\,, \\ v(xy) &= (vx)y\,. \end{aligned} \tag{7}$$

An operator A on V is a quaternionic-linear map of V into itself:

$$A[(v+w)x] = (Av)x + (Aw)x\,. \tag{8}$$

Our space of states can be converted into the quaternionic space as follows. If e_1, e_2, e_3 are quaternionic units and $v \in \mathcal{H}$ we define[1]

$$ve_1 = -iTe_1, \qquad ve_2 = Te_2, \qquad ve_3 = -iv\,. \tag{9}$$

[1] Our definitions differ from the ones adopted in [4].

The quaternionic basis is spun by the vectors $\Phi_1, \Phi_3, \ldots, \Phi_{2n+1}, \ldots$. Indeed, we have

$$\begin{aligned} v &= \sum_k ((a_k - ib_k)\Phi_{2k-1} + ((c_k - id_k)\Phi_{2k}) \\ &= \sum_k (a_k - ib_k + (c_k - id_k)T)\Phi_{2k-1} \\ &= \sum_k \Phi_{2k-1}(a_k e_0 + d_k e_1 + c_k e_2 + b_k e_3) \equiv \sum_k \Phi_{2k-1} q_k . \end{aligned}$$

Now, if A commutes with T, it is, by virtue of Eqs (8), (9), a quaternionic operator. Let us define the matrix elements $A^{(kl)}$ by

$$Av = \sum_{k,l} \Phi_{2k-1} A^{(kl)} q_l . \tag{10}$$

This definition coincides with the one given by Eqs (3), (5). In order to check this it is sufficient to consider onedimensional quaternionic space. Let

$$v = (a - ib)\Phi_1 + (c - id)\Phi_2 \equiv \Phi\tilde{q}, \qquad \tilde{q} = a + de_1 + ce_2 + be_3 .$$

Now, let us take A of form (5); the resulting transformation reads in components

$$\begin{pmatrix} a - ib \\ c - id \end{pmatrix} \to \begin{pmatrix} a_0 - ia_3 & -ia_1 - a_2 \\ -ia_1 + a_2 & a_0 + ia_3 \end{pmatrix} \begin{pmatrix} a - ib \\ c - id \end{pmatrix} .$$

The same transformation can be written as

$$\tilde{q} \to q\tilde{q}, \qquad q = a_0 + a_k e_k$$

which establishes the equivalence.

3. The quaternionic Berry's phase

Let us consider the family of Hamiltonians of the following form

$$H(g) = U(g) H_0 U^+(g) , \tag{11}$$

where H_0 is some fixed hermitean operator while $G \ni g \to U(g)$ is an unitary representation of some Lie group G. It has been shown in [6] that the Berry phase for such a set of Hamiltonians is essentially determined by the geometry of homogeneous space G/S, where $S \subset G$ is the stability subgroup of H_0. Let us briefly recall the result obtained there. First, let us note that the family of Hamiltonians is parametrized by the points x of G/S. For any $U(x)$ we put

$$U^{+}(x)\partial_\mu U(x) = \eta^i_\mu(x)S_i + \omega^a_\mu(x)T_a\,, \tag{12}$$

where $\omega^a \equiv \omega^a_\mu dx^\mu$, $\eta^i \equiv \eta^i_\mu dx^\mu$ are the Cartan forms while S_i, resp. T_a, are the generators of S, resp. G/S.

Let

$$H_0 = \sum_n E_n \Pi_n \tag{13}$$

be a spectral decomposition of H_0 and

$$S_i^{(n)} \equiv \Pi_n S_i \Pi_n\,, \qquad T_a^{(n)} \equiv \Pi_n T_a \Pi_n\,. \tag{14}$$

The Berry matrix for a given closed curve $\gamma \subset G/S$, for a given energy level E_n, is the holonomy matrix obtained by the parallel transport along γ by means of the connection

$$\frac{dD}{dt} \equiv \frac{\partial}{\partial t} + \frac{dx^\mu}{dt}\left(\omega^a_\mu T_a^{(n)} + \eta^i_\mu S_i^{(n)}\right)\,. \tag{15}$$

Assume now we are dealing with time-reversal invariant fermionic system. Let the family of Hamiltonians depending on external parameters be given as above and let

$$TU(g) = U(g)T\,, \tag{16a}$$

$$T\Pi_n = \Pi_n T\,, \qquad n = 0,1,\ldots\,. \tag{16b}$$

The above conditions obviously imply

$$TH(g) = H(g)T\,. \tag{17}$$

It follows from Eq. (16a) that the representation $G \ni g \to U(g)$ is pseudoreal (quaternionic); also, by virtue of Eq. (16b), the Π_n matrices are quaternionic. Therefore $T_a^{(n)}$ and $S_i^{(n)}$ are quaternionic and the Berry matrix, determined by connection (15) can be put in quaternionic form (note that connection (15) has quaternionic structure due to the fact that ω's and η's are imaginary).

The above presented scheme allows us to determine the quaternionic Berry's matrix for a wide class of time-reversal invariant fermionic systems (there are, however, significant exceptions, see below).

Let us first discuss the family of Hamiltonians studied extensively in [4]. For any representation $\{J_k\}$ of SU(2) algebra and any 3×3 symmetric traceless matrix Q we define

$$H(Q) = \sum_{i,j} Q_{ij} J_i J_j \,. \tag{18}$$

One should also impose some normalization condition on Q in order to exclude the variations of Q which change the energy levels without affecting the geometry of eigenspaces. One imposes the condition $\mathrm{Tr}\, Q^2 = {}^2/_3$; such Q is called unit quadrupole. It is not difficult to show [4] that the spectrum of $H(Q)$ is quaternionically simple, *i.e.* its degeneracy is minimal one allowed by Kramers rule.

The geometry of $H(Q)$ can be described as follows.

Let $D(g)$, $g \in \mathrm{SU}(2)$ be the representation generated by J_i's. Then any $H(Q)$, with Q being a unit quadrupole, can be written as

$$H(Q) = D(g) H_\Theta D^+(g) \,, \tag{19a}$$

$$H_\Theta = \cos\Theta \Big(J_3^2 - \frac{\vec{J}^2}{3} \Big) + \frac{\sin\Theta}{\sqrt{3}} (J_1^2 - J_2^2) \,, \qquad 0 \le \Theta \le \frac{\pi}{3} \,. \tag{19b}$$

The T-operator is most easily defined in the canonical basis where $J_{1,3}$ are real while J_2 is purely imaginary. Then

$$T = \mathrm{e}^{-i\pi J_2} K \,. \tag{20}$$

$H(Q)$ is obviously invariant under T. For odd integer J, $D(g)$ is quaternionic ($T^2 = -I$), and Berry's phase is quaternionic as well. It is also not difficult to determine the invariance subgroup of H_Θ. For $\Theta = 0$, resp. $\Theta = \frac{\pi}{3}$ it is U(1) — subgroup generated by J_3, resp. J_2. For other values of Θ one has only discrete subgroup (the so-called quaternionic subgroup).

Let us consider the family of Hamiltonians (19) for Θ fixed, g varying over SU(2). Then we can apply the geometric approach summarized above. For $\Theta = 0, \frac{\pi}{3}$ our parameter space is basically two-sphere S^2 while for other values of Θ it is the whole SU(2)-manifold (however, in both cases some care must be exercised due to the remaining discrete symmetry subgroups). The adiabatic connections are given by the relevant Cartan forms, multiplied by appropriate generators written in quaternionic form. This makes the whole structure quite transparent. However, for general J, our geometric method fails if we consider the families of Hamiltonians with g and Θ varying simultaneously. The only exception (apart from the trivial case $J = {}^1/_2$) is provided by $J = {}^3/_2$, then all Hamiltonians $H(Q)$ with Q's unital are unitarily equivalent [4]. The underlying group-theoretical structure looks as follows. Let Q_α, $\alpha = 0,\ldots,4$ be a basis of the space of quadrupoles, orthogonal with respect to the scalar product $(Q,Q') = \frac{3}{2}\,\mathrm{Tr}(QQ')$. Then the operators

$$T_\alpha \equiv H(Q_\alpha)\,, \tag{21}$$

generate fourdimensional representation of fivedimensional Clifford algebra. The commutators $[T_\alpha, T_\beta]$, $0 \le \alpha \le \beta \le 4$, span tendimensional Lie algebra of Spin (5). Let Spin (5) $\ni g \to U(g)$ be the representation generated by $[T_\alpha, T_\beta]$; then

$$H(Q^g) = U(g)H(Q)U^+(g)\,, \tag{22}$$

where $Q \to Q^g$ is the corresponding action of SO(5) in fivedimensional real vector space. The stability subgroup of a fixed Hamiltonian is the lift (to Spin(5)) of SO(4) invariance subgroup of a corresponding Q. Therefore we can again apply here our geometric approach to rederive the results of Avron *et al.* [4].

4. General examples of Hamiltonians with quaternionic Berry's phase

The geometrical approach to Berry's phase introduced in [6] allows us to construct the whole families of Hamiltonians for which the Berry matrices can be described in terms of quaternionic holonomies of connections defined over homogeneous spaces. Let G be any compact simple Lie group, $G \ni g \to U(g)$ - a unitary irreducible representation of G acting in the space of states. Assume that $U(g)$ is pseudoreal (quaternionic). Denote by X_k the generators of G in the representation U. Due to the pseudoreality of U there exists an antiunitary operator T such that $T^2 = -I$ and

$$TX_kT^{-1} = -X_k\,. \tag{23}$$

Let $H(X)$ be any element of universal enveloping algebra such that $H(X) = H(-X)$; for example, one can take any even polynomial in X's. Then $H(X)$ commutes with T and has a quaternionic structure. The same applies to

$$H(g) = U(g)H(X)U^+(g)\,. \tag{24}$$

Therefore the family of Hamiltonians $H(g)$, $g \in G$, exhibits the quaternionic structure and Kramers degeneracy. If $S \subset G$ is the stability subgroup of $H(X)$, the effective parameter space is G/S. The Berry connection is given by formula (15) with relevant Cartan forms and is a quaternionic matrix-valued function.

It is possible to classify all quaternionic representations of compact simple Lie groups [7]. This clasification is given below.

$SU(n) : (\lambda_1, \ldots, \lambda_{n-1})$ is pseudoreal iff:

(a)$\lambda_i = \lambda_{n-i}$, $i = 1, 2, \ldots$,
(b) $n = 2(2m+1)$,
(c) λ_{2m+1} is odd;

$SO(2n+1) : (\lambda_1, \ldots, \lambda_n)$ is pseudoreal iff:

(a) $n = 4k+1$ or $n = 4k+2$
(b) λ_1 is odd;

$Sp(n) : (\lambda_1, \ldots, \lambda_n)$ is pseudoreal iff:

(a) $\lambda_1 + \ldots + \lambda_n$ is odd;

$SO(2n) : (\lambda_1, \ldots, \lambda_n)$ is pseudoreal iff:

(a) $n = 4k+2$,
(b) $\lambda_1 + \lambda_2$ is odd;

G_2, F_4, E_6, E_8 have no pseudoreal representations;

$E_7 : (\lambda_1, \ldots, \lambda_{n-1})$ is pseudoreal iff $\lambda_2 + \lambda_3 + \lambda_6$ is odd.

Therefore, we can easily describe all families of Hamiltonians of spin type (*i.e.* finitedimensional) obtained by the action of irreducible representations of compact simple Lie group for which the Berry phase/matrix can be put in a quaternionic form.

REFERENCES

[1] M.V. Berry, *Proc. R. Soc. London* **A392**, 45 (1984).
[2] C.A. Mead *Phys. Rev. Lett.* **59**, 161 (1987).
[3] L. Sadun, J. Segert, *Phys. Rev. Lett.* **A22**, L111 (1989).
[4] J.E. Avron *et al.*, *Comm. Math. Phys.* **124**, 529 (1989).
[5] F. Dyson, *J. Math. Phys.* **3**, 140 (1964).
[6] S. Giller, *et al.*, *Int. J. Mod. Phys.* **A4**, 1453 (1989).
[7] M.L. Mehta, *J. Math. Phys.* **7**, 1824, 1833 (1966).