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DYNAMIC LIE ALGEBRA STRUCTURE OF QUANTAL SYSTEM AND BERRY'S PHASE FACTOR*

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At present, Berry's topological phase factor and the studies of its relevant problem have drawn considerable attention[1]. It concerns the theoretical analysis of chiral anomaly, etc.[2], which is also experimentally confirmed[3]. In general, the explicit determination of the Berry's phase for a quantal system with adiabatically-changing parameters depends on the solution of the eigenvalue problem of its Hamiltonian $\hat{H}[R(t)]$ in an explicit form. The variation of the parameters $R(t)=(R_1(t), R_2(t),\cdots,R_N(t))$ sweeps a curve $C:\{R(t)\}$ on the parameter manifold $\mu:\{R\}$. When $R(0)=R(T)$, C is a loop. However, in many practical problems, the eigenvalue problem of $\hat{H}[R(t)]$ cannot be solved in an explicit form and some methods dealing with the special problems are proposed for this reason.

In this report, according to the structure theory of Lie algebra, we will discuss a class of rather general cases: $\hat{H}[R(t)]$ possesses a non-symmetry dynamic Lie algebra structure, i.e.

$$\hat{H}\equiv\hat{H}[R(t)]=\sum_{j=1}^{N}R_j(t)\hat{T}_j, \qquad (1)$$

where $\hat{T}_j\,(j=1,2,\cdots,N)$ are the generators of a semisimple Lie algebra $\mathscr{L}$.

I. LIE ALGEBRA STRUCTURE DECOMPOSITION OF HAMILTONIAN

According to the Lie algebra structure theorem[5], the Lie algebra $\mathscr{L}$ can be decomposed into a direct sum of some simple Lie algebras $L_j\,(j=1,2,\cdots,s)$, i.e. $\mathscr{L}=L_1\oplus L_2\oplus\cdots\cdots\oplus L_s$ and the Hamiltonian $\hat{H}[(R)]$ is correspondingly decomposed into $\hat{H}=\hat{H}_1\oplus\hat{H}_2\oplus\cdots\oplus\hat{H}_s$, where $\hat{H}_j\equiv H_j[R(t)]\in L_j$. It is easily proved that the Schrödinger equation $i\hbar\partial/\partial t\cdot\hat{U}(t)=\hat{H}\cdot\hat{U}(t)$ about the evolution matrix $\hat{U}(t)$ can be

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decomposed as

$$\begin{cases} i\hbar\partial/\partial t\ \hat{U}_j(t) = \hat{H}_j[R(t)]\,\hat{U}_j(t),\ j=1,2,\cdots,S; \\ \hat{U}(t) = \hat{U}_1(t)\cdot\hat{U}_2(t)\cdot\cdots\cdot\hat{U}_s(t). \end{cases} \tag{2}$$

Therefore, the discussion about the time-evolution problem with $\mathscr{L}$ as a semisimple Lie algebra can be reduced to the several cases with simple Lie algebras. In the following discussions, we assume that $\mathscr{L}$ is a simple Lie algebra without losing the generality. On the Cartan-Weyl basis $\{\hat{h}_i, \hat{E}_{\alpha_j} \mid i=1,2,\cdots,l;\ j=1,2,\cdots,D=N-l\}$ of $\mathscr{L}$, we have

$$\hat{H} \equiv \hat{H}[R(t)] = \sum_{k=1}^{l} g_k[R(t)]\hat{h}_k + \sum_{j=1}^{D} f_j[R(t)]\hat{E}_{\alpha_j}, \tag{3}$$

where $\hat{h}_i$ is a generator of the Cartan subalgebra $\mathscr{H}$ of $\mathscr{L}$ and $g_j[R(t)]$ and $f_j[R(t)]$ are the linear combinations of $R_i(t)$.

In order to solve the eigenvalue problem of $\hat{H}[R(t)]$, we make an Ansätz:

$$\begin{cases} \hat{H}[R(t)] = \hat{g}[R]\cdot\hat{H}_c[R]\cdot\hat{g}[R]^{+} \in \mathscr{L}, \\ \hat{H}_c[R] = \sum_{k=1}^{l} y_k[R]\hat{h}_k \in \mathscr{H}, \end{cases} \tag{4}$$

where

$$\hat{g}[R] = \prod_{j=1}^{D} \exp[iX_j[R]\hat{E}_{\alpha_j}] \equiv \prod_{j=1}^{D} \hat{g}_j[R] \tag{5}$$

is an element of the Lie group of $\mathscr{L}\cdot x_j = x_j[R]$ and $y=y_k[R]$ will be determined by the coefficient equation of the operator equation

$$\sum_{k=1}^{l} g_k[R]\hat{h}_k + \sum_{j=1}^{D} f_j[R]\hat{E}_{\alpha_j} = \sum_{k=1}^{D} y_k[R]\left\{\left[\prod_{j=1}^{D}\hat{g}_j[R]\right]\cdot\hat{h}_k\cdot\left[\prod_{j'=1}^{D}\hat{g}^{+}_{D+1-j}[R]\right]\right\}. \tag{6}$$

In fact, from the commutation relations of $\hat{h}_i$ and $\hat{E}_{\alpha_j}$ [5] we obtain that

$$\begin{cases} \exp[ix\hat{E}_\alpha]\cdot\hat{h}_k\cdot\exp[-ix\hat{E}_\alpha] = \hat{h}_k - ix\alpha_k\hat{E}_\alpha, \\ \exp[ix\hat{E}_\alpha]\cdot\hat{E}_{-\alpha}\exp[-ix\hat{E}_\alpha] = \hat{E}_{-\alpha} + ix\alpha^k\hat{h}_k + \frac{1}{2}x^2(\alpha,\alpha)\hat{E}_\alpha, \\ \exp[ix\hat{E}_\alpha]\cdot\hat{E}_\beta\cdot\exp[-ix\hat{E}_\alpha] = \sum_{k=0}^{4} C_k\hat{E}_\beta + k\alpha, \quad \text{for } \alpha+\beta\neq 0, \end{cases} \tag{7}$$

where α_k and α^k are separately the covariant component and the contravariant component of a root α; C_k's are the constants relating to the structure of $\mathscr{L}$. By using Eq. (7), the right-hand side of Eq. (6) can be written as

$$\sum_{k=1}^{l} G_k(x_{j'}, y_{k'})\hat{h}_k + \sum_{j=1}^{D} F_j(x_{j'}, y_{k'})\hat{E}_{\alpha_j},$$

i.e. there is a system of non-linear equation about N unknown variables x_j and y_k to be determined, i.e.

$$g_k[R] = G_k(x_{j'}, y_{k'}), \quad f_j(R) = F_j(x_{j'}, y_{k'}). \tag{8}$$

Its solutions are a set of local coordinates for the manifold μ and the set $(x_1, x_2, \cdots, x_D)$ determines a submanifold $\mathscr{N}$, i.e. $\mathscr{N} = \{x \equiv (x_1, x_2, \cdots, x_D)\}$. The closed curve C: $\{R(t) | R(0) = R(T)\}$ on $\mathscr{M}$ corresponds to a closed curve C: $\{x[\widetilde{R}(t)] \mid x[R(0)] = x[R(T)]\}$ on $\mathscr{N}$.

II. Berry's Phase Factor and Its Geometrical Properties

After $\hat{H}[R(t)]$ is written as the form (4), we can construct the eigenfunction $|\Sigma, \Lambda[R]\rangle = \hat{g}[R] | \Sigma, \Lambda\rangle$ of $\hat{H}[R(t)]$ from the standard basis $|\Sigma, \Lambda\rangle$ of an irreducible representation Γ_Σ of $\mathscr{L}$. In fact, it can be verified from $\hat{H}_k |\Sigma, \Lambda\rangle = \Lambda_k |\Sigma, \Lambda\rangle$ that

$$\begin{cases} \hat{H}[R(t)] \,|\Sigma, \Lambda[R(t)]\rangle = E_\Lambda[R(t)] \,|\Sigma, \Lambda[R(t)]\rangle, \\ E_\Lambda[R(t)] = \sum_{k=1}^{l} \Lambda_k y_k[R(t)], \end{cases} \tag{9}$$

where Σ is the highest weight and Λ_k is a component of a weight Λ.

Then, when the adiabatic conditions

$$\left| \frac{\hbar \langle \Sigma\Lambda | \hat{g}^+ \cdot \dot{\hat{g}} | \Sigma\Lambda' \rangle}{\sum_{j=1}^{l} (\Lambda_j - \Lambda_j') y_j(R)} \right| \ll 1, \Lambda \neq \Lambda' \tag{10}$$

hold, the adiabatic approximation solution of the Schrödinger equation $i\hbar\partial/\partial t \,|\psi(t)\rangle = \hat{H}[R(t)] \,|\psi(t)\rangle$ is

$$|\psi(T)\rangle = \exp\left[\frac{1}{i\hbar}\int_0^T E_\Lambda[R(t)]\,dt\right] \exp[\,i\nu_\Lambda(T)] \,|\Sigma\Lambda[R(0)]\rangle, \tag{11}$$

where the Berry's topological phase $\nu_\Lambda(T)$ for the manifold $\mathscr{M}$ can be expressed as an element of holonomy group on the submanifold $\mathscr{N}$, i.e.

$$\nu_\Lambda(T) = i\int_0^T \langle \Sigma\Lambda[R(t)] \,|\, \frac{d}{dt} \,|\Sigma\Lambda[R(t)]\rangle dt' = i\int \langle \Sigma\Lambda \,|\hat{g}[R]^+ D_R \hat{g}[R]\rangle dR$$

$$= -\int_c \langle \Sigma\Lambda \,|\sum_{j=1}^{D} \left(\prod_{k=j+1}^{D} \hat{g}_k\right)^+ \hat{E}_{\alpha_j} \cdot \left(\prod_{k=j+1}^{D} \hat{g}_k\right) |\Sigma\Lambda\rangle dx_j, \tag{12}$$

where the $U(1)$-connection 1-form $A_\Lambda = i\ \langle \Sigma\Lambda \mid \hat{g}[R]^+ \nabla_R \hat{g}[R]\ \rangle dR$ defined on the manifold $\mathscr{M}$ has a projection

$$A_\Lambda |_{\mathscr{N}} = -\ \langle \Sigma\Lambda \mid \sum_{j=1}^{D} \left(\prod_{k=j+1}^{D} \hat{g}_k \right)^+ \cdot \hat{E}_{\alpha_j} \cdot \left(\prod_{k=j+1}^{D} \hat{g}_k \right) \mid \Sigma\Lambda\ \rangle dx_j \tag{13}$$

on the submanifold $\mathscr{N}$. The above fact means that the Berry's phase factor defined on the N-dimensional manifold $\mathscr{M}$ is only related to the connection and holonomy group on its $N-l=D$-dimensional submanifold $\mathscr{N}$; the Berry's phases for all the parameter manifolds $\mathscr{M}$ with the same submanifold $\mathscr{N}$ are completely determined by the geometrical properties of $\mathscr{N}$ and the embedding ways of $\mathscr{N}$ in these manifolds $\mathscr{M}$.

III. Example: $Su(2)$ Case

Now let us consider a practical example of the $Su(2)$ case: a spin-J neutral particle moves in a slowly-changing uniform magnetic field $\boldsymbol{B} = \sum_{k=1}^{3} B_k(t)\boldsymbol{e}_k$ with period T. The Hamiltonian for the problem is

$$\hat{H} \equiv \hat{H}[\boldsymbol{B}(t)] = v \cdot \hat{J} \cdot \boldsymbol{B}(t) = \sum_{k=1}^{3} vB_k(t)\hat{J}_k \in Su(2).$$

By using Eqs. (4)—(8), $\hat{H}$ is rewritten as

$$\begin{aligned} &\hat{H}[\boldsymbol{B}(t)] = \hat{g}[\boldsymbol{B}] \cdot vB(t) \cdot \hat{g}[\boldsymbol{B}]^+,\ v \in C, \\ &\hat{g}[\boldsymbol{B}(t)] = \exp[-i\hat{J}_z\beta(t)/\hbar]\exp[-iJ_y\,\theta(t)/\hbar], \end{aligned} \tag{14}$$

where $B(t) = \left[\sum_{i=1}^{3} B_i^2(t)\right]^{\frac{1}{2}}$, $\mathrm{tg}\beta(t) = B_2(t)/B_1(t)$ and $\cos\theta(t) = B_3(t)B/(t)$. According to the angular momentum theory, we can construct the eigenfunctions $|J, M[\boldsymbol{B}]\ \rangle = \hat{g}[\boldsymbol{B}]\ |J, M\rangle$ of $\hat{H}[\boldsymbol{B}(t)]$ from the common eigenfunctions $|\ J,\ M\ \rangle$ of $(\hat{J}^2,\ \hat{J}_3)$. The corresponding eigenvalues are $E_M[\boldsymbol{B}] = M \cdot B(t)\ v\ \hbar$. By using Eq. (12), the expression on the 2-dimensional submanifold $S^2\{\boldsymbol{B} \mid |\boldsymbol{B}|^2 = l\}$ of the Berry's phase on the manifold $\mathscr{M}\{(B_1, B_2, B_3) = \boldsymbol{B}\}$ is obtained as

$$v_M(T) = -M\oint_{\tilde{C}} [1 - \cos\theta(t)]\ d\beta(t) = -M\Omega(\tilde{C}), \tag{15}$$

where $\tilde{C}$ is a projection (on the unit sphere S^2) of the closed curve $C: \{\boldsymbol{B}(t) \mid \boldsymbol{B}(0) = \boldsymbol{B}(T)\}$ of the 3-dimensional manifold $\mathscr{M}$ and $\Omega(\tilde{C})$ is a solid angle subtended by $\tilde{C}$ with respect to the point $\boldsymbol{B} = 0$. Thus, the Berry's phase on $\mathscr{M}\{\boldsymbol{B}\}$ only depends on the geometry of the submanifold S^2.

IV. Generalizations and Discussions

(1) The above discussions in this report can be extended to any case with the Hamiltonians as the form

$$\hat{H}[R]=u[R]\ \hat{H}_0\, u[R]^+, \tag{16}$$

where $u(R)$ is a unitary representation of a Lie group and the spectra of $\hat{H}_0$ can be explicitly solved. For example, the Hamiltonian that produces the coherent state is

$$\hat{H}=\hbar\omega_0(t)[\hat{a}^+-\alpha^*(t)][\hat{a}-\alpha(t)],$$

where $\alpha(t)=x(t)+iy(t)\in C$, and $\hat{a}^+$ and $\hat{a}$ are respectively the creation operator and annihilation operator of boson. $\hat{H}$ can be written as

$$\hat{H}=D(\alpha)\hbar\omega_0(t)\,\hat{a}^+\hat{a}\,D(\alpha)^+,$$

where $D(\alpha)=\exp[\alpha\hat{a}^+-\alpha^*\hat{a}]$ is a unitary representation of the Heisenberg-Weyl group. From the states $|n\rangle$ of harmonic oscillator that $\hat{a}^+a|n\rangle=n|n\rangle$ and $\hat{a}|0\rangle=0$, we can construct the eigenfunction

$$|n[\alpha]\rangle=D(\alpha)|n\rangle=[n!]^{-\frac{1}{2}}\cdot[\hat{a}^+-a^*(t))]^n|\alpha\rangle \tag{17}$$

of $\hat{H}$, where $|\alpha\rangle=D(\alpha)|n\rangle$ is a coherent state of the harmonic oscillator. By a simple calculation, the Berry's phase is obtained as

$$v_n(T)=\int_C[dx\cdot Y-dY\cdot x]=-2\iint_{S:\{\partial S=C\}}dx\Lambda dY.$$

This result is reached under a more general condition than that in Ref. [8].

(2) The above discussion is also extended to rather general cases: $\hat{H}[R]=[u[R]H_0u^+[R]]^n$, ($n=1, 2, \cdots$.). For example, we have $\hat{H}=[\boldsymbol{B}\cdot\hat{J}]^2$ for the nuclear quadrupole resonance[9].

(3) We can also discuss the higher-order corrections of the problem in the case that the adiabatic conditions are broken, by making use of high-order approximation method[7] or the scheme for diagonalization in Ref. [10] with the results in this report as a zeroth apporximation.

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