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LETTER TO THE EDITOR

A gauge theory for a quantum system with isospin

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Abstract. A quantum system with external symmetry is made into a principal fibre bundle with a non-Abelian Lie group as the structure group, and is equipped with a connection. A gauge theory for a non-rigid molecule on the basis of the observation that the vector bundle associated with the principal fibre bundle provides a setting for quantum mechanics of the internal molecular motion.

Classical dynamics of particles with internal degrees of freedom can be described in terms of a principal bundle over the cotangent bundle of the spacetime manifold [5]. In contrast to this internal symmetry, we intend to develop the quantum theory of a system of particles with external symmetry. Namely, we are interested in a molecule which is a system of particles or atomic nuclei in the Born–Oppenheimer approximation.

The physical properties of a quantum mechanical system depend upon the types of molecules out of which the system is built, but as critically upon the overall geometrical way in which the various constituents are put together. On the other hand, the symmetry group often greatly simplifies complex problems. In fact, it offers one an understanding of the way in which mathematical properties of wavefunctions of a quantum system depend upon the physical symmetry of the system.

In a series of papers [2, 3], Iwai first developed a gauge theory for the quantum planar three-body system. He provided a mathematical meaning of non-rigidity of molecules. As an application of the connection theory due to Guichardet [1], he also established a gauge theory for non-rigid molecules on the basis of the observation that the vector bundle associated with the principal fibre bundles gives rise to a setting for quantum mechanics of the internal molecular motion. From the viewpoint of Berry's phase, Wu also pointed out that the rotational and vibrational motions are not separable in the planar three-body problem [7]. In fact, he showed that the corrected symplectic structure gives the correct quantization in the planar three-body system [8]. On the basis of Guichardet's work, Iwai demonstrated that the internal motion of the non-rigid molecule can be well described in terms of the gauge theory or the connection theory in differential geometry [2, 3].

In this letter, we shall establish the quantum theory of a non-rigid molecule with isospin as external symmetry. A quantum system with external symmetry is made into a principal fibre bundle with SU(2) as the structure group, and is equipped with a connection. The base manifold of this bundle is called the internal space. A gauge theory for non-rigid molecules on the basis of the observation that the vector bundle associated with the principal fibre bundle provides a setting for quantum mechanics of the internal motion. This also illustrates that non-vanishing curvature gives rise to the non-separability of motions.

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For simplicity, we consider a principal fibre bundle with the structure group SU(2). The total space is $\mathscr{C}^4 \cong \mathscr{R}^8$. The system is in $\mathscr{R}^8 = Q$ with an orthonormal system $\{f_i\}_{i=0}^7$.

The left action of SU(2) on Q is expressed with respect to the basis $\{f_i\}$ in the form

$$\begin{pmatrix} g & 0 \\ 0 & g \end{pmatrix} \tag{1}$$

where

$$g = \begin{pmatrix} u_1 + \mathrm{i}u_2 & u_3 + \mathrm{i}u_4 \\ -u_3 + \mathrm{i}u_4 & u_1 - \mathrm{i}u_2 \end{pmatrix}$$

$$u_1 = \cos\alpha$$

$$u_2 = \sin\alpha\cos\beta$$

$$u_3 = \sin\alpha\sin\beta\cos\gamma$$

$$u_4 = \sin\alpha\sin\beta\sin\gamma$$

Proposition 1. The system $\dot{Q} = \mathscr{R}^8 - \{0\}$ is made into a principal fibre bundle with structure group SU(2)

$$\pi : \dot{Q} \to M \simeq \dot{\mathscr{R}}^5 \qquad M := \dot{Q}/\mathrm{SU}(2).$$

Proof. We introduce in $\dot{Q}$ the structure of the algebra by setting the following operations on basis.

$$f_0^2 = f_0 \qquad f_j^2 = -f_0 \qquad j \neq 0$$

$$f_j f_0 = f_0 f_j = f_j$$

$$f_{ij} = -f_{ji} \qquad i \neq j \qquad i, j \neq 0$$

$$f_1 f_2 = -f_3 \qquad f_4 f_5 = f_1 \qquad f_4 f_6 = f_2$$

$$f_1 f_3 = f_2 \qquad f_2 f_3 = -f_1 \qquad f_4 f_7 = f_3$$

$$f_1 f_4 = f_5 \qquad f_2 f_4 = f_6 \qquad f_3 f_4 = f_7$$

$$f_1 f_5 = -f_4 \qquad f_2 f_5 = f_7 \qquad f_3 f_5 = -f_6$$

$$f_1 f_6 = -f_7 \qquad f_2 f_6 = -f_4 \qquad f_3 f_6 = f_5$$

$$f_1 f_7 = f_6 \qquad f_2 f_7 = -f_5 \qquad f_3 f_7 = -f_4$$

$$f_5 f_6 = -f_3 \qquad f_5 f_7 = f_2 \qquad f_6 f_7 = -f_1.$$

For each x in Q, $x = \xi_0 f_0 + \Sigma_{j=1}^7 \xi_j f_j$, $\xi_j \in \mathscr{R}$, we set

$$\varepsilon = (\cos\alpha) f_0 + (\sin\alpha\cos\beta) f_1 - (\sin\alpha\sin\beta\cos\gamma) f_2 + (\sin\alpha\sin\beta\sin\gamma) f_3.$$

Then the SU(2) action on Q, given by (1), is written as the left action:

$$x \to \varepsilon x. \tag{2}$$

From (2), we have the corresponding fundamental vector field $\{F_i\}_{i=1}^3$, the infinitesimal generator of the SU(2) action on $\dot{Q}$ as

$$F_1 = \tfrac{1}{3}\{(-\xi_1+\xi_2-\xi_3)f_0+(\xi_0+\xi_3+\xi_2)f_1+(\xi_3-\xi_0-\xi_1)f_2+(-\xi_2-\xi_1+\xi_0)f_3 + (-\xi_5+\xi_6-\xi_7)f_4+(\xi_4+\xi_7+\xi_6)f_5+(\xi_7-\xi_4-\xi_5)f_6+(-\xi_6-\xi_5+\xi_4)f_7\}$$

$$F_2 = \tfrac{1}{2}\{(\xi_2-\xi_3)f_0+(\xi_3+\xi_2)f_1+(-\xi_0-\xi_1)f_2+(-\xi_1+\xi_0)f_3+(\xi_6-\xi_7)f_4 + (\xi_7+\xi_6)f_5+(-\xi_4-\xi_5)f_6+(-\xi_5+\xi_4)f_7\}$$

$$F_3 = -\xi_3 f_0+\xi_2 f_1-\xi_1 f_2+\xi_0 f_3-\xi_7 f_4+\xi_6 f_5-\xi_5 f_6+\xi_4 f_7$$

where f_k are naturally identified with $\partial/\partial\xi_k$. In fact, the vector fields F_i are vertical, and the vector fields Y orthogonal to F_i are horizontal [4]; i.e.

$$K_x(Y_x, F_x) = 0 \qquad x \in \dot{Q}$$

when K_x is the inner product naturally induced in the tangent space $T_x(\dot{Q})$. We choose the horizontal vector fields V_k, $k = 1, 2, 3, 4, 5$, as follows:

$$V_1 = \xi_0 f_0+\xi_1 f_1+\xi_2 f_2+\xi_3 f_3+\xi_4 f_4+\xi_5 f_5+\xi_6 f_6+\xi_7 f_7$$

$$V_2 = \xi_4 f_0+\xi_5 f_1+\xi_6 f_2+\xi_7 f_3+\xi_0 f_4+\xi_1 f_5+\xi_2 f_6+\xi_3 f_7$$

$$V_3 = -\xi_5 f_0+\xi_4 f_1-\xi_7 f_2+\xi_6 f_3+\xi_1 f_4-\xi_0 f_5+\xi_3 f_6-\xi_2 f_7$$

$$V_4 = -\xi_6 f_0+\xi_7 f_1+\xi_4 f_2-\xi_5 f_3+\xi_2 f_4-\xi_3 f_5-\xi_0 f_6+\xi_1 f_7$$

$$V_5 = \xi_7 f_0+\xi_6 f_1-\xi_5 f_2-\xi_4 f_3-\xi_3 f_4-\xi_2 f_5+\xi_1 f_6+\xi_0 f_7.$$

The linear subspace $W_{x,\mathrm{hor}}$ of $T_x(\dot{Q})$ spanned by all the horizontal vectors at x is called the horizontal subspace.

Proposition 2. The connection forms are Lie-algebra-value one-forms (in terms of the basis of Lie algebra of SU(2)):

$$\omega_1 = \|\xi\|^{-2}[-\xi_1\,d\xi^0+\xi_0\,d\xi^1+\xi_3\,d\xi^2-\xi_2\,d\xi^3-\xi_5\,d\xi^4+\xi_4\,d\xi^5+\xi_7\,d\xi^6-\xi_6\,d\xi^7]$$

$$\omega_2 = \|\xi\|^{-2}[\xi_2\,d\xi^0+\xi_3\,d\xi^1-\xi_0\,d\xi^2-\xi_1\,d\xi^3+\xi_6\,d\xi^4+\xi_7\,d\xi^5-\xi_4\,d\xi^6-\xi_5\,d\xi^7]$$

$$\omega_3 = \|\xi\|^{-2}[-\xi_3\,d\xi^0+\xi_2\,d\xi^1-\xi_1\,d\xi^2+\xi_0\,d\xi^3-\xi_7\,d\xi^4+\xi_6\,d\xi^5-\xi_5\,d\xi^6+\xi_4\,d\xi^7]$$

where $\|\xi\|^2 = \Sigma_{j=0}^7 (\xi_j)^2$.

Let e_1, e_2, e_3 be a basis for the Lie algebra $\mathscr{G}$ of SU(2) and c_{jk}^m, $m, k, j = 1, 2, 3$ the structure constants of $\mathscr{G}$ with respect to e_1, e_2, e_3, that is $[e_j, e_k] = \Sigma_m c_{jk}^m e_m$, $c_{jk}^m = 2i\varepsilon_{jkm}$, $j, k = 1, 2, 3$,
where

$$\varepsilon_{jkm} = \begin{cases} \operatorname{sgn}\begin{pmatrix} 1 & 2 & 3 \\ j & k & m \end{pmatrix} \\ 0 \qquad \text{in other cases.} \end{cases}$$

Let $\omega = \Sigma_i \omega_i e_i$ and $\Omega = \Sigma_m \Omega^m e_m$. One can obtain the curvature Ω by applying the structure equation

$$\Omega^m = d\omega_m + \tfrac{1}{2}\sum_{j,k} c_{jk}^m \omega_j \wedge \omega_k \qquad m = 1, 2, 3$$

where ω_m is obtained in proposition 2.

To express Ω^m in terms of coordinates on internal space M, one can express $\pi:\dot{Q}\to M$ explicitly in terms of basis elements in Q. To avoid lengthy pages, we omit the expressions here.

To set up quantum mechanics for internal motion, we associate complex vector bundles to the principal SU(2) bundle $\pi:\dot{Q}\to M$ as follows [6]. For each j, $j=0,\frac{1}{2},1,\ldots$, let D^j denote unitary representation of SU(2) and $\mathscr{C}^{2j+1}$ its representation space. We have $(D^j(g)z)_k=\Sigma_{m=j}^{-j}D^j_{km}(g)z_j$, $z\in\mathscr{C}^{2j+1}$, $g\in\mathrm{SU}(2)$, $D^j_{km}(g)$: matrix elements. For a basis $|jm\rangle$ with $J_3|jm\rangle=m|jm\rangle$, Casimir operator J^2, we have

$$J^2=\sum_i (J_i)^2=\tfrac{1}{2}(J_+J_-+J_-J_+)+(J_3)^2$$

$$[J^2,J_i]=[J^2,J_\pm]=0$$

$$J^2|jm\rangle=j(j+1)|jm\rangle.$$

Define a left action of SU(2) on $\dot{Q}\times\mathscr{C}^{2j+1}$ by $(x,z)\to(gx,D^j(g)z)$ which gives an equivalence relation in $\dot{Q}\times\mathscr{C}^{2j+1}$. We denote the quotent manifold by $\dot{Q}\times_{\mathrm{SU}(2)}\mathscr{C}^{2j+1}$ which is made into a complex vector bundle $V_j=(\dot{Q}\times_{\mathrm{SU}(2)}\mathscr{C}^{2j+1},\pi_j,M)$ via the following commutative diagram:

$$\begin{array}{ccc} \dot{Q}\times\mathscr{C}^{2j+1} & \xrightarrow{\;q_j\;} & \dot{Q}\times_{\mathrm{SU}(2)}\mathscr{C}^{2j+1} \\ {\scriptstyle pr}\downarrow & & \downarrow{\scriptstyle \pi_j} \\ \dot{Q} & \xrightarrow{\;\pi\;} & M \end{array}$$

Projection maps are related by $\pi_j\circ q_j=\pi\circ pr$. The internal states of the system are described by the cross sections in the complex vector bundle V_j. The V_j is a trivial bundle, and hence the cross sections become $\mathscr{C}^{2j+1}$-valued functions on the internal space M. To illustrate this idea, we proceed as follows:

A $\mathscr{C}^{2j+1}$-valued function f on $\dot{Q}$ is said to be D^j-equivalent if it satisfies $f(gx)=D^j(g)f(x)$. For each D^j-equivalent function, there corresponds a cross section in the complex vector bundle V_j, and vice versa. Let $q_j^{\#}$ be the one-to-one correspondence from the cross section to the D^j-equivariant function.

On the other hand, let σ denote the cross section of $\pi:\dot{Q}\to M$. Then any point x of $\dot{Q}$ is of the form $g\sigma(u)$, $u\in M$. Therefore we have $f(x)=D^j(g)f(\sigma(u))$. One can then identify $\Phi=f\circ\sigma$ with a cross section. The components of f are $f_k(x)=\Sigma_{m=j}^{-j}D^j_{km}(g)\Phi_m(u)$. More precisely, the correspondence can be traced by the following commutative diagram:

$$\begin{array}{ccc} V_j & \xrightarrow{\;q^{\#}\;} & V_j \\ {\scriptstyle f}\uparrow & & \uparrow \\ \dot{Q} & \xrightarrow{\;\varepsilon\;} & \dot{Q} \\ {\scriptstyle \sigma}\uparrow & & \uparrow \\ M & \longrightarrow & M. \end{array}$$

On the other hand, we apply the Casimir operator

$$\hat{J}^2D^j(g)=j(j+1)D^j(g)$$

$$\hat{J}^2=\sum\hat{J}_k^2$$

to cross sections in the complex vector bundle V_j which can also be regarded as $\mathscr{C}^{2j+1}$-valued functions on ther internal space M.

Furthermore, one can construct the Hilbert space of square-integrable sections, and construct connection, curvature on the complex vector bundle V_j. To set up quantum mechanics for internal states of the quantum system, it is to obtain the internal Hamiltonian operator acting on cross sections in V_j by direct calculations or by applying the technique of geometric quantization.

One of the crucial parts of the above geometric setting of quantum system is that the SU(2) action (in proposition 1) can be described by introducing an amazing algebraic structure on the operations of basis elements of the total space of the principal fibre bundle. It would be interesting to know how to build up the parameter spaces setting in Berry's phase situation [8]. It is also interesting to set up the SU(3) case or higher degree of freedom for the internal motion of the quantum system by applying Bott's periodicity formula.

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