A Geometrical Characteristic of the Mixing Effect Induced by Non-Abelian Berry’s Phase

— Case of Nuclear Quadrupole System Rotating about Two Axes —

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A geometrical characteristic of the mixing effect induced by the non-Abelian Berry’s phase appearing in a nuclear quadrupole system \((I = 3/2)\) rotating about two axes is examined by using the rotating frame formulation. We show that the geometry-dependent parts of the mixing effect appear in the magnitude of the probability amplitude of the spin states and the rate of non-trivial mixing among these states after one period of motion of the system. These values depend only on the geometrical parameters which determine the trajectory traced by the principal-axis defined as the direction of the symmetry axis of the quadrupolar interaction.

§1. Introduction

Non-Abelian Berry’s phase is the extended version of Berry’s phase to degenerate systems formulated by Wilczek and Zee.\(^1\) Such a generalization is needed because there were two fundamental assumptions in Berry’s original formulation.\(^2\) One is the adiabatic change of the system, and the other is the non-degeneracy of the eigenstate. The former assumption was removed by Aharonov and Anandan,\(^3\) and they have shown that the non-adiabatic Berry’s phase reflects the geometrical structure of the projective Hilbert space. A more important implication of their results is that the geometrical phase is included in the total phase change of the wave function. Compared with this non-adiabatic generalization, the non-Abelian generalization that removes the later assumption seems to be difficult to obtain because of its non-commutable structure. Moreover, the effect of the non-adiabatic Berry’s phase (Aharonov-Anandan phase) appears in the phase change of the wave function, whereas that of the non-Abelian Berry’s phase (Wilczek-Zee phase) causes mixing among the degenerate eigenstates.

Since Berry’s formulation, many experiments have been performed to observe the effect of Berry’s phase. Of these experiments, nuclear quadrupole resonance (NQR) experiment performed by Tycko\(^4\) is notable because it involves the degenerate spin states. Zee\(^5\) has pointed out that if Tycko’s experiment, in which a single-rotor was used, is extended to rotation around more than one axis, then the effect of the non-Abelian Berry’s phase must appear. An experiment based on this suggestion was performed by Zwanziger, Koenig and Pines\(^6\) by applying a double-rotor NQR technique. They showed that the observed NQR spectrum agrees with the numerical simulations taking account of the non-Abelian Berry’s phase. Although this result seems to reflect the effect of the non-Abelian Berry’s phase appearing in the NQR
spectrum, the geometrical characteristic of the effect of the non-Abelian Berry’s phase is not clarified in their analysis.

Appelt, Wäckerle and Mehring\(^7\) have extended Tycko’s experiment to the non-adiabatic region. The importance of their experiment is not only determining the NQR spectrum in the non-adiabatic region but also the use of the rotating frame formulation to analyze the effect of Berry’s phase. The fact that the results derived from the rotating frame formulation is identical with that derived from the calculations of Berry’s phase indicates that the gauge term appearing in the rotating frame formulation is equivalent to Berry’s gauge potential (Berry’s connection). Based on this equivalence, it is natural to apply this formulation to a system rotating about more than one axis, in which, as shown by Zee, the effect of non-Abelian Berry’s phase must appear. According to these considerations, we have demonstrated the non-trivial mixing among the spin states after one period of motion of the principal-axis induced by the non-Abelian Berry’s phase in a nuclear quadrupole system rotating about two axes,\(^8\)

The purpose of this article is to identify a geometrical characteristic of the mixing effect induced by the non-Abelian Berry’s phase in a nuclear quadrupole system rotating about two axes by using the rotating frame formulation.

This article is organized as follows. First of all, the preliminaries for analyzing a nuclear quadrupole system (\(I = \frac{3}{2}\)) rotating about two axes are given in §2. In §3, we briefly review the original framework of the non-Abelian Berry’s phase and non-Abelian Berry’s gauge potential, and we give the non-Abelian gauge potential for the nuclear quadrupole system rotating about two axes. In §4, we derive the Hamiltonian of the nuclear quadrupole system transformed into the double-rotor system. We show that the transformed Hamiltonian includes the non-Abelian Berry’s gauge potential derived in §3 by using an adiabatic approximation. In §5, we analyze the transformed Hamiltonian and identify a geometrical characteristic of the mixing effect induced by the non-Abelian Berry’s phase. A conclusion is given in §6. In the Appendix, we give the details of the calculations.

§2. Preliminaries

2.1. Hamiltonian of the nuclear quadrupole system

The static Hamiltonian of the nuclear quadrupole system is given by

\[
H_Q = \hbar \omega_Q \left[ I_z^2 - \frac{1}{3} I (I + 1) \right],
\]

where \(\omega_Q\) is the strength of the quadrupolar interaction and \(z\)-axis is aligned along the principal-axis defined as the direction of the symmetry axis of the quadrupolar interaction.

2.2. Frames

To treat the motion of the principal-axis in the double-rotor system, we define three frames. We call these frames the laboratory frame, rotating frame and principal-axis frame. The laboratory frame \((x, y, z)\) is fixed and is time-independent.
A Geometrical Characteristic of the Mixing Effect

The rotating frame \((\bar{x}, \bar{y}, \bar{z})\) is defined as that in which the principal-axis is fixed and the angle between the \(\bar{z}\)-axis and the principal-axis fixed to \(\beta_2\). The angle between the \(z\)-axis and \(\bar{z}\)-axis is fixed to \(\beta_1\). This rotating frame rotates around the \(z\)-axis with the angular frequency \(\omega_1\) and it rotates around \(\bar{z}\)-axis with the angular frequency \(\omega_2\). The principal-axis frame \((\tilde{x}, \tilde{y}, \tilde{z})\) is defined as that in which the principal-axis is the \(\tilde{z}\)-axis. These situations are shown in Fig. 1.

The laboratory frame and the rotating frame are related by an Euler rotation. In our frames, the Euler angle is \((\beta_1, \omega_1 t, \omega_2 t)\), and thus the Euler rotation matrix \(M(t)\) is

\[
\begin{pmatrix}
\cos \omega_2 t \cos \omega_1 t \\
- \cos \beta_1 \sin \omega_1 t \sin \omega_2 t \\
- \sin \omega_2 t \cos \omega_1 t \\
- \cos \beta_1 \sin \omega_1 t \cos \omega_2 t \\
\sin \beta_1 \sin \omega_1 t
\end{pmatrix}
\begin{pmatrix}
\cos \omega_2 t \sin \omega_1 t \\
+ \cos \beta_1 \cos \omega_1 t \sin \omega_2 t \\
- \sin \omega_2 t \sin \omega_1 t \\
+ \cos \beta_1 \cos \omega_1 t \cos \omega_2 t \\
- \sin \beta_1 \cos \omega_1 t
\end{pmatrix}
\begin{pmatrix}
\sin \beta_1 \sin \omega_2 t \\
\sin \beta_1 \cos \omega_2 t \\
\sin \beta_1 \cos \omega_2 t \\
\cos \beta_1
\end{pmatrix}.
\]

The unit vector aligned along the principal-axis is expressed in these frames, \(\mathbf{X}(t)\)
in the laboratory frame and $X'$ in the rotating frame, and these are related by

$$X' = M(t) \cdot X(t),$$  \hspace{1cm} (2.2)

where the coordinates of the principal-axis in the two frames are

$$X(t) = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = \begin{pmatrix} \sin \theta(t) \cos \phi(t) \\ \sin \theta(t) \sin \phi(t) \\ \cos \theta(t) \end{pmatrix},$$  \hspace{1cm} (2.3)

$$X' = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \sin \beta_2 \cos \alpha \\ \sin \beta_2 \sin \alpha \\ \cos \beta_2 \end{pmatrix}.$$

Thus the time-dependent functions of $X(t)$ can be expressed by $\beta_1, \beta_2, \omega_1, \omega_2$ and $\alpha$. The following functions are used in later calculations:

$$\cos \theta(t) = \sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_1 t) + \cos \beta_1 \cos \beta_2,$$  \hspace{1cm} (2.5)

$$\sin \theta(t) = \sqrt{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_1 t) + \cos \beta_1 \cos \beta_2)^2},$$  \hspace{1cm} (2.6)

$$\frac{d\theta(t)}{dt} = \frac{-\omega_1 \sin \beta_1 \sin \beta_2 \cos(\alpha + \omega_1 t) - \cos \beta_1 \cos \beta_2}{\sqrt{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_1 t) + \cos \beta_1 \cos \beta_2)^2}},$$  \hspace{1cm} (2.7)

$$\frac{d\phi(t)}{dt} = \frac{-1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_1 t) + \cos \beta_1 \cos \beta_2)^2}{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_1 t) + \cos \beta_1 \cos \beta_2)^2} \times \left\{ \omega_1 \left[ \sin^2 \beta_2 + \sin^2 \beta_1 \cos^2 \beta_2 - 2 \sin \beta_1 \sin \beta_2 \cos \beta_1 \cos \beta_2 \sin(\alpha + \omega_1 t) \\
- \sin^2 \beta_1 \sin^2 \beta_2 \sin^2(\alpha + \omega_1 t) \right] \\
+ \omega_2 \left[ \sin^2 \beta_2 \cos \beta_1 - \sin \beta_1 \sin \beta_2 \cos \beta_2 \sin(\alpha + \omega_1 t) \right] \right\}. $$  \hspace{1cm} (2.8)

Note that $\omega_2$ determines the time-dependence of these functions.

The coordinates of the trajectory in $S^2$ traced by the unit vector aligned along the principal-axis, $X(t) = (x(t), y(t), z(t))$, are

$$x(t) = \cos \alpha \sin \beta_2 \cos(\omega_1 t \cos \omega_2 t - \cos \beta_1 \sin \omega_1 t \sin \omega_2 t)$$
$$- \sin \alpha \sin \beta_2 \sin \omega_1 t \cos \omega_1 t + \cos \beta_1 \sin \omega_1 t \cos \omega_2 t$$
$$+ \cos \beta_2 \sin \beta_1 \sin \omega_1 t,$$  \hspace{1cm} (2.9)

$$y(t) = \cos \alpha \sin \beta_2 \cos(\omega_1 t \sin \omega_2 t + \cos \beta_1 \cos \omega_1 t \sin \omega_2 t)$$
$$- \sin \alpha \sin \beta_2 \sin \omega_1 t \sin \omega_1 t - \cos \beta_1 \cos \omega_1 t \cos \omega_2 t$$
$$- \cos \beta_2 \sin \beta_1 \cos \omega_1 t,$$  \hspace{1cm} (2.10)

$$z(t) = \cos \alpha \sin \beta_2 \sin \beta_1 \sin \omega_2 t + \sin \alpha \sin \beta_2 \sin \beta_1 \cos \omega_2 t$$
$$+ \cos \beta_2 \cos \beta_1.$$  \hspace{1cm} (2.11)

Defining $\kappa \equiv \omega_1/\omega_2$, $x(t)$ and $y(t)$ are given by

$$x(t) = \frac{1}{2} \cos \alpha \sin \beta_2 \{(1 + \cos \beta_1) \cos[(\kappa + 1)\omega_2 t] + (1 - \cos \beta_1) \cos[(\kappa - 1)\omega_2 t]\}.$$
$y(t) = \frac{1}{2} \cos \alpha \sin \beta_2 \{(1 + \cos \beta_1) \sin[(\kappa + 1)\omega_2 t] + (1 - \cos \beta_1) \sin[(\kappa - 1)\omega_2 t]\}
+ \frac{1}{2} \sin \alpha \sin \beta_2 \{(1 + \cos \beta_1) \cos[(\kappa + 1)\omega_2 t] - (1 - \cos \beta_1) \cos[(\kappa - 1)\omega_2 t]\}
+ \sin \beta_1 \cos \beta_2 \cos(\kappa \omega_2 t)$.

(2.13)

§3. Non-Abelian Berry’s phase and gauge potential

When an adiabatically changing Hamiltonian $H(t)$ has $k$-degeneracy, the adiabatic theorem guarantees that the eigenvalue equation

$$H(t)|n_a(t)\rangle = E_n|n_a(t)\rangle$$

(3.1)

holds at any instant, where $|n_a(t)\rangle(a = 1, \cdots, k)$ is the set of orthonormal instantaneous eigenstates of $H(t)$, and $a$ labels the degenerate eigenstates. At any instant of the time evolution, there is a degree of freedom of the unitary transformation $U(t)$ for the instantaneous eigenstates, and thus the true wave function $|\psi_a(t)\rangle$ is given by $|\psi_a(t)\rangle = \sum_b |n_b(t)\rangle U_{ba}(t)$. Substituting this true wave function into the Schrödinger equation, we obtain the simultaneous set of differential equations

$$\frac{dU_{ba}(t)}{dt} = -\sum_c \left< n_b(t) \left| \frac{d}{dt} n_c(t) \right| \right> U_{ca}(t).$$

(3.2)

In general, the adiabatically changing Hamiltonian $H(t)$ depends on some parameters $\lambda_j$, and in this case (3.2) becomes

$$\frac{dU_{ba}(\lambda_j)}{d\lambda_j} = -\sum_c \left< n_b(\lambda_j) \left| \frac{d}{d\lambda_j} n_c(\lambda_j) \right| \right> U_{ca}(\lambda_j).$$

(3.3)
The formal solution of the above simultaneous set of differential equations is given by

\[ U_{ba} = \left[ P \exp \left( i \sum_j A_j^d \lambda_j \right) \right]_{ba}, \tag{3.4} \]

\[ A_j^d = i \left( n_b(\lambda_j) \left| \frac{d}{d\lambda_j} n_c(\lambda_j) \right| \right), \tag{3.5} \]

where \( U \) is the non-Abelian Berry’s phase and \( A_j^d \) is Berry’s gauge potential.

Within this framework, we derive the non-Abelian gauge potential for the nuclear quadrupole system rotating about two axes. The Hamiltonian (2.1) can be parametrized for the double-rotor system as

\[ H(\theta, \phi) = e^{-i\phi I_z} e^{-i\theta I_y} H_Q e^{i\theta I_y} e^{i\phi I_z}, \tag{3.6} \]

and the instantaneous eigenstate becomes \( |n(\theta, \phi) \rangle = e^{-i\phi I_z} e^{-i\theta I_y} |n \rangle \), where \( |n \rangle \) is the eigenstate of the static Hamiltonian \( H_Q \). Substituting the eigenstate into (3.5), Berry’s gauge potential is obtained as

\[ A = A^\phi d\phi + A^\theta d\theta, \tag{3.7} \]

\[ A^\phi_{nm} = \langle n | (I_z \cos \theta - I_x \sin \theta) | m \rangle \tag{3.8} \]

\[ A^\theta_{nm} = \langle n | I_y | m \rangle. \tag{3.9} \]

From this expression, the gauge potential for the \( | \pm 3/2 \rangle \) sector is obtained as \( A_{|3/2 \rangle} = m \cos \theta d\phi \). Thus, \( A_{|3/2 \rangle} \) is the Abelian gauge potential. In addition, that for the \( | \pm 1/2 \rangle \) sector is obtained as

\[ A_{|1/2 \rangle} = \left( \frac{\sigma_3}{2} \cos \theta - \sigma_1 \sin \theta \right) d\phi + \sigma_2 d\theta, \tag{3.10} \]

where \( \sigma_i (i = 1, 2, 3) \) are Pauli matrices. This is the non-Abelian gauge potential.

\section*{§4. Rotating frame formulation and adiabatic approximation}

If the system is in a time-dependent frame, then the Hamiltonian is changed as follows. Accompanying the time-dependent change of the frame, the basis of the static Hamiltonian \( |\psi(t)\rangle \) is transformed to \( U(t)|\psi(t)\rangle \), where \( U(t) \) is the time-dependent unitary transformation of the basis. Substituting this transformed basis into the Schrödinger equation, we obtain

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = \left[ U^{-1}(t)H(t)U(t) - i\hbar U^{-1}(t) \frac{dU(t)}{dt} \right] |\psi(t)\rangle. \tag{4.1} \]

The second term on the right-hand side is called the “gauge term”, and the transformed Hamiltonian is called the “effective Hamiltonian”.

We treat the case of the nuclear quadrupole system rotating about two axes. For the double-rotor system, we need two time-dependent unitary transformations,
$U_1(t) = \exp[-i\theta(t)I_y]$ and $U_2(t) = \exp[-i\phi(t)I_z]$. The static Hamiltonian \((2.1)\) is transformed by \((4.1)\) as

$$
\tilde{H}_Q(t) = U_2^{-1}(t)U_1^{-1}(t)H_Q U_1(t)U_2(t)
\equiv \hbar \omega_Q \left[I_z^2 - \frac{1}{3}I(I+1)\right] - \hbar \left[(I_z \cos \theta(t) - I_z \sin \theta(t))\frac{d\phi(t)}{dt} + I_y \frac{d\theta(t)}{dt}\right].
$$

(4.2)

This transformed Hamiltonian can be expressed in the matrix representation by choosing the direction of the $\tilde{z}$-axis for the quantization axis as

$$
\hbar \frac{\omega - \frac{3}{2}f(t)}{\frac{\sqrt{3}}{2}[g(t) + ih(t)]} 0 0
\frac{\sqrt{3}}{2}[g(t) - ih(t)] -\omega - \frac{3}{2}f(t) g(t) + ih(t) 0
0 g(t) - ih(t) -\omega + \frac{3}{2}f(t) g(t) + \frac{1}{2}f(t)
0 0 \sqrt{3}[g(t) - ih(t)] \omega + \frac{3}{2}f(t)
$$

(4.3)

where we define $f(t) \equiv \cos \theta(t)d\phi(t)/dt$, $g(t) \equiv \sin \theta(t)d\phi(t)/dt$ and $h(t) \equiv d\theta(t)/dt$, for convenience.

Here, we consider an adiabatic approximation. Under this approximation, the relation $\omega_Q \gg \omega_1, \omega_2$ is satisfied, and thus the following relations hold for the elements of \((4.3)\):

$$
|2\omega_Q - f(t)| \gg \left|\frac{\sqrt{3}}{2}[g(t) \pm ih(t)]\right|,
$$

(4.4)

$$
|f(t)| \sim |g(t) \pm ih(t)|.
$$

(4.5)

Thus the adiabatic Hamiltonian is obtained as

$$
\tilde{H}_Q^{ad}(t) = \hbar \left(\begin{array}{cccc}
\omega - \frac{3}{2}f(t) & 0 & 0 & 0 \\
0 & -\omega - \frac{3}{2}f(t) & g(t) + \frac{1}{2}f(t) & 0 \\
0 & g(t) - \frac{1}{2}f(t) & -\omega + \frac{3}{2}f(t) & 0 \\
0 & 0 & 0 & \omega + \frac{3}{2}f(t)
\end{array}\right).
$$

(4.6)

From this adiabatic Hamiltonian, it is clear that the mixing effect appears only in the $|\pm 1/2\rangle$ sector. In the following, we treat only this sector. With this approximation, the transformed Hamiltonian \((4.2)\) reduces to

$$
\tilde{H}_Q^{(1/2)}(t) = \hbar \omega_Q \left[\left(\frac{\sigma_3}{2}\right)^2 - \frac{1}{3}I(I+1)\right] - \hbar \left[\left(\frac{\sigma_3}{2}\cos \theta(t) - \sigma_1 \sin \theta(t)\right)\frac{d\phi(t)}{dt} + \sigma_2 \frac{d\theta(t)}{dt}\right].
$$

(4.7)

This adiabatic and transformed Hamiltonian indicates that the non-Abelian Berry’s gauge potential \((3.10)\) is included as the gauge terms.
§5. Geometrical dependence of the mixing effect

The problem of clarifying the mixing effect induced by the non-Abelian Berry’s phase reduces to the analysis of the transformed Hamiltonian (4.7), which includes the non-Abelian Berry’s gauge potential, the origin of the non-Abelian Berry’s phase. When the adiabatic condition, \( \omega_Q \gg \omega_1, \omega_2 \), is satisfied, then the time-dependent terms in the transformed Hamiltonian (4.7) can be treated as the perturbation compared with the first term of (4.7). The time-dependent functions \( f(t) \), \( g(t) \) and \( h(t) \) are expanded as

\[
\begin{align*}
    f(t) &= \sum_{n=-\infty}^{\infty} f_n e^{in(\alpha + \omega_2 t)}, \\
    g(t) &= \sum_{n=-\infty}^{\infty} g_n e^{in(\alpha + \omega_2 t)}, \\
    h(t) &= \sum_{n=-\infty}^{\infty} h_n e^{in(\alpha + \omega_2 t)}, 
\end{align*}
\]

where the Fourier coefficients are obtained by direct calculation as

\[
\begin{align*}
    f_n &= \omega_2 \Gamma_n^F(\beta_1, \beta_2, \kappa), \\
    g_n &= \omega_2 \Gamma_n^G(\beta_1, \beta_2, \kappa), \\
    h_n &= \omega_2 \Gamma_n^H(\beta_1, \beta_2, \kappa). 
\end{align*}
\]

Here, \( \Gamma_n^F(\beta_1, \beta_2, \kappa) \), \( \Gamma_n^G(\beta_1, \beta_2, \kappa) \) and \( \Gamma_n^H(\beta_1, \beta_2, \kappa) \) are functions that depend only on the geometrical parameters \( \beta_1, \beta_2 \) and \( \kappa \). The explicit forms are given in the Appendix.

Substituting these expansions into (4.7) and dividing into static and dynamical parts, we obtain

\[
\begin{align*}
    H_Q^{1/2}(t) &= H_0 + V(t) \\
    &= \hbar \omega_Q \left[ \left( \frac{\sigma_3}{2} \right)^2 - \frac{1}{3} (I + 1) \right] - \hbar \omega_2 \left( \frac{\sigma_3}{2} \Gamma_0^F - \sigma_1 \Gamma_0^G \right) \\
    &\quad - \hbar \omega_2 \sum_{n=-\infty}^{\infty} \left[ \left( \frac{\sigma_3}{2} \Gamma_n^F - \sigma_1 \Gamma_n^G + \sigma_2 \Gamma_n^H \right) e^{in(\alpha + \omega_2 t)} \right] \\
    &\equiv \hbar H'_0 + \hbar \omega_2 \sum_{n=1}^{\infty} \left( K_n e^{in\omega_2 t} + K_n^\dagger e^{-in\omega_2 t} \right), \\
    K_n(\beta_1, \beta_2, \kappa) &= -e^{ina} \left( \frac{\sigma_3}{2} \Gamma_n^F - \sigma_1 \Gamma_n^G + \sigma_2 \Gamma_n^H \right), \\
    K_n^\dagger(\beta_1, \beta_2, \kappa) &= -e^{-ina} \left( \frac{\sigma_3}{2} \Gamma_n^{F*} - \sigma_1 \Gamma_n^{G*} + \sigma_2 \Gamma_n^{H*} \right), 
\end{align*}
\]

where the sum \( \sum' \) is over all integer \( n \) except \( n = 0 \). Here, we note that the gauge terms in (4.7) are composed of two parts, the static part and the harmonic part. The
static part lifts the degeneracy of the first term of (5.7) as the effect of the Abelian Berry’s phase, whereas the effect of the harmonic part is unique to the non-Abelian case.

To see the effect of the harmonic part, we diagonalize the static part of the transformed Hamiltonian (5.8),

\[ H'_0 = \begin{pmatrix} -\omega_Q - \frac{1}{2}\omega_2 F_0^F(\beta_1, \beta_2, \kappa) & \omega_2 F_0^G(\beta_1, \beta_2, \kappa) \\ \omega_2 F_0^G(\beta_1, \beta_2, \kappa) & -\omega_Q + \frac{1}{2}\omega_2 F_0^F(\beta_1, \beta_2, \kappa) \end{pmatrix}. \]

This matrix can be diagonalized as

\[ H^D \equiv P^{-1} H'_0 P = \begin{pmatrix} E_- & 0 \\ 0 & E_+ \end{pmatrix}, \]

\[ E_+ = -\omega_Q + \frac{1}{2}\omega_2 \sqrt{[F_0^F(\beta_1, \beta_2, \kappa)]^2 + 4[F_0^G(\beta_1, \beta_2, \kappa)]^2}, \]

\[ E_- = -\omega_Q - \frac{1}{2}\omega_2 \sqrt{[F_0^F(\beta_1, \beta_2, \kappa)]^2 + 4[F_0^G(\beta_1, \beta_2, \kappa)]^2}, \]

\[ P = \begin{pmatrix} \cos \frac{\xi}{2} & -\sin \frac{\xi}{2} \\ \sin \frac{\xi}{2} & \cos \frac{\xi}{2} \end{pmatrix}, \]

\[ \tan \xi = -\frac{2[F_0^G(\beta_1, \beta_2, \kappa)]}{F_0^F(\beta_1, \beta_2, \kappa)} \]

Note that the diagonalizing matrix \( P \) depends only on the geometrical parameters, so that \( P = P(\beta_1, \beta_2, \kappa). \)

We consider the effect of the harmonic part in (5.8). It is clear that these terms cause transitions between the levels \( E_+ \) and \( E_- \) when the resonance condition \( (E_+ - E_-)/\hbar = n'\omega_2 \) is nearly satisfied for some integer \( n' \). The energy difference induced by the static part of the gauge potential is

\[ E_+ - E_- = \omega_2 \sqrt{[F_0^F(\beta_1, \beta_2, \kappa)]^2 + 4[F_0^G(\beta_1, \beta_2, \kappa)]^2}. \]

This shows that the energy difference is proportional to \( \omega_2 \) if the geometrical parameters \( \beta_1, \beta_2 \) and \( \kappa \) are fixed. The wave function for the transformed Hamiltonian (5.8) can be expanded as \( |\phi(t)\rangle = \sum_i c_i(t) \exp(-iE_i t/\hbar) |i\rangle \), where \( |i\rangle \) and \( E_i(i = \pm) \) are eigenstates and eigenvalues of the diagonalized Hamiltonian \( H^D \), respectively. Substituting this wave function into the Schrödinger equation and assuming that the resonance condition is nearly satisfied for some integer \( n' \), we obtain the simultaneous differential equations

\[ \begin{cases} \frac{dc_-(t)}{dt} = \omega_2 e^{-i\omega_2 t(\beta_1, \beta_2, \kappa)} (-|K_{n'+1}(\beta_1, \beta_2, \kappa)|+|K_{n'+1}(\beta_1, \beta_2, \kappa)|) c_+(t), \\ \frac{dc_+(t)}{dt} = \omega_2 e^{i\omega_2 t(\beta_1, \beta_2, \kappa)} (+|K_{n'}(\beta_1, \beta_2, \kappa)|-|K_{n'}(\beta_1, \beta_2, \kappa)|) c_-(t), \end{cases} \]
where we define the small number \(\varepsilon'(\beta_1, \beta_2, \kappa) = \varepsilon/\omega_2\) as \(E_+ - E_- = n'\omega_2 + \varepsilon\). If the resonance condition is not satisfied, then we can ignore the mixing effect because it becomes very small. We note that the matrix representation of \(\langle -|K'_n(\beta_1, \beta_2, \kappa)|j\rangle\) is

\[
P^{-1}(\beta_1, \beta_2, \kappa) \left[ e^{im'\alpha} \left( \frac{\sigma_3}{2} \Gamma_n^{F} - \sigma_1 \Gamma_n^{G} + \sigma_2 \Gamma_n^{H} \right) \right] P(\beta_1, \beta_2, \kappa), \tag{5.19}
\]

and the matrix elements depend only on the geometrical parameters \((\beta_1, \beta_2, \kappa)\). Thus \(\langle -|K'_n(\beta_1, \beta_2, \kappa)|+\rangle\) is rewritten as \(K'_n(\beta_1, \beta_2, \kappa)\). The solutions of this simultaneous set of differential equations under the initial conditions \(c_-(0) = 1\) and \(c_+(0) = 0\) are

\[
|c_+(t)|^2 = A(\beta_1, \beta_2, \kappa) \sin^2 [\Omega(\beta_1, \beta_2, \kappa)\omega_2 t] \quad \text{if} \quad \frac{\varepsilon'(\beta_1, \beta_2, \kappa)}{2} \neq 0,
\]

\[
|c_-(t)|^2 = 1 - |c_+(t)|^2,
\]

\[
\Omega(\beta_1, \beta_2, \kappa) = \sqrt{\frac{\varepsilon'(\beta_1, \beta_2, \kappa)^2}{4} + \left| K'_{n'}(\beta_1, \beta_2, \kappa) \right|^2}, \tag{5.22}
\]

where the amplitude \(A(\beta_1, \beta_2, \kappa)\) is obtained as

\[
4 \left| K_{n'}^{-1}(\beta_1, \beta_2, \kappa) \right|^2 \left( \frac{\varepsilon'(\beta_1, \beta_2, \kappa)}{2} \pm \sqrt{\frac{\varepsilon'(\beta_1, \beta_2, \kappa)^2}{4} + \left| K_{n'}^{-1}(\beta_1, \beta_2, \kappa) \right|^2} \right)^2 \left( \frac{\varepsilon'(\beta_1, \beta_2, \kappa)}{2} \mp \sqrt{\frac{\varepsilon'(\beta_1, \beta_2, \kappa)^2}{4} + \left| K_{n'}^{-1}(\beta_1, \beta_2, \kappa) \right|^2} \right)^2.
\]

This is the well-known Rabi formula. These solutions show that \(|c_\pm(t)|^2\) has a periodic time-dependence and, as we have shown in a previous paper,\(^8\) in general the period of \(|c_\pm(t)|^2\) does not coincide with that of the motion of the principal-axis.

This result shows that the amplitude \(A\) depends only on the geometrical parameters \(\beta_1, \beta_2\) and \(\kappa\). In other words, the magnitude of the amplitude \(|c_\pm(t)|^2\) does not depend on the change in the angular frequencies \(\omega_1\) and \(\omega_2\) if the ratio \(\kappa = \omega_1/\omega_2\) is kept constant. Thus we conclude that this is the geometry-dependent part of the mixing effect induced by the non-Abelian Berry’s phase appearing in a nuclear quadrupole system rotating about two axes.

In addition to this geometry-dependent part, the difference between the initial value \(|c_\pm(0)|^2\) and the final value \(|c_\pm(T)|^2\), which is defined as the value after one period of motion of the principal-axis, has the geometry-dependence

\[
|c_+(T)|^2 - |c_+(0)|^2 = A(\beta_1, \beta_2, \kappa) \sin^2 [2m\pi \Omega(\beta_1, \beta_2, \kappa)], \tag{5.24}
\]

where \(m\) is an integer that is determined from the period of motion of the principal-axis, \(T = m \times (2\pi/\omega_2)\).
§6. Conclusion

We have analyzed the effect of the non-Abelian Berry’s phase appearing in a nuclear quadrupole system rotating about two axes by using the rotating frame formulation. We found some geometry-dependent parts of the mixing effect induced by the non-Abelian Berry’s phase. These are the magnitude of the probability amplitude of each state $|\pm\rangle$ and the difference between the initial and final value of $|c_{\pm}(t)|^2$. These quantities do not depend on the change in the angular frequencies $\omega_1$ and $\omega_2$ if the ratio $\kappa = \omega_1/\omega_2$ is kept constant in the adiabatic region, but, rather, are determined by the geometrical parameters $\beta_1, \beta_2$ and $\kappa$. Since these parameters also determine the trajectory in $S^2$ traced by the unit vector aligned along the principal-axis, we explicitly clarify the geometrical dependence of the effect of the non-Abelian Berry’s phase.

To examine the effect of the non-Abelian Berry’s phase, Segert\(^9,10\) has studied a family of Hamiltonians, $H_k = H_0 + k \cdot V$, where $H_0$ is a rotationally invariant operator, $V$ is a vector operator, and $k$ is a unit vector varying in $\mathbb{R}^3$. He has shown that the transition probability between the approximately degenerate eigenstates of $H_k$ takes the form $W'_{\alpha'} = A' \sin^2(\Omega't')$, where $A'$ and $\Omega'$ depend on the geometrical parameter and eigenvalue of vector operator and $t'$ is the angle of rotation about the rotation axis. The analysis using the rotating frame formulation of the same system was studied by Ligare.\(^11\) In his analysis, the effective Hamiltonian remains static. This fact implies that if we analyze the effective Hamiltonian in the diagonalized eigenstates, then the time evolution of this system is Abelian. (In other words, the change induced by the time evolution appears only in the phase change of the diagonalized eigenstates.) This situation is similar to that considered by Tycko,\(^4\) Appelt, Wäckerle and Mehring,\(^7\) and, as pointed out by Zee,\(^5\) the non-Abelian character of the gauge potential is lost. On the other hand, the effective Hamiltonian of the nuclear quadrupole system rotating about two axes is non-static, and there are no eigenstates which diagonalize the effective Hamiltonian (5.8). This fact implies that the non-Abelian character exists in our case.

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Appendix A

--- Fourier Coefficients $f_n, g_n$ and $h_n$ ---

In this appendix, we show the Fourier coefficients of the time-dependent functions $f(t)$, $g(t)$ and $h(t)$. These coefficients are calculated as

$$f_n = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} e^{-in(\alpha+\omega_2 t)} \cos(t) \frac{d\phi(t)}{dt} dt, \quad (A.1)$$
\( g_n = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} e^{-in(\alpha+\omega_2 t)} \sin \theta(t) \frac{d\phi(t)}{dt} \, dt, \quad (A\cdot2) \)

\( h_n = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} e^{-in(\alpha+\omega_2 t)} \frac{d\theta(t)}{dt} \, dt. \quad (A\cdot3) \)

Substituting the explicit forms of the time-dependent functions into the above integrals, we obtain

\[
f_n \equiv \omega_2 \Gamma^F_n(\beta_1, \beta_2, \kappa),
\]

\[
= \omega_2 [-\kappa \sin^3 \beta_1 \sin^3 \beta_2 F^3_n(\beta_1, \beta_2)
- (3\kappa \sin^2 \beta_1 \sin \beta_2 \cos \beta_1 \cos \beta_2 + \sin^2 \beta_1 \sin \beta_2 \cos \beta_2) F^2_n(\beta_1, \beta_2)
+ (\kappa \sin \beta_1 \sin^3 \beta_2 + \kappa \sin \beta_1 \sin \beta_2 \cos \beta_2 + \sin \beta_1 \sin^3 \beta_2 \cos \beta_1
- 2\kappa \sin \beta_1 \sin \beta_2 \cos \beta_1 \cos \beta_2 - \sin \beta_1 \sin \beta_2 \cos \beta_1 \cos \beta_2) F^1_n(\beta_1, \beta_2)
+ (\kappa \sin^2 \beta_2 \cos \beta_1 \cos \beta_2 + \kappa \sin^2 \beta_1 \cos \beta_1 \cos \beta_2 + \sin^2 \beta_2 \cos \beta_1 \cos \beta_2)]
\]

\[
g_n \equiv \omega_2 \Gamma^G_n(\beta_1, \beta_2, \kappa),
\]

\[
= \omega_2 [-\kappa \sin^2 \beta_1 \sin \beta_2 G^2_n(\beta_1, \beta_2)
- (2\kappa \sin \beta_1 \sin \beta_2 \cos \beta_1 \cos \beta_2 + \sin \beta_1 \sin \beta_2 \cos \beta_2) G^1_n(\beta_1, \beta_2)
+ (\kappa \sin^2 \beta_2 + \kappa \sin^2 \beta_1 \cos \beta_2 + \sin^2 \beta_2 \cos \beta_1)]
\]

\[
h_n \equiv \omega_2 \Gamma^H_n(\beta_1, \beta_2, \kappa),
\]

\[
= \omega_2 [-\sin \beta_1 \sin \beta_2 H^1_n(\beta_1, \beta_2)].
\]

In the above expressions, \( F^m_n(\beta_1, \beta_2) \), \( G^m_n(\beta_1, \beta_2) \) and \( H^m_n(\beta_1, \beta_2) \) are functions that depend only on \( \beta_1 \) and \( \beta_2 \), and their explicit forms are

\[
F^m_n(\beta_1, \beta_2) = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} \frac{e^{-in(\alpha+\omega_2 t)} \sin^m(\alpha + \omega_2 t)}{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_2 t) + \cos \beta_1 \cos \beta_2)^2} \, dt,
\]

\[
G^m_n(\beta_1, \beta_2) = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} \frac{e^{-in(\alpha+\omega_2 t)} \sin^m(\alpha + \omega_2 t)}{\sqrt{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_2 t) + \cos \beta_1 \cos \beta_2)^2}} \, dt,
\]

\[
H^m_n(\beta_1, \beta_2) = \frac{\omega_2}{2\pi} \int_0^{2\pi/\omega_2} \frac{e^{-in(\alpha+\omega_2 t)} \cos^m(\alpha + \omega_2 t)}{\sqrt{1 - (\sin \beta_1 \sin \beta_2 \sin(\alpha + \omega_2 t) + \cos \beta_1 \cos \beta_2)^2}} \, dt.
\]

References