

High-order adiabatic approximations related to non-Abelian Berry's phase factors and nuclear quadrupole resonance

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A high-order adiabatic-approximation method is proposed to study the time evolution of degenerate quantum-mechanical systems with slowly changing Hamiltonians. We not only discuss the quantum adiabatic theorem, induced gauge structure, and non-Abelian Berry's phase factors in the first-order approximation, but we also give nonadiabatic corrections for problems in the second-order approximation. With the nuclear quadrupole resonance as an explicit example, we analyze the above-mentioned questions in detail and point out the observable effects of non-Abelian Berry's phase factors for nonadiabatic transitions between two instantaneous states in an improvement of Tycko's experiment.

I. INTRODUCTION

As a new concept in quantum physics, the Abelian Berry's phase factor (ABPF) has been found in many areas of physics^{1,2} and verified by some experiments.^{3,4} With respect to it, a few methods used to study nonadiabatic effects in the time evolution of quantum-mechanical systems with slowly changing parameters were proposed by different authors.⁵⁻¹⁰ One of these methods is the high-order adiabatic approximation (HOAA) presented by the author for both the nondegenerate and degenerate cases with an invariant single symmetry.^{7,8} This method has been applied to other problems of time evolution.¹¹⁻¹³

In fact, the degenerate case with varying symmetry (e.g., the symmetry is a rotation around an axis whose direction is varying) is more usual. It is necessary to generate the original HOAA method to this case. Under the adiabatic limit, Wilczek and Zee have studied the evolution of a degenerate system with a varying symmetry in first-order approximation.¹⁴ The concepts of the induced gauge structure (IGS) and non-Abelian Berry's phase factor (NABPF) represented by them have been further developed by those same authors.¹⁵⁻¹⁷ In this paper, we will pay attention to the nonadiabatic case for the problem.

This paper is arranged as follows. In Sec. II we formulate the HOAA method for the degenerate quantum system with varying symmetry. In Sec. III we apply the first-order approximation to the degenerate quantum adiabatic theorem and calculation of NABPF's with nuclear quadrupole resonance (NQR) as a detailed example. In

Sec. IV nonadiabatic transitions from an instantaneous state to another in NQR are analyzed by making use of the HOAA method. Finally, the observable effects of the NABPF are pointed out in Tycko's experiment under nonadiabatic conditions.

II. HOAA METHOD FOR DEGENERATE CASE

In the simple degenerate case considered in this paper, the Hamiltonian $\hat{H} = \hat{H}[R]$ depends on time though the slowly changing parameters $(R_1(t), R_2(t), \dots, R_N(t)) = R(t)$ and a set of its instantaneous eigenstates $|n\alpha[R]\rangle$ ($\alpha = 1, 2, \dots, D_n$) with the eigenvalue $E_n[R]$ transforms as an irreducible representation $\Gamma^{(n)}$ under a varying symmetry group, which is an isomorphism of a fixed group G at any instant. For the accidentally degenerate case that the eigenstates can equally well transform as a reducible representation, which frequently occurs in systems of physical interest, we need further work on the basis of this paper and now do not consider it.

We define $f' = f(\tau)$, $\dot{f} = (d/d\tau)f(\tau)$, and $|n\dot{\alpha}[f]\rangle = (d/d\tau)|n\alpha[f]\rangle$ for any function f of variable τ as follows. Let

$$|\phi(t)\rangle = \sum_n \sum_{\alpha=1}^{D_n} C_{n\alpha}(t) \exp\left\{\frac{1}{i\hbar} \int_{t_0}^t E_n[R'] dt'\right\} |n\alpha[R]\rangle \quad (1)$$

be a solution of the Schrödinger equation $i\hbar(\partial/\partial t)|\phi(t)\rangle = \hat{H}[R]|\phi(t)\rangle$. It is easy to see that $C_{n\alpha}(t)$ satisfies

$$\dot{C}_{n\alpha}(t) + \sum_{\beta=1}^{D_n} \langle n\alpha[R] | n\dot{\beta}[R] \rangle C_{n\beta}(t) = - \sum_{n' \neq n} \exp\left\{\frac{i}{\hbar} \int_{t_0}^t (E_n[R'] - E_{n'}[R']) dt'\right\} \sum_{\beta=1}^{D_{n'}} \langle n\alpha[R] | n'\dot{\beta}[R] \rangle C_{n'\beta}(t). \quad (2)$$

Because the left-hand side of (2) concerns different states $|n\beta[R]\rangle$ ($\beta = 1, 2, \dots, D_n$) for the same eigenvalue $E_n[R]$, the original HOAA method in Refs. 7 and 8 cannot be used to solve (2) directly. However, if $\hat{H}[R(t)]$ has a single symme-

try at any instant and G is the corresponding symmetry group, then $|n\alpha[R(t)]\rangle$ and $|n\alpha[R(t+\Delta t)]\rangle$ at different times t and $t+\Delta t$ are the basis for the same irreducible representation of the same symmetry group. According to the orthogonality theorem of group representations, we have

$$\langle n\alpha[R]|n\dot{\beta}[R]\rangle = \lim_{\Delta t \rightarrow 0} \left\langle n\alpha[R] \left| \frac{|n\beta[R(t+\Delta t)]\rangle - |n\beta[R(t)]\rangle}{\Delta t} \right. \right\rangle = \delta_{\alpha\beta} \langle n\alpha[R]|n\dot{\alpha}[R]\rangle. \quad (3)$$

Therefore, the left-hand side of (2) can be diagonalized and the original HOAA method can work in this case.

Now, we return to the case with varying symmetry. In order to solve (2) order by order, we introduce an adiabatic perturbing parameter $\epsilon = 1/T$ [T is the characteristic time of system, e.g., the period of $R(t)$] and define

$$s = t/T, \quad b_{n\alpha}(s) = C_{n\alpha}(sT), \quad Q(s) = R(Ts) \quad (4)$$

and D_n vectors $b_n(s)$ and $D_n \times D_n$ matrices $\tilde{A}(n, n', s)$:

$$b_n(s) = (b_{n1}(s), b_{n2}(s), \dots, b_{nD_n}(s))^T, \quad (5)$$

$$\tilde{A}(n, n', s)_{\alpha\beta} = \langle n\alpha[Q]|n'\dot{\beta}[Q]\rangle.$$

Then, the integral equation of (2) is written as

$$b_n(s) - b_n(s_0) + \int_{s_0}^s \tilde{A}(n, n, \tau) b_n(\tau) d\tau$$

$$= - \sum_{n' \neq n} \int_{s_0}^s e^{iT\alpha_{nn'}(\tau, s_0)} \tilde{A}(n, n', \tau) b_{n'}(\tau) d\tau, \quad (6)$$

where $\alpha_{nn'}(s, s_0) = (1/\hbar) \int_{s_0}^s (E_n[Q'] - E_{n'}[Q']) ds'$.

Using a similar procedure to that in the original HOAA method, we successively integrate the right-hand side of (6) by parts and then differentiate both the right- and left-hand sides of the resulting equation, obtaining

$$\dot{b}_n^{[0]}(s) + \tilde{A}(n, n, s) b_n^{[0]}(s) = 0, \quad (9a)$$

$$\dot{b}_n^{[K]}(s) + \tilde{A}(n, n, s) b_n^{[K]}(s) = - \sum_{l=0}^{K-1} \sum_{n' \neq n} \frac{d}{ds} \left[e^{iT\alpha_{nn'}(s, s_0)} \left(\frac{i}{\dot{\alpha}_{nn'}(s, s_0)} \frac{d}{ds} \right)^K \left(\frac{\tilde{A}(n, n', s) b_n^{[K-l-1]}(s)}{i\alpha_{nn'}(s, s_0)} \right) \right]$$

$$\equiv F_n^{[K]}(s). \quad (9b)$$

Because Eq. (9b) for $b_n^{[K]}(s)$ ($n=1, 2, \dots$) only include $b_n^{[0]}(s)$, $b_n^{[1]}(s)$, \dots , $b_n^{[K-2]}(s)$, and $b_n^{[K-1]}(s)$ ($n=1, 2, \dots$), we can solve the above Eq. (9b) successively from the first-order approximation solutions, the solutions of (9a).

III. ADIABATIC APPROXIMATIONS AND NABPF IN NQR

Under the adiabatic limit $T \rightarrow \infty$ ($\epsilon \rightarrow 0$), which explicitly means that $\hat{H}[R]$ changes so slowly that the adiabatic conditions

$$\left| \frac{\hbar \langle n\alpha[R]|m\dot{\beta}[R]\rangle}{E_n[R] - E_m[R]} \right| = \left| \frac{\hbar \epsilon \langle n\alpha[Q]|m\dot{\beta}[Q]\rangle}{E_n[Q] - E_m[Q]} \right| \ll 1,$$

$m \neq n$ (10)

$$\dot{b}_n(s) + \tilde{A}(n, n, s) b_n(s)$$

$$= - \sum_{k=0}^{\infty} \sum_{n' \neq n} \epsilon^{K+1} \frac{d}{ds} \left[\exp[iT\alpha_{nn'}(s, s_0)] \times \left(\frac{i}{\dot{\alpha}_{nn'}(s, s_0)} \frac{d}{ds} \right)^K \times \left(\frac{\tilde{A}(n, n', s) b_{n'}(s)}{i\dot{\alpha}_{nn'}(s, s_0)} \right) \right]. \quad (7)$$

When $R(t)$ changes slowly enough, $\epsilon = 1/T$ is so small that $b_n(s)$ can be expanded into a rapidly converging power series in ϵ : i.e.,

$$b_n(s) = \sum_{K'=0}^{\infty} \epsilon^{K'} b_n^{[K']}(s)$$

$$\equiv \sum_{K'=0}^{\infty} \epsilon^{K'} [b_{n1}^{[K']}(s), b_{n2}^{[K']}(s), \dots, b_{nD_n}^{[K']}(s)]^T. \quad (8)$$

Substituting (8) into (7) we obtain an equality between two power series in ϵ . Because coefficients of each power of ϵ must be separately equal, there are approximate equations

are satisfied, it is shown in Eqs. (2) and (9) that we only need to take solutions of (9a) in path-ordered integral forms:

$$b_n^{[0]}(s) = \tilde{K}_n(s, s_0) b_n^{[0]}(s_0), \quad (11)$$

$$\tilde{K}_n(s, s_0) = \mathcal{P} \exp \left[- \int_{s_0}^s \tilde{A}(n, n, s') ds' \right].$$

Equation (11) results in the quantum adiabatic theorem: if a system is initially in an eigenstate $|n\alpha[Q, (s_0)]\rangle$ of $\hat{H}[Q(s_0)]$, then it will be evolved into a state

$$|\Psi(s)\rangle = \exp \left[\frac{1}{i\hbar} \int_{s_0}^s E_n[Q'] ds' \right] \times \sum_{\alpha'=1}^{D_n} [\tilde{K}_n(s, s_0)]_{\alpha'\alpha} |n\alpha'[Q]\rangle \in \mathcal{V}_{(s_0)}^{[n]} \quad (12)$$

in eigenspace $\mathcal{V}_{(s)}^{[n]}$; $\{|x\rangle | \hat{H}[Q(s)]|x\rangle = E_n[Q(s)]|x\rangle\}$

under the adiabatic conditions (10).

The adiabatic propagator $\tilde{K}_n(s, s_0)$ is called the non-Abelian Berry's phase factor (NABPF). With respect to it, a non-Abelian gauge structure is defined as follows. The gauge potential one-form $\mathcal{A}(n, Q)$ in the parameter manifold $\mu\{Q\}$ is given by

$$\mathcal{A}(n, Q)_{\alpha\beta} = \langle n\alpha[Q] | d | n\beta[Q] \rangle, \quad \alpha, \beta = 1, 2, \dots, D_n \quad (13)$$

and the gauge group corresponds to local unitary freedom in choosing the basis $|n\alpha[Q]\rangle$. Under unitary transformation $U(Q)$,

$$|n\alpha[Q]\rangle \rightarrow |n\alpha[Q]\rangle' = \sum_{\beta=1}^{D_n} U(Q)_{\beta\alpha} |n\beta[Q]\rangle, \quad (14)$$

we have

$$\mathcal{A}(n, Q) \rightarrow \mathcal{A}'(n, Q) = U^\dagger(Q) \mathcal{A}(n, Q) U(Q) + U^\dagger(Q) dU(Q), \quad (15)$$

$$\mathcal{F}(n, Q) = d\mathcal{A}(n, Q) + \mathcal{A}(n, Q) \wedge \mathcal{A}(n, Q) \rightarrow \mathcal{F}'(n, Q) = U^\dagger(Q) \mathcal{F}(n, Q) U(Q).$$

Following the above discussion, we consider the nuclear quadrupole resonance (NQR) in concrete terms. According to Zee,¹⁵ the spin quadrupole Hamiltonian describing Tycko's experiment is

$$\hat{H}(s) \equiv \hat{H}[\mathbf{n}] = \omega_0 (\mathbf{n} \cdot \hat{\mathbf{J}})^2, \quad \hbar \equiv 1, \quad (16)$$

where $\mathbf{n} = \mathbf{n}(s) = (\sin\alpha(s)\cos\beta(s), \sin\alpha(s)\sin\beta(s), \cos\alpha(s))$ is the direction of the principal axis for the quadrupole coupling with a coupling constant ω_0 . By making use of angular momentum theory, we immediately obtain instantaneous eigenvectors

$$\begin{aligned} |J, \pm M(s)\rangle &= |J \pm M[\alpha(s), \beta(s)]\rangle \\ &= e^{-i\hat{J}_z \beta(s)} e^{-i\hat{J}_y \alpha(s)} |J, M\rangle, \\ M &= J, J-1, \dots, \frac{1}{2} \text{ or } 0 \end{aligned} \quad (17)$$

of $\hat{H}[\mathbf{n}]$ with eigenvalues $E_M[\mathbf{n}] = \omega_0 M^2$, where $|J, \pm M\rangle$ are the standard angular momentum bases. The instantaneous states $|JM(s)\rangle$ and $|J, -M(s)\rangle$ form a doubly degenerate sector.

From (17) we compute

$$\begin{aligned} \tilde{A}(M, M, S) &= \text{diag}[-iM\dot{\beta}(s)\cos\alpha(s), iM\dot{\beta}(s)\cos\alpha(s)] \\ &= -iM\dot{\beta}(s)\cos\alpha(s)\sigma_3 \quad \text{for } M \neq \frac{1}{2}, \end{aligned} \quad (18a)$$

$$\tilde{A}(\frac{1}{2}, \frac{1}{2}) = \begin{bmatrix} -\frac{i}{2}\dot{\beta}(s)\cos\alpha(s) & \alpha_+(\frac{1}{2}) \\ \alpha_-(\frac{1}{2}) & \frac{i}{2}\dot{\beta}(s)\cos\alpha(s) \end{bmatrix}, \quad (18b)$$

$$\tilde{A}(M, M+1, S) = \text{diag}[\alpha_-(M+1), \alpha_+(-M-1)], \quad (18c)$$

$$\tilde{A}(M, M-1, S) = \text{diag}[\alpha_+(M-1), \alpha_-(-M+1)], \quad (18d)$$

$$\tilde{A}(M, N, S) = 0 \quad (N \neq M, M \pm 1), \quad (18e)$$

and thereby obtain the induced gauge potentials defined by (13),

$$\mathcal{A}(M, \mathbf{n}) = -iM\cos\alpha(s)\sigma_3 d\beta, \quad M \neq \frac{1}{2}, \quad (19a)$$

$$\begin{aligned} \mathcal{A}(\frac{1}{2}, \mathbf{n}) &= -\frac{i}{2} \{ [\cos\alpha(s)\sigma_3 - (J + \frac{1}{2})\sin\alpha(s)\sigma_1] d\beta \\ &\quad + (J + \frac{1}{2})\sigma_2 d\alpha \}, \end{aligned} \quad (19b)$$

as the same as that obtained in Ref. 15. Here,

$$\begin{aligned} \alpha_\pm(M) &= \alpha_\pm(M, S) \equiv \frac{1}{2} [i\dot{\beta}(s)\sin\alpha(s) \mp \dot{\alpha}(s)] \\ &\quad \times [J(J+1) - M(M\pm 1)]^{1/2}. \end{aligned} \quad (20)$$

Now, we denote M or $-M$ by \tilde{M} as follows and then calculate the NABPF's in NQR by solving the adiabatic approximation equation (9a). For $m \neq \frac{1}{2}$, we obtain the NABPF

$$\begin{aligned} \tilde{K}_M(s, s_0) &= \exp[-iM\Omega(s, s_0)\sigma_3], \\ \Omega(s, s_0) &= -\int_{s_0}^s \cos\alpha(s') \dot{\beta}(s') ds'. \end{aligned} \quad (21)$$

For a cycle evolution that $\mathbf{n}(s_0) = \mathbf{n}(s_0+1)$, $\Omega(s_0+1, s_0)$ is just the solid angle subtended by a loop $C: \{\mathbf{n}(s) | \mathbf{n}(s_0) = \mathbf{n}(s_0+1)\}$ in the parameter manifold $S^2: \{\mathbf{n} \in \mathbb{R}^3 | |\mathbf{n}| = 1\}$. For $M = \frac{1}{2}$, it is very difficult to compute NABPF's in general situations, because they are path-ordered integrals of noncommutative matrix one-forms. However, the explicit expression of the NABPF for a specific case with $\alpha = \text{const}$ can be obtained as

$$\tilde{K}_{1/2}(s, s_0) = \mathcal{P} \exp \left[-\int_{s_0}^s \tilde{A}'(\frac{1}{2}, \frac{1}{2}) dS' \right] = \frac{-1}{\lambda} \begin{bmatrix} \lambda \cos\Gamma(s, s_0) - i \cos\alpha \sin\Gamma(s, s_0) & i(J + \frac{1}{2}) \sin\alpha \sin\Gamma(s, s_0) \\ i(J + \frac{1}{2}) \sin\alpha \sin\Gamma(s, s_0) & \lambda \cos\Gamma(s, s_0) + i \cos\alpha \sin\Gamma(s, s_0) \end{bmatrix} \quad (22)$$

by solving (9a) directly, where

$$\lambda = [1 + (J + \frac{1}{2})(J - \frac{1}{2})\sin^2\alpha]^{1/2},$$

$$\Gamma(s, s_0) = \frac{1}{2} \lambda [\beta(s) - \beta(s_0)].$$

It is easy to see from the above discussion that the NABPF $\tilde{K}_{1/2}(s, s_0)$ as a unitary matrix transforms the

two states $|J, M(s)\rangle$ and $|J, -M(s)\rangle$ into two linear combinations of them separately in an adiabatic evolution. Because $\mathcal{A}(\frac{1}{2}, \frac{1}{2})$ is proportional to a fixed matrix $\cos\alpha\sigma_3 - (J + \frac{1}{2})\sin\alpha\sigma_1$, the non-Abelian character is lost for the case with fixed α according to Zee (see Ref. 15).

According to Simon¹⁸ and Segert,¹⁷ the NABPF can be interpreted as a holonomy group element of the Hilbert

bundle over the parameter manifold and the Schrödinger equation uniquely determines the corresponding connection—the induced gauge potential.

In our discussion the two-dimensional eigenspace

$$V_M = \{C_+ |J, +M(s)\rangle + C_- |J, -M(s)\rangle | C_\pm \in \mathbb{C}\}$$

is a fiber over a point on the parameter manifold S^2 . With no loss of generality, we can set $E_M[\mathbf{n}] = 0$. When the Hamiltonian $\hat{H}[\mathbf{n}]$ changes along a loop C on the base space S^2 , the state of the system at $s = s_0 + 1$ is a un-

itary transformation of the initial state by the unitary matrix

$$\bar{u}[c] = \bar{K}_M(s_0 + 1, s_0) = \mathcal{P} \exp \left[- \oint_C \mathcal{A}(M, \mathbf{n})_\mu d\mathbf{n}^\mu \right].$$

For all the loops on S^2 , the corresponding unitary matrices form the holonomy group, which is non-Abelian for the case that $M = \frac{1}{2}$ and α is not fixed. For the case with $M \neq \frac{1}{2}$, the holonomy group is an Abelian subgroup $U(1)$ of $U(2)$:

$$\left\{ u(C) = \exp \left[-iM\sigma_3 \oint_C \cos\alpha(s)\alpha\beta(s) \right] \mid C \text{ is a loop on } S^2 \right\}.$$

From the above discussions, we can observe manifestations of properties of the NABPF in adiabatic transitions; for $M \neq \frac{1}{2}$, there only exists the transition from $|JM(s_0)\rangle$ to $|JM(s)\rangle$ because of diagonalization of $\bar{K}_M(s, s_0)$; for $M = \frac{1}{2}$, because $\bar{K}_{1/2}(s, s_0)$ is nondiagonal, there exists a transition both from $|JM = \frac{1}{2}(s_0)\rangle$ to $|JM = \frac{1}{2}(s)\rangle$ and from $|JM = \frac{1}{2}(s_0)\rangle$ to $|JM' = -\frac{1}{2}(s)\rangle$. Then, we have the selection rules

$$\Delta\tilde{M} = \tilde{M}' - \tilde{M} = \begin{cases} 0 & \text{for } \tilde{M} \neq \pm\frac{1}{2}, \\ 0, \mp 1 & \text{for } \tilde{M} = \pm\frac{1}{2}, \end{cases} \quad (23)$$

from $|JM(s_0)\rangle$ to $|JM'(s)\rangle$. The difference in the selection rule between the two cases for $M \neq \frac{1}{2}$ and $M = \frac{1}{2}$ may be observed in an experiment.

IV. NONADIABATIC EFFECTS IN NQR

When the principal axis of the quadrupole coupling is changed so fast that the adiabatic condition in NQR,

$$|\sin\alpha(s)\dot{\beta}(s)/(\omega_0 T)| \ll 1, \quad (24)$$

does not hold, we need to consider the lowest-order approximation leading to nonadiabatic corrections—the second-order approximation.

In NQR the evolution with an initial state $|J, M(s_0)\rangle$ ($M \geq 2$) only is concerned with the Abelian holonomy subgroup structure. The initial conditions for this case are

$$\begin{aligned} b_M^{[0]}(s_0) &= \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_n^{[0]}(s_0) = 0 \quad (n' \neq M), \\ b_n^{[K]}(s_0) &= 0 \quad (K \geq 1) \end{aligned} \quad (25)$$

from which we obtain explicit solutions of the first-order approximate equations:

$$\begin{aligned} b_M^{[0]}(s) &= \bar{K}_M(s, s_0) b_M^{[0]}(s_0) \\ &= \exp[-iM\Omega(s, s_0)] \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad M \neq \pm\frac{1}{2}, \pm\frac{3}{2}, \\ b_n^{[0]}(s) &= 0, \quad n' \neq M. \end{aligned} \quad (26)$$

Solving second-order approximate equations

$$\dot{b}_{M+1}^{[1]}(s) + \bar{A}(M+1, M+1, s) b_{M+1}^{[1]}(s) = i \frac{d}{ds} \left[\frac{\exp[i(2M+1)(s-s_0)\omega_0 T - iM\Omega(s, s_0)]}{(2M+1)\omega_0} \alpha_+(M) \right] \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (27a)$$

$$\dot{b}_{M-1}^{[1]}(s) + \bar{A}(M+1, M+1, s) b_{M-1}^{[1]}(s) = -i \frac{d}{ds} \left[\frac{\exp[-i(2M-1)(s-s_0)\omega_0 T - iM\Omega(s, s_0)]}{(2M-1)\omega_0} \alpha_-(M) \right] \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (27b)$$

from (25) and (26), we have

$$b_{M\pm 1}^{[1]}(s) = \pm i \int_{s_0}^s d\tau \exp[i(M\pm 1)\Omega(s, \tau)] \frac{d}{d\tau} \left[\frac{\exp[\pm i(2M\pm 1)(s-s_0)\omega_0 T - iM\Omega(s, s_0)]}{(2M\pm 1)\omega_0} \alpha_\pm(M, \tau) \right] \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (28)$$

and thereby obtain the probabilities

$$P(|JM(s_0)\rangle \rightarrow |JM\pm(s)\rangle) = \left| \frac{1}{T} b_{M\pm 1}^{[1]}(s) \right| \quad (29)$$

from $|JM(s_0)\rangle$ to $|JM\pm(s)\rangle$, which can be finally computed for a certain variation of $\mathbf{n}(s)$: e.g.,

$$P(|JM(s_0)\rangle \rightarrow |JM\pm(s)\rangle) \simeq \frac{4 \sin^2\alpha [J(J+1) - M(M\pm 1)]}{(2M\pm 1)^2} \left[\frac{\omega}{\omega_0} \right]^2 \sin^2\{[\omega \cos\alpha + (M\pm \frac{1}{2})\omega_0]T(s-s_0)\} \quad (30)$$

for the case with $\dot{\beta}(s) = \omega T = \text{const}$ and $\alpha(s) = \text{const } \alpha$. Here the terms of $(\omega/\omega_0)^3$ have been neglected. Then we have the selection rules of transition from $|J\tilde{M}(s_0)\rangle$ to $|J\tilde{M}'(s)\rangle$:

$$\Delta\tilde{M} = \tilde{M}' - \tilde{M} = \pm 1, \quad \tilde{M} \neq \pm \frac{1}{2}, \quad \tilde{M}' \neq \pm \frac{3}{2} \quad (31)$$

under second-order approximations.

Now we consider nonadiabatic effects in NQR concerning the non-Abelian holonomy group structure for the following cases.

(i) The second-order approximate equations for evolution with the initial state $|J\tilde{M} = \frac{3}{2}(s_0)\rangle$ are

$$\dot{b}_{\frac{1}{2}}^{[1]}(s) + \tilde{A}(\frac{1}{2}, \frac{1}{2}, s)b_{\frac{1}{2}}^{[1]}(s) = \left[\frac{\exp[-2i\omega_0 T(s-s_0)]\alpha_-(\frac{3}{2})}{2\omega_0} \tilde{A}(\frac{1}{2}, \frac{3}{2}, s)b_{\frac{3}{2}}^{[0]}(s) \right], \quad (32a)$$

$$\dot{b}_{\frac{3}{2}}^{[1]}(s) + \tilde{A}(\frac{3}{2}, \frac{3}{2}, s)b_{\frac{3}{2}}^{[1]}(s) = i \frac{d}{ds} \left[\frac{\exp[4i\omega_0 T(s-s_0)]\alpha_+(\frac{3}{2})}{4\omega_0} \tilde{A}(\frac{3}{2}, \frac{3}{2}, s)b_{\frac{3}{2}}^{[0]}(s) \right], \quad (32b)$$

$$\dot{b}_n^{[1]}(s) = 0, \quad n \neq \frac{1}{2}, \frac{5}{2}, \quad (32c)$$

where the first-order approximate solutions

$$b_{\frac{3}{2}}^{[0]}(s) = \exp[-i\frac{3}{2}\Omega(s, s_0)] \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_n^{[0]}(s) = 0, \quad n' \neq \frac{3}{2} \quad (33)$$

are obtained from the initial conditions

$$b_{\frac{3}{2}}^{[0]}(s_0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_n^{[0]}(s_0) = 0, \quad n' \neq \frac{3}{2}, \quad b_n^{[l]}(s_0) = 0, \quad l \geq 1. \quad (34)$$

Equation (32b) is independent of the NABPF and its solutions can be given by (28). Equation (32a) depends on the NABPF and its solution takes the form

$$\begin{bmatrix} a \neq 0 \\ b \neq 0 \end{bmatrix}$$

because of a nondiagonal $\tilde{K}_{1/2}(s, s_0)$. Thus, there exists not only the transition from $|J_{\frac{3}{2}}(s_0)\rangle$ to $|J_{\frac{1}{2}}(s)\rangle$, but also the transition from $|J_{\frac{3}{2}}(s_0)\rangle$ to $|J, -\frac{1}{2}(s)\rangle$. Here we have considered the formal solutions of (9b):

$$b_n^{[K]}(s) = \int_{s_0}^s \tilde{K}_n(s, \tau) F_n^{[K]}(\tau) d\tau. \quad (35)$$

(ii) The second-order approximate equations for evolution with the initial state $|J\tilde{M} = \frac{1}{2}(s_0)\rangle$ are

$$\dot{b}_{\frac{3}{2}}^{[1]}(s) + \tilde{A}(\frac{3}{2}, \frac{3}{2}, s)b_{\frac{3}{2}}^{[1]}(s) = -i \frac{d}{ds} \left[\frac{\exp[2i\omega_0 T(s-s_0)]\alpha_-(\frac{1}{2})}{2\omega_0} \tilde{A}(\frac{3}{2}, \frac{1}{2}, s)b_{\frac{1}{2}}^{[0]}(s) \right], \quad \dot{b}_n^{[1]}(s) = 0, \quad n' \neq \frac{3}{2}, \quad (36)$$

where the first-order approximate solutions

$$b_{\frac{1}{2}}^{[0]}(s) = ([\tilde{K}_{1/2}(s, s_0)]_{11}, [\tilde{K}_{1/2}(s, s_0)]_{21})^T = \tilde{K}_{1/2}(s, s_0) \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_n^{[0]}(s) = 0, \quad n' \neq \frac{1}{2} \quad (37)$$

are obtained from the initial conditions

$$b_{\frac{1}{2}}^{[0]}(s_0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_n^{[0]}(s_0) = 0, \quad n' \neq \frac{1}{2}, \quad b_n^{[l]}(s_0) = 0, \quad l \geq 1. \quad (38)$$

Because of nondiagonal $\tilde{K}_{1/2}(s, s_0)$, $b_{\frac{1}{2}}^{[0]}(s)$ takes the form

$$\begin{bmatrix} a \neq 0 \\ b \neq 0 \end{bmatrix}$$

and thereby $b_{\frac{3}{2}}^{[1]}(s)$ given by (36) and (35) takes the form

$$\begin{bmatrix} a' \neq 0 \\ b' \neq 0 \end{bmatrix};$$

i.e., there exist the transitions both from $|J_{\frac{1}{2}}(s_0)\rangle$ to $|J_{\frac{3}{2}}(s)\rangle$ and from $|J_{\frac{1}{2}}(s_0)\rangle$ to $|J, -\frac{3}{2}(s_0)\rangle$.

According to the qualitative analyses in (i) and (ii) and other similar discussion, we obtain the selection rules

$$\Delta\tilde{M} = \tilde{M}' - \tilde{M} = \begin{cases} \pm 1, \mp 2 & \text{for } \tilde{M} = \pm \frac{1}{2}, \\ +1, -1, \mp 2 & \text{for } \tilde{M} = \pm \frac{3}{2} \end{cases} \quad (39)$$

for transitions from $|J\tilde{M}(s_0)\rangle$ to $|J\tilde{M}'(s)\rangle$ under the second-order approximation. They manifest the physical effects of

the NABPF in a nonadiabatic situation and are expected to be observed in Tycko's experiment improved by breaking the adiabatic conditions.

For concrete situations the above predictions can be quantitatively given, e.g., for the cases with $\beta(s) = \text{const}\omega T$ and $\alpha(s) = \text{const}\alpha$, a solution of (36) is

$$\begin{aligned}
 b_{3/2}^{[1]}(s) &= \frac{T}{8\lambda} \left[\frac{\omega}{\omega_0} \right] \sin\alpha (b_+(s), b_-(s))^T, \\
 b_+(s) &= -[J(J+1) - \frac{3}{4}]^{1/2} \left\{ (\cos\alpha + \lambda) \left[\exp \left[\frac{i}{2} [(\lambda - 3\cos\alpha)\omega + 4\omega_0]T(s-s_0) \right] - 1 \right] \right. \\
 &\quad \left. + (\lambda - \cos\alpha) \left[\exp \left[\frac{i}{2} [(\lambda + 3\cos\alpha)\omega - 4\omega_0]T(s-s_0) \right] - 1 \right] \right\}, \\
 b_-(s) &= (J + \frac{1}{2}) [J(J+1) + \frac{3}{4}]^{1/2} \sin\alpha \left[\exp \left[\frac{i}{2} [(\lambda + 3\cos\alpha)\omega + 4\omega_0]T(s-s_0) \right] \right. \\
 &\quad \left. - \exp \left[\frac{-i}{2} [(\lambda + 3\cos\alpha)\omega - 4\omega_0]T(s-s_0) \right] \right],
 \end{aligned} \tag{40}$$

which explicitly gives the probabilities

$$\begin{aligned}
 P(|J_{\frac{1}{2}}(s_0)\rangle \rightarrow |J_{\frac{3}{2}}(s)\rangle) &= \left| \frac{1}{T} b_{3/2+3/2}^{[1]}(s) \right|^2 = \frac{1}{64\lambda^2} \left[\frac{\omega}{\omega_0} \right]^2 \sin^2\alpha [J(J+1) - \frac{3}{4}] \\
 &\quad \times ((\cos^2\alpha + 5\lambda^2) + (\cos^2\alpha - \lambda^2)\cos[\frac{1}{2}\lambda\omega T(s-s_0)]) \\
 &\quad - 2\lambda(\cos\alpha + \lambda)\cos\{\frac{1}{2}(\lambda - 3\cos\alpha)\omega - \omega_0\}T(s-s_0)\} \\
 &\quad + 2\lambda(\cos\alpha - \lambda)\cos\{\frac{1}{2}(\lambda + 3\cos\alpha)\omega - \omega_0\}T(s-s_0)\},
 \end{aligned} \tag{41a}$$

$$\begin{aligned}
 P(|J_{\frac{1}{2}}(s_0)\rangle \rightarrow |J - \frac{3}{2}(s)\rangle) &= \left| \frac{1}{T} b_{3/2-3/2}^{[1]}(s) \right|^2 \\
 &= \frac{1}{16\lambda^2} \left[\frac{\omega}{\omega_0} \right]^2 \sin^2\alpha [J(J+1) + \frac{3}{4}] \sin^2[\frac{1}{2}\lambda\omega T(s-s_0)]
 \end{aligned} \tag{41b}$$

of transitions from $|J\tilde{M} = \frac{1}{2}(s_0)\rangle$ to $|J\tilde{M}' = \pm\frac{3}{2}(s)\rangle$.

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