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Test of Quantum Adiabatic Approximation via Exactly-Solvable Dynamics of High-Spin Precession

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Abstract

By invoking the Rabi rotation technique, the Schrödinger wavefunction of a neutral particle with a magnetic moment and a high-spin is exactly solved in a harmonically-changing magnetic field. This result is then applied to illustrate what the accuracy of the quantum adiabatic approximation is exactly and how the non-adiabatic transition vanishes in accompaniment with the appearence of Berry's geometrical phase. The discussion of this paper verifies C. N. Yang's point of view about the generalization of the quantum adiabatic approximation in connection with Berry's phase.

Because of Berry's remarkable discovery [1], a number of theoretical and experimental investigations have been focused on the geometrical and topological behaviours of the quantum mechanical system with time-dependent parameters [2]. As Berry showed, if the frequency of variation of its Hamiltonian is small enough in comparison with its natural transition frequency, so that the adiabatic conditions hold, the system always remains in an instantaneous eigenstate of the time-dependent Hamiltonian for the whole process of evolution and a geometrical phase, the Berry's phase, appears in addition to the dynamical phase of the Schrödinger wavefunction for the system. Notice that Berry's proof about this conclusion is based on the quantum adiabatic approximation method (QAAM) [3–5].

Considering that the Berry's phase was ignored in the original QAAM (see the standard texts of quantum mechanics [4, 5], one (CPS) of the authors developed the QAAM in connection with the Berry's phase and the treatment of the non-adiabatic effects for many cases [6–10]. However, we have to point out that only very little is well known at present about the quantitative validity of the original QAAM and its generalization. One of the purposes of this paper is to test the accuracy and validity of the QAAM through an exact solution to the Schrödinger equation of a neutral particle with a magnet and a high-spin in a harmonically-changing magnetic field. Such a solution is obtained by generalizing Rabi's rotating framework technique, which was proposed for the case of spin-1/2 [11]. Another purpose is to consider C. N. Yang's insight on the QAAMs with and without Berry's phase [12] in terms of this exact solution of the Schrödinger equation. In Yang's point, the QAAM incorporating Berry's phase was considered as an approximation of next order while the original QAAM without Berry's phase is thought as that of lowest order.

Consider a neutral particle with a magnetic moment and arbitrary spin j in a harmonically-changing external magnetic field

$$\boldsymbol{B} = \boldsymbol{B}(t) = B_0 (\sin\theta \cos\omega t, \sin\theta \sin\omega t, \cos\theta), \tag{1}$$

where θ is constant. Its Hamiltonian,

$$\hat{H} = \hat{H}(t) = \mu \boldsymbol{B}(t) \cdot \hat{\boldsymbol{J}} = \mu B_0 (J_x \sin\theta \cos\omega t + J_y \sin\theta \sin\omega t + J_x \cos\theta), \tag{2}$$

is written in terms of the angular momentum operators $\hat{\boldsymbol{J}} = (J_x, J_y, J_z)$. Here, the time-dependent magnetic field rotates around the z-axis with a constant frequency ω, and a constant angle θ with respect to the z-axis. The Schrödinger equation governed by such a Hamiltonian is time-dependent and thus it is difficult to solve it exactly.

However, a straight-forward physical consideration teaches us to transform into a moving framework of reference rotating along with the motion of the magnetic field, $\boldsymbol{B}(t)$. In such a frame of reference, one should "see" a time-independent Hamiltonian. This idea is motivated by Rabi's work [11] for spin-1/2, although it was not stated explicitly by Rabi himself. Since the case of spin-1/2 is associated with the two-dimensional representation of angular momentum, we naturally invoke quantum rotation transformation in angular momentum theory to deal with the quantum dynamics of high-spin precession in a $2j + 1$-dimensional representaton for arbitrary j. The main difference of the present mathematical derivation from that in the case of spin-1/2 is to use the operator computation instead of the 2×2 matrix computation for spin-1/2.

Let us invoke a transformation:

$$R_z(\omega t) = e^{-iJ_z \omega t/\hbar} \tag{3}$$

to the rotating frame of reference for the wavefunction, $|\psi(t)\rangle$, governed by the original Hamiltonian, $H(t)$, the rotated wavefunction

$$|\phi(t)\rangle = R_z(\omega t)^\dagger |\psi(t)\rangle \tag{4}$$

is easily proved to satisfy an effective Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle = \hat{H}_R |\phi(t)\rangle \tag{5}$$

with the effective Hamiltonian

$$H_R = R_z(\omega t)^\dagger H(t) R(\omega t) + \frac{1}{-i\hbar} R(\omega t)^\dagger \frac{\partial}{\partial t} R(\omega t) = \omega_0 [J_z \cos\alpha + J_x \sin\alpha] \tag{6}$$

where

$$\sin\alpha = \frac{\mu B_0}{\omega_0}\sin\theta,$$

$$\lambda = \frac{\omega}{\mu B_0},$$

$$\omega_0(\lambda)^2 \equiv \omega_0^2 = (\mu B_0)^2(1 - 2\lambda\cos\theta + \lambda^2). \tag{7}$$

Obviously, the effective Hamiltonian, H_R, "seen" in the rotating framework of reference has not explicit time-dependence. So we can solve its evolution in this frame of reference.

In fact, using the rotation operator

$$R_y(\alpha) = e^{-iJ_y\alpha/\hbar} \tag{8}$$

one can rewrite H_R in the following form:

$$H_R = R_y(\alpha)\omega_0 J_z R_y(\alpha)^\dagger. \tag{9}$$

Then, it is not difficult to prove that the eigenstates

$$|j, m(\alpha)\rangle = R_y(\alpha)|j, m\rangle, \quad m = j, j-1, \ldots, -j, \tag{10}$$

are the rotations of the standard angular momentum basis $|j, m\rangle$, which correspond to the eigenvalues

$$E_m = m\hbar\omega_0, \tag{11}$$

respectively.

Therefore, if the initial state of the system is $|\psi(0)\rangle$ at $t = 0$, then the exact wavefunction follows from eqs (9)–(11), directly:

$$|\psi(t)\rangle = \sum_m \langle jm(\alpha)|\psi(0)\rangle\, e^{-im\omega_0 t}\, e^{-iJ_z\omega t/\hbar}|j, m(\alpha)\rangle$$
$$= \sum_{m,m'} \langle jm(\alpha)|\psi(0)\rangle d^j_{m'm}(\alpha)\, e^{-i(m\omega_0 + m'\omega)t}|j, m'\rangle. \tag{12}$$

Here, the d-function

$$d^j_{m',m}(\alpha) = \langle j, m'|e^{-iJ_y\alpha/\hbar}|j, m\rangle$$

in angular momentum theory has been used explicitly.

Let us use the above exact solution (12) to test the QAAM. If the system is initially in an instantaneous eigenstate of $H(0)$,

$$|\psi(0)\rangle = e^{-iJ_y\theta/\hbar}|j, m = M\rangle$$
$$= \sum_{m'}\langle j, m'(\alpha)|e^{-iJ_y\theta/\hbar}|j, M\rangle|j, m'(\alpha)\rangle$$
$$= \sum_{m'} d^j_{m',M}(\theta - \alpha)|j, m'(\alpha)\rangle,$$

the exactly-solvable solution (12) is specified as

$$|\psi(t)\rangle = \sum_{m,m'=-j}^{j} d^j_{m'M}(\theta - \alpha) d^j_{m,m'}(\alpha)\, e^{-im'\omega_0 t - im\omega t}|j, m\rangle$$
$$\equiv \sum_{m,m'} F^M_{m,m'}\left(\cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}\right) e^{-im'\omega_0 t - im\omega t}|j, m\rangle. \tag{13}$$

Notice that $d^j_{m,n}(\beta)$ here is the linear combination of $(\cos\beta/2)^k\,(\sin\beta/2)^l$ ($k, l = 0, 1, 2, \ldots$). If the variation of $\boldsymbol{B}(t)$ is slow enough, then $\lambda = \omega/\mu B_0$ is so small that the deviation of α from θ is of the order $O^1(\omega/\mu B_0)$, i.e.,

$$\sin\alpha = [1 + \lambda\cos\theta - O^2(\lambda)]\sin\theta. \tag{14}$$

This is because eq. (7) results in

$$\omega_0 = \mu B_0[1 - \lambda\cos\theta + O^2(\lambda)]. \tag{15}$$

Now, we are just in the position to exactly see how the adiabatic approximation appears. Since it is required for a real evolution that $\boldsymbol{B}(t)$ must be changed by a finite difference in a sufficiently-long time, T, e.g., $\boldsymbol{B}(t)$ is traversed by a period, i.e., $\omega T = 2\pi$, we cannot neglect all terms of the order $\lambda = \omega/\mu B_0$ in expression (13). Using eqs (13) and (14), one formally writes

$$|\psi(T)\rangle = \sum_{m,m'}\left[F^M_{m,m'}\left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\right) + O^1(\lambda)\right]$$
$$\times e^{-i\mu m' B_0 T}\, e^{i[\omega T(m'\cos\theta - m)]}\, e^{im'\omega T O^1(\lambda)}|j, m\rangle. \tag{16}$$

Notice that

$$\sum_{m'} F^M_{m,m'}\left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\right) e^{-im'\omega_0 T} = d^j_{m,M}(\theta)\, e^{-iM\omega_0 T}. \tag{17}$$

Taking a reasonable limit by letting $\lambda = \omega/\mu B_0$ approach zero but letting ωT remain of a finite value, one has

$$|\psi(T)\rangle = \sum_m d^j_{m,M}(\theta)\, e^{-i(M\omega_0 + m\omega)T}|j, m\rangle$$
$$= e^{-iM\mu B_0 T}\, e^{iM\omega T\cos\theta}|j, M(\theta; T)\rangle \tag{18}$$

where

$$|j, M(\theta, T)\rangle = e^{-iJ_z\omega T/\hbar}\, e^{-iJ_y\theta/\hbar}|j, M\rangle \tag{19}$$

is just an instantaneous eigenstate of $H(T)$ at time $t = T$. Physically, this limit means that a very strong magnetic field is changed with a finite frequency. The result can also be given by the generalized QAAM. Here,

$$\nu_M(T) = -M\omega T\cos\theta \tag{20}$$

is a Berry's geometric phase in addition to the dynamic phase $m\mu BT$.

It is pointed out that, in the original QAAM, there does not appear the Berry's phase $\nu_M(T)$ in eq. (18). This is because it neglects all terms of the order $O^1(\lambda) = O^1(\omega/muB_0)$ both in the coefficients $F^M_{m,n}$ and the oscillating phase $T\omega_0(\omega/\mu B_0)$ in eq. (16). (Notice that $F^N_{m,n}$s are the component amplitudes of the wavefunction.) But a reasonable QAAM should only neglect terms of the order $O^1(\lambda)$ in the amplitudes but not that in the phase $T\omega_0(\omega/\mu B_0)$ for oscillation. The above discussions just enjoy Yang's point on QAAM [12]: The original QAAM without Berry's phase can be regarded as the lowest order approximation while that with Berry's phase as an approach of next order. The recent experiments on Berry's phase have partiality for the latter since the former ignores too much of the practical problems.

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