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Berry's Phases of the Alkali Atom in a SlowlyChanging Strong Magnetic Field and Non-Adiabatic Transition[1]

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Abstract

In this paper the high-order adiabatic approximation (HOAA) method is formulated in a new form so that the calculation is greatly simplified. Using this improved HOAA method, we study the Berry phase effects of the Alkali atom in a slowly-changing strong magnetic field and also the non-adiabatic transitions between the instantaneous angular momentum states. The possible observability is also pointed out.

I. Introduction

Time evolution of quantum system governed by a changing Hamiltonian can be geometrically analyzed and its adiabatic case leads to the famous Berry's topological phase and the corresponding induced gauge structure[1,2]. For the non-adiabatic case, a few methods calculating non-adiabatic transitions, such as the schemes for successively diagonalizing (SSD)[3–5], the high-order adiabatic approximation (HOAA) method[6–9], the generalized WKB approximation (GWKBA)[10,11] and the extended Born-Oppenheimer (EBO) approximation[12,13] (for the case that the changing parameters are dynamic variables), were proposed with respect to the Berry's phase and the induced gauge field respectively. However all the discussions[3–13] only concern with the case of precession of spin $\frac{1}{2}$ as an example, which is an ideal model rather than a practical physics system. Thus, it is worth paying attention to a practical physics system — a Alkali atom with a higher orbit angular momentum state in a slowly-changing strong magnetic field:

$$\vec{B}(t) = B(t)(\sin\theta(t)\cos\phi(t), \sin\theta(t)\sin\phi(t), \cos\theta(t)) .$$

The Hamiltonian for the problem is

$$\hat{H}(t) = \hat{H}[\vec{B}(t)] = \frac{\hbar^2}{2\mu}\hat{p}^2 + V(r) + \alpha\vec{B}\cdot(\hat{\vec{L}} + 2\hat{\vec{S}}) , \tag{1}$$

where $\alpha = e/(2\mu c), \mu$ is the reduced mass and the $L - S$ coupling has been neglected for the sufficiently strong magnetic field $\vec{B}(t)$.

II. General Formulation of Improved HOAA Method

We consider the simple degenerate case that the Hamiltonian depending on the slowly-changing parameters $R(T) = (R_1(t), R_2(t), \cdots, R_N(t))$ has a set of degenerate instantaneous

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eigenstates $|n\alpha[R]\rangle(\alpha = 1, 2, \cdots, D_n)$ with the eigenvalues $E_n[R] = E_n(t)$ transforming as an irreducible representation $\Gamma^{[n]}$ under a varying symmetry group, which is an isomorphism of a fixed group G. Let $\hbar = 1$ and

$$|\phi(t)\rangle = \sum_n \sum_{\alpha=1}^{D_n} C_{n\alpha}(t) \exp\left[-i \int_0^t E_n(t')dt'\right] |n\alpha[R]\rangle \tag{2}$$

be a solution of the time-dependent Schrödinger's equation

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle .$$

Then

$$\begin{aligned}\dot{C}_{n\alpha}(t) + \sum_{\beta=1}^{D_n} \langle n\alpha[R]|n\dot{\beta}[R]\rangle C_{n\beta}(t) = &-\sum_{m\neq n} \exp\left[-i\int_0^t (E_n[R'] - E_m[R'])dt'\right] \\ &\times \sum_{\beta=1}^{D_m} \langle n\alpha[R]|m\dot{\beta}[R]\rangle C_{m\beta}(t) ,\end{aligned} \tag{3}$$

where we have defined

$$f' = f(\tau') , \qquad \dot{f} = \frac{d}{d\tau} f(\tau)$$

and

$$|n\dot{\alpha}[f]\,\rangle = \frac{d}{d\tau}|n\alpha[f]\,\rangle$$

for a function $f = f(\tau)$ of τ.

In Refs. [6]–[8], the right-hand side of Eq. (3) is expanded as a series of the adiabatic parameter $(1/T)$ through the integration by part (T is a characteristic time of the system such as the period of $\vec{B}(t)$). Because the infinite terms are contained in the series, the calculation is very complicated. Now, in order to avoid this complexity, we simply regard the right-hand side of Eq. (4) as a perturbation from a physical consideration that the right-hand side completely vanishes when $\hat{H}$ does not depend on time, it is very small when $\hat{H}$ slightly depends on time. Using the perturbation theory of linear differential equation, we obtain

$$C_{n\alpha}(t) = \sum_{k=0}^{\infty} C_{n\alpha}^{[k]} , \tag{4a}$$

$$\dot{C}_{n\alpha}^{[0]}(t) + \sum_{\beta=0}^{D_n} \langle n\alpha[R]|n\dot{\beta}[R]\rangle C_{n\beta}^{[0]}(t) = 0 , \tag{4b}$$

$$\begin{aligned}\dot{C}_{n\alpha}^{[k]}(t) + \sum_{\beta=0}^{D_n} \langle n\alpha[R]|n\dot{\beta}[R]\rangle C_{n\beta}^{[k]} = &-\sum_{m\neq n} \exp\left[-i\int_0^t (E_n[R'] - E_m[R'])dt'\right] \\ &\times \sum_{\beta=1}^{D_m} \langle n\alpha[R]|m\dot{\beta}[R]\rangle C_{m\beta}^{[k-1]}(t) , \quad k = 1, 2, \cdots .\end{aligned} \tag{4c}$$

So long as we can obtain the first order solution $C_{n\alpha}^{[0]}(t)$, we can easily obtain the higher-order solution from Eq. (4c) since the equations of $C_{n\alpha}^{[k]}(t)$ only concern with $C_{n\alpha}^{[k-1]}(t)(k \geq 1)$.

According to Refs. [7] and [9], for the case with an invariant symmetry group,

$$\langle n\alpha[R]|n\dot{\beta}[R]\rangle = \delta_{\alpha\beta}\langle n\alpha[R]|n\dot{\alpha}[R]\rangle \equiv -\delta_{\alpha\beta} i\dot{\gamma}_{n\alpha}(t)\,,$$

then, we have

$$C^{[0]}_{n\alpha}(t) = C_{n\alpha}(0)\exp[i\gamma_{n\alpha}(t)]\,, \tag{5}$$

where

$$\gamma_{n\alpha}(t) = i\int_0^t \langle n\alpha[R']|n\dot{\alpha}[R']\rangle dt' \tag{6}$$

is just the Berry's phase.

When the adiabatic condition

$$\left|\frac{\langle n\alpha[R]|m\dot{\beta}[R]\rangle}{E_n[R]-E_m[R]}\right| \ll 1 \qquad (m \neq n) \tag{7}$$

holds, the parameter $R(t)$ changes so slowly that all the higher-order terms $C^{[k]}_{n\alpha}(t)\ (k \geq 1)$ in Eq. (4a) can be neglected and the first-order approximation solution $C^{[0]}_{n\alpha}$ describes the evolution of the system sufficiently in the adiabatic case.

III. Berry's Phase for the Alkali Atom

According to the angular momentum theory, we rewrite the Hamiltonian as

$$\hat{H}(t) = R_L(t)R_S(t)\Big[\frac{\hbar^2}{2\mu}p^2 + V(r) + \alpha B(t)(\hat{L}_z + 2\hat{S}_z)\Big]R_S^\dagger(t)R_L^\dagger(t)\,, \tag{8}$$

where

$$R_L(t) = e^{-i\phi(t)\hat{L}_z}e^{-i\theta(t)\hat{L}_y} \tag{9}$$

and

$$R_S(t) = e^{-i\phi(t)\hat{S}_z}e^{-i\theta(t)\hat{S}_y} \tag{10}$$

are the reduced rotation operators respectively on the coordinate space and the spin space. Then, we immediately obtain the instantaneous eigenstates

$$|\sigma(t)\rangle \equiv |n,l,m,m_s(t)\rangle = R_L(t)R_S(t)R_{nl}(r)|l,m\rangle \otimes |S,m_s\rangle \tag{11}$$

with the corresponding eigenvalues

$$E_{\sigma(t)} = E_{nlmm_s}(t) = E_{nl} + \alpha B(t)(m+2m_s)\,, \tag{12}$$

where $\sigma. = (n,l,m,m_s)$, $|l,m\rangle$ and $|S,m_s\rangle$ are the standard angular momentum states and $R_{nl}(r)$ is the Coulomb radial function.

The direct calculation leads to

$$\begin{aligned}\Big\langle \sigma'(t)\Big|\frac{d}{dt}\sigma(t)\Big\rangle = \delta_{ll'}\delta_{nn'}\{&\delta_{m_s m_s'}[-i\dot{\phi}(t)m\cos\theta\delta_{mm'} + F_+(t)f_+(l,m)\delta_{m',m+1} \\ &+F_-(t)f_-(l,m)\delta_{m',m-1}] + \delta_{m,m'}[-i\dot{\phi}(t)m_s\cos\theta\delta_{m_s,m_s'} \\ &+F_+(t)f_+(\tfrac{1}{2},m_s)\delta_{m_s',m_s+1} + F_-(t)f_-(\tfrac{1}{2},m_s)\delta_{m_s',m_s-1}]\}\,,\end{aligned} \tag{13}$$

where

$$\begin{aligned}F_\pm(t) &= \frac{1}{2}[i\sin\theta\dot{\phi}(t) \mp \dot{\theta}(t)]\,, \\ f_\pm(j,m) &= [(j\mp m)(j\pm m+1)]^{1/2}\,.\end{aligned} \tag{14}$$

Then, we obtain the explicit expression of Berry's phase

$$\gamma_{mm_s}(t) = \gamma_{nlmm_s}(t) = i\int_0^t \left\langle \sigma(t')\Big|\frac{d}{dt'}\sigma(t')\right\rangle dt' = -(m_s+m)[\Omega(t)+\phi(t)]\,, \tag{15}$$

where

$$\Omega(t) = \int_0^t (1-\cos\theta(t'))\dot{\phi}(t')dt'\,, \tag{16}$$

which is just the solid angle

$$\Omega(C) = \int_0^{2\pi} (1-\cos\theta[\phi])d\phi \tag{17}$$

subtended by the loop $C : \{\vec{B}(t)|\vec{B}(0) = \vec{B}(T)\}$ with respect to the point $\vec{B} = 0$ on the parameter manifold $M : \{\vec{B}\}$ for a cycle evolution that $\vec{B}(0) = \vec{B}(T)$. For the atom with the spin-up electron state and the orbit angular momentum state that the observable $\hat{L}_z$ has a definite value $\bar{m}$ at $t = 0$, the polarization of the atom with spin-up electron state is characterized by the probability P_0 that atom is in the orbit angular momentum state $|\,l,m\rangle$ at $t = T$. Using Eqs. (2), (4a) and (5), we obtain

$$\begin{aligned} P_0 = &\left[1-\sin^2\theta\cdot\sin^2\left(\alpha\int_0^T B(t')dt'\right)\right]\sum_{m'm''} d^l_{\bar{m}m'}(\theta_0)d^l_{mm'}(\theta_0)\cdot d^l_{\bar{m}m''}(\theta_0) \\ &\cdot d^l_{mm''}(\theta_0)\cos\left[(m'-m'')\left(\alpha\int_0^T B(t')dt'+\Omega[C]\right)\right] \end{aligned} \tag{18}$$

in terms of the d-function of the angular momentum theory. The solid angle $\Omega[C]$ appearing in the above equation manifests an observable effect of the Berry's phase.

IV. Non-Adiabatic Transitions

When $\vec{B}(t)$ changes so fast that the adiabatic condition

$$\frac{[|\sin\theta\dot{\phi}(t)|^2+|\dot{\theta}|^2]^{1/2}}{|\alpha B(t)|} \ll 1 \tag{19}$$

does not hold, the non-adiabatic effects appear as the transitions between $|\sigma(t=0)\rangle$ and $|\sigma(t=T)\rangle$. Let

$$|\psi(t)\rangle = \sum_\sigma C_\sigma e^{-i\int_0^t E_\sigma(t')dt'}|\sigma(t)\rangle \tag{20}$$

be a solution of $i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$. Then

$$\begin{aligned} &\dot{C}_{n\,l\,m\,m_s}(t) - i\dot{\gamma}_{m\,m_s}(t)C_{n\,l\,m\,m_s}(t) = \\ &-\{F_+(t)e^{-i\beta(t)}[f_+(l,m)C_{n\,l\,m+1\,m_s}(t)+e^{-i\beta(t)}f_+(\tfrac{1}{2},m_s)C_{n\,l\,m\,m_s+1}(t)] \\ &+F_-(t)e^{i\beta(t)}[f_-(l,m)C_{n\,l\,m-1\,m_s}(t)+e^{i\beta(t)}f_-(\tfrac{1}{2},m_s)C_{n\,l\,m\,m_s-1}(t)]\}\,, \end{aligned} \tag{21}$$

where

$$\beta(t) = \alpha\int_0^t B(t')dt'\,.$$

If the initial state of the atom at $t=0$ is $|n,l,\bar{m},\bar{m}_s(t=0)\rangle$, the initial conditions for Eq.

(21) are

$$C^{[0]}_{nl\bar{m}\bar{m}_s}(0) = 1\,, \quad C^{[0]}_{nlmm_s}(0) = 0\,, \quad ((m, m_s) \neq (\bar{m}, \bar{m}_s))\,,$$
$$C^{[k]}_{nlmm_s}(0) = 0\,, \quad (k = 1, 2, \cdots)\,, \tag{22}$$

then we have the first-order approximation solution

$$C^{[0]}_{nlmm_s}(t) = e^{i\gamma_{mm_s}(t)}\delta_{m\bar{m}}\delta_{m_s\bar{m}_s} \tag{23}$$

and the second-order approximation equations

$$\dot{C}^{[1]}_{nl\,\bar{m}-1\,m_s}(t) - i\dot{\gamma}_{\bar{m}-1\,m_s}(t)C^{[1]}_{nl\,\bar{m}-1\,m_s}(t) = -F_+(t)e^{-i\beta(t)}f_+(l, \bar{m}-1)C^{[0]}_{nl\,\bar{m}\,m_s}(t)\,, \tag{24a}$$

$$\dot{C}^{[1]}_{nl\,\bar{m}+1\,m_s}(t) - i\dot{\gamma}_{\bar{m}+1\,m_s}(t)C^{[1]}_{nl\,\bar{m}+1\,m_s}(t) = -F_-(t)e^{i\beta(t)}f_-(l, \bar{m}+1)C^{[0]}_{nl\,\bar{m}\,m_s}(t)\,, \tag{24b}$$

$$\dot{C}^{[1]}_{nl\,\bar{m}\,\bar{m}_s-1}(t) - i\dot{\gamma}_{\bar{m}\,\bar{m}_s-1}(t)C^{[1]}_{nl\,\bar{m}\,\bar{m}_s-1}(t) = -F_+(t)e^{-2i\beta(t)}f_+(\tfrac{1}{2}, \bar{m}_s-1)C^{[0]}_{nl\,\bar{m}\,m_s}(t)\,, \tag{24c}$$

$$\dot{C}^{[1]}_{nl\,\bar{m}\,\bar{m}_s+1}(t) - i\dot{\gamma}_{\bar{m}\,\bar{m}_s+1}(t)C^{[1]}_{nl\,\bar{m}\,\bar{m}_s+1}(t) = -F_-(t)e^{2i\beta(t)}f_-(\tfrac{1}{2}, \bar{m}_s+1)C^{[0]}_{nl\,\bar{m}\,m_s}(t)\,. \tag{24d}$$

Their solutions define the transition probabilities

$$P(\bar{\sigma} \longrightarrow \sigma) = |C^{[1]}_{\sigma}|^2\,, \qquad \bar{\sigma} = (n, l, \bar{m}, m_s)\,.$$

The selection rule for the transitions under the second-order approximation is

$$\Delta m = \pm 1\,, \qquad \Delta m_s = \pm 1\,.$$

A similar discussion gives the selection rules

$$\Delta m = \pm 1, \pm 2, \cdots, \pm(k-1)\,, \quad (k \leq l)\,,$$
$$\Delta m = \pm 1, \pm 2, \cdots, \pm l\,, \quad (k > l)\,,$$
$$\Delta m_s = \pm 1$$

under the k' th-order adiabatic approximation. These transitions manifests the non-adiabatic effects accompanied with Berry's phases.

Now, we calculate the explicit transition probabilities. Because the exact transition probability can be worked out by using some tricks in a particular case that $\theta(t)$=constant and $\dot{\phi}(t)$=constant, we now consider a more complicated case

$$\theta(t) = \theta_0 - \frac{kt}{T}\,, \quad \phi(t) = \frac{2\pi}{T}t\,, \quad B(t) = \text{constant}\, B\,.$$

From Eqs. (24a) and (24b), we obtain the transition probabilities

$$\begin{aligned} P(|l, m(0)\rangle \longrightarrow |l, m \pm 1(T)\rangle) &= |C^{[1]}_{nl\,m\pm 1\,m_s}(T)|^2 \\ &= \frac{|f_\pm(l,m)|^2}{T^2\alpha^2 B^2}\Big\{\Big|\int_0^t [\cos\Gamma_\pm(t')\cdot A_\pm(t') - \sin\Gamma_\pm(t')B_\pm(t')]dt'\Big|^2 \\ &\quad + \Big|\int_0^t [\cos\Gamma_\pm(t')\cdot B_\pm(t') + \sin\Gamma_\pm(t')A_\pm(t')dt'\Big|^2\Big\}\,, \end{aligned} \tag{25}$$

where

$$\Gamma_{\pm}(t) = \pm\frac{2\pi}{k}\sin\left(\theta_0 - \frac{kt}{T}\right) \pm \alpha BT,$$
$$A_{\pm}(t) = k\pi\cos\left(\theta_0 - \frac{kt}{T}\right) + \frac{1}{2}\left[2m\cos\left(\theta_0 - \frac{kt}{T}\right) \pm \alpha BT\right], \tag{26}$$
$$B_{\pm}(t) = \mp\sin\left(\theta_0 - \frac{kt}{T}\right)\left[2m\cos\left(\theta_0 - \frac{kt}{T}\right) \pm \alpha BT\right].$$

V. Discussion

It is easy to observe that the external magnetic field $\vec{B}(t)$ can not cause the transition between two states with different quantum numbers (n, l) and the effects related to Berry's phase only appear with respect to the magnetic quantum number (m, m_s). Thus, the discussion about adiabatic and non-adiabatic evolutions only concern with a given irreducible representation of SO(3).

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