Commun. Theor. Phys. 13(1990)63–70

Physical Effects of U(1)–Induced Gauge Field and Their Non–Adiabatic Corrections for the Cases with Arbitrary Spin[1]

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(Received August 18, 1989)

Abstract

By making use of the improved Born–Oppenheimer approximate method, we deal with the separation of spin variable and space variable of neutral particle with arbitrary spin in inhomogeneous magnetic field and non–adiabatic corrections for the problems are thereby computed as perturbations. We also analysis the geometrical properties of loop phase of the induced gauge potential and point out its observable effects relating to Bitter and Dubbers' experiment. Finally, we discuss the transitions between the instantaneous spin states as non–adiabatic effects resulting from *inhomogeneity of the magnetic field.*

I. Introduction

After topological Berry's phase was discovered[1,2], it was recognized by Simon that Berry's phase factor is precisely the holonomy in a Hermitian bundle over the parameter space and the quantum adiabatic theorem defines a connection in such a bundle[3]. The connection naturally gives a gauge structure–the induced gauge structure and the gauge group corresponds to the local unitary freedom in choosing the phases of the instantaneous eigenstates of the Hamiltonian with slowly changing parameters. Wilczek and Zee discussed its non–Abelian generalization for degenerate quantum mechanical systems[4]. With molecular system as an example, later on Moody, Shapre and Wilczek analysed the implications of induced gauge structure when the parameters are themselves the dynamical variable in large system[5]. It was shown from their work that for a quantum system (e.g. a molecule) with two sets of variables, the fast one (e.g. electric degree of freedom) and slow one (e.g. nuclear degree of freedom), after resolving the dynamics of the fast variable under the adiabatic condition that the Born–Oppenheimer (B–O) approximation holds, an involved external vector field within the effective Hamiltonian about the slow variables is just the aforementioned connection, i.e. the induced gauge potential.

[1] Work supported in part by the National Natural Science Foundation of China.

Now, a natural question is whether one can observe the direct effects of the induced gauge field when the parameters are dynamical variable. Jackiw's answer was that "only more indirect effects can be tested" and the presence of induced gauge potential is established by studying the energy spectrum of the complete system[2]. However, in this paper, a direct observable effects for a particle with arbitrary spin in an inhomogeneous magnetic field and thereby a new interpretation of Bitter and Dubbers' experiment[6] (B–D experiment) is naturally given (This experiment was also interpreted from the point of view of moving reference system and its non-adiabatic corrections was discussed with high-order adiabatic approximation method[7] by Sun, one of the authors, and Zhang[8]). The key point of our discussion in this paper is that the spin variable and the space variable for the particle are taken as the fast variable and the slow variable in B–O approximation respectively.

We arrange this paper as follows. In Sec. II, the improved B–O approximate method is extended to deal with the separation of the spin and space components for a particle in a slightly inhomogeneous magnetic field, and the general formulations are given for computing arbitrary order non-adiabatic effects. In Sec. III we use the first-order approximation to discuss the direct effects of induced gauge field for spin precession and corresponding geometrical properties. In Sec. IV, we compute the non-adiabatic corrections in practice and analyse their effects in experiments.

II. Formulation of Generalised B–O Approximation for Spin

A particle whose spin degree of freedom and space degree of freedom interact each other through an external field $\{F_\mu(x)\} \equiv F(x)$ $(x = (x_1, x_2, x_3) \in$ the physical space $R^3)$, can be described with the following Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + V(x) + \hat{h}[F(x), s]\,, \tag{1}$$

where $\hat{h}[F(x), s]$ is the interacting Hamiltonian.

Let $\hat{h}[F(x), s]$ have non-degenerate eigenfuctions $|n[F]\rangle$ $(n = 1, 2, \cdots N)$ with eigenvalues $\mathcal{E}_n[F]$ for a frozen $F = F(x)$ in arbitrary x. In terms of $|n[F]\rangle$, we can expand the solution $|\phi\rangle$ of the time-independent Schrödinger equation $\hat{H}|\phi\rangle = E|\phi\rangle$ as

$$|\phi\rangle = \sum_{n=1}^{N} \phi_n(x)|n[F(x)]\rangle\,, \tag{2}$$

we then have

$$\hat{H}_n\phi_n(x) + \sum_{m=1}^{N} \hat{O}_{nm}(x)\phi_m(x) = E\phi_n(x) \tag{3}$$

by direct computation, where

$$\hat{H}_n = -\frac{\hbar^2}{2M}[\nabla - iA(n)]^2 + V(x) + \mathcal{E}_n(x)\,, \tag{4a}$$

$$A(n) = i\langle n[F(x)]|\nabla|n[F(x)]\rangle\,, \tag{4b}$$

$$\hat{O}_{nm}(x)=\begin{cases} -\dfrac{\hbar^2}{2M}\sum_{n'\neq n}\langle n[F]|\bigtriangledown n'[F]\rangle\langle n'[F]|\bigtriangledown n[F]\rangle\equiv\tilde{O}\,, & n=m\,,\\ -\dfrac{\hbar^2}{2M}\{2\langle n[F]|\bigtriangledown m[F]\rangle\bigtriangledown+\langle n[F]|\bigtriangledown^2|m[F]\rangle\}\,, & n\neq m\,.\end{cases}\tag{4c}$$

Defining

$$\psi=\begin{bmatrix}\phi_1(x)\\ \phi_2(x)\\ \vdots\\ \phi_N(x)\end{bmatrix},\qquad \hat{O}=\begin{bmatrix}\hat{O}_{11} & \hat{O}_{12} & \cdots & \hat{O}_{1N}\\ \hat{O}_{21} & \hat{O}_{22} & \cdots & \hat{O}_{2N}\\ & & \cdots & \\ \hat{O}_{N1} & \hat{O}_{N2} & \cdots & \hat{O}_{NN}\end{bmatrix},\tag{5}$$

$$\hat{\mathcal{H}}_0=\text{diag}\cdot[\hat{H}_1\,,\ \hat{H}_2\,,\ \cdots\hat{H}_N]\,.\tag{6}$$

We rewrite the above system of equations (3) in a matrix form

$$[\hat{\mathcal{H}}_0+\hat{O}]\psi=E\psi\,.\tag{7}$$

It can be seen from Eqs. (3) and (4) that when the external field $F(x)$ is completely homogeneous, the elements of matrix operator $\hat{O}$ in Eq. (7) vanish; spin and space components completely separate each other. Then, from the physical consideration, when $F(x)$ slightly depends on x, these elements are very small and $\hat{O}$ can be regarded as a perturbation. We can use the standard perturbation theory to solve Eq. (7) order by order, and obtain

$$\begin{aligned}&\psi=\psi^{[0]}+\psi^{[1]}+\psi^{[2]}+\cdots\,,\\ &E=E^{[0]}+E^{[1]}+E^{[2]}+\cdots\\ &\mathcal{H}\psi^{[0]}=E^{[0]}\psi^{[0]}\,,\\ &\mathcal{H}\psi^{[l]}+\hat{O}\psi^{[l-1]}=\sum_{l'=0}^{l}E^{[l-l']}\psi^{[l']}\,.\end{aligned}\tag{8}$$

For example, we can explicitly obtain the second order approximate solution

$$\begin{aligned}&E^{[1]}_{kn}=O_{nn}\,,\\ &\psi^{[1]}_{nk}=\sum_{k',n'\neq k,n}\frac{\langle\Phi^{[0]}_{n'k'}|\hat{O}_{n'n}|\Phi^{[0]}_{nk}\rangle}{E^{[0]}_{n'k'}-E^{[0]}_{nk}}\psi^{[1]}_{n'k'}\,,\end{aligned}\tag{9}$$

where the first–order approximate solutions $\psi^{[0]}_k$'s are given by

$$\begin{cases}\psi^{[0]}_{1k}=[\Phi^{[0]}_{1k}(x)\,,\ O\,,\ \cdots\ O]^T\,,\\ \psi^{[0]}_{2k}=[O\,,\ \Phi^{[0]}_{2k}(x)\,,\ O\,,\ \cdots O]^T\,,\\ \cdots\\ \psi^{[0]}_{Nk}=[O\,,\ O\,,\ \cdots\ \Phi^{[0]}_{Nk}]^T\,,\end{cases}\tag{10a}$$

$$\hat{H}_n \Phi^{[0]}_{nk}(x) = E^{[0]}_{nk} \Phi^{[0]}_{nk}(x) . \tag{10b}$$

Here k labels the levels of the effective Hamiltonian $\hat{H}_n$.

According to Eq. (9), when the external field $F(x)$ is so homogeneous that the adiabatic conditions

$$\left| \frac{\langle \Phi^{[0]}_{n'k'} | \hat{O}_{n'n} | \Phi^{[0]}_{nk} \rangle}{E^{[0]}_{n'k'} - E^{[0]}_{nk}} \right| \ll 1 , \qquad k', n' \neq k, n \tag{11}$$

holds, the second order approximate solutions can be neglected and one only needs to take first order approximate solutions defined by Eq. (10b). From the explicit form of Eq. (10b)

$$\left\{ -\frac{\hbar^2}{2M} (\nabla - iA(n))^2 + V(x) + \mathcal{E}_n(x) \right\} \Phi^{[0]}_{nk}(x) = E^{[0]}_{nk} \Phi^{[0]}_{nk}(x) , \tag{12}$$

we see that the effects of the spin component on the space component under the B–O approximation provide with a U(1)–vector field $A(n) = A(n, x)$ and a scalar field $\mathcal{E}_n(x)$.

III. Geometry of Induced Gauge Field for Spin Precession

In the following discussions, we consider the spin precession relating to B–D experiment as an example of the above discussions. In an inhomogeneous magnetic field

$$\vec{B} = \vec{B}(x) = (B_1(x), B_2(x), B_3(x)) ,$$

the Hamiltonian of a particle with spin s is

$$\hat{H} = -\frac{\hbar^2}{2M} \nabla^2 + h[\vec{B}(x) s] \equiv -\frac{\hbar^2}{2M} \nabla^2 + g\vec{B}(x) \cdot \hat{\vec{s}} . \tag{13}$$

By making use of the angular momentum theory, $h(\vec{B}s)$ can be rewritten as

$$h[\vec{B}s] = e^{-i\hat{s}_3\phi/\hbar} e^{-i\hat{s}_2\theta/\hbar} [\hbar\omega_0 \hat{s}_3] e^{i\hat{s}_2\theta/\hbar} e^{i\hat{s}_3\phi/\hbar} , \tag{14a}$$

$$\begin{cases} \omega_0 = gB = g[B_1^2 + B_2^2 + B_3^2]^{1/2} , \\ \phi = \operatorname{arctg} \dfrac{B_2}{B_1} , \\ \theta = \operatorname{arctg} \dfrac{B_3}{[B_1^2 + B_2^2]^{1/2}} . \end{cases} \tag{14b}$$

Then, we immediately obtain the eigenvectors

$$|m_s[\vec{B}]\rangle = e^{-i\hat{s}_3\phi/\hbar} e^{-i\hat{s}_2\theta/\hbar} |sm_s\rangle , \qquad (m_s = s, s-1, \cdots - s) \tag{15}$$

of $h[\vec{B}s]$ with eigenvalues $\mathcal{E}_{m_s}[B] = \hbar\omega_0 m_s$, where $|sm_s\rangle$ is a standard angular momentum state satisfying

$$\hat{s}_3 |sm_s\rangle = m_s \hbar |sm_s\rangle , \qquad \hat{s}^2 |sm_s\rangle = s(s+1)\hbar^2 |sm_s\rangle . \tag{16}$$

In the B-O approximation, the effective equations about the space components $\phi_{m_s}(x)$ in full eigenfunction

$$\psi = \sum_{m_s=-s}^{s} \Phi_{m_s}(x)|m_s[B]\rangle$$

of $\hat{H}$ are

$$-\frac{\hbar^2}{2M}[\nabla - i\vec{A}(m_s,x)]^2\Phi_{m_s}(x) + m_s\hbar\omega_0(x)\Phi_{m_s}(x) = E\Phi_{m_s}(x) \ , \tag{17a}$$

$$\vec{A}(m_s,x) = m_s\cos\theta(x)\,\nabla\,\phi(x) \ , \qquad m_s = s, s-1\cdots - s \ . \tag{17b}$$

Its solutions for the cases with $\omega(x) = g\cdot B$ =const. are

$$\Phi_m^{[0]}(x) = (2\pi)^{-3/2}\cdot\exp\Big\{i\int_{x_0}^{x} A(m_s,x)_\mu dx^\mu\Big\}\cdot\exp(ik_\mu x^\mu) \tag{18}$$

with eigenvalues

$$E_{m_s\vec{k}} = \frac{\hbar^2|\vec{k}|^2}{2M} + m_s\hbar\omega_0 \ .$$

In this paper, we define

$$A_\mu D^\mu = A_1D_1 + A_2D_2 + A_3D_3$$

for any 3-vectors A and D.

The path-dependent phase $\int_{x_0}^{x} A(m_s,x)_\mu dx^\mu$ appearing in $\Phi_{m_s}^{[0]}(x)$ is just the Aharonov-Borm (A-B) phase of the induced gauge field. When the particle is subjected to a cycle magnetic field $\vec{B}(x)$ ($\vec{B}(x_0) = \vec{B}(x_1)$) from x_0 to x_1, this phase becomes a loop phase, which is similar to the Berry's phase. In fact, a mapping $\vec{B}$ from $R^3(x):\{x\}$ to $R^3(\vec{B}):\{\vec{B}\}$ enables a path $l:\{x(t)\}$ with starting point x_0 and end point x_1 of the particle in $R^3(x)$ corresponding to a closed path (loop) $C:\{\vec{B}(x):\vec{B}(x_0)=\vec{B}(x_1)\}$ in $R^3(\vec{B})$. Under this mapping, the $A-B$ phase

$$ABP = \int_{x_0}^{x_1} A(m_s,x)_\mu dx^\mu$$

defined on the path l is written as a loop integration along the loop C, i.e.

$$\begin{aligned}\gamma_{m_s}(c) = ABP &= i\int_{x_0}^{x_1}\langle m_s[\vec{B}]\Big|\frac{\partial}{\partial x_\mu}\Big|m_s[\vec{B}]\rangle dx_\mu \\ &= i\oint_c\langle m_s[\vec{B}]\Big|\frac{\partial}{\partial B_\mu}\Big|m_s[\vec{B}]\rangle dB_\mu \ ,\end{aligned} \tag{19}$$

However, this phase is over-defined by a loop C in $R^3(\vec{B})$, because two loops $C\{\vec{B}(x)\}$ and $C'\{\vec{B}'(x)\}$ have the same projective loop $\hat{C}$ on S^2:

$$\{\vec{n}(x)|\vec{n}(x) = \vec{B}(x)/|\vec{B}(x)|\} = \{\theta(x),\phi(x)\}$$

($\vec{n}(x)$ is a Kronecker mapping), and have the same phase, i.e. $\gamma_{m_s}(c) = \gamma_{m_s}(c')$. Thus, $\gamma_{m_s}(c)$ is defined by a class of loops $[c] = \{c'|\{c' = \lambda(x)\vec{B}(x)\}$, $\lambda(x)$ is a real functions of $x \in R^3(x)\}$, i.e. any loop in the class $[c]$ corresponds to the same phase $\gamma_{m_s}(c)$. If $C, C' \in [C]$ then $\gamma_{m_s}(c) = \gamma_{m_s}(c')$. Thus the $\gamma_{m_s}(c)$ can be regarded as a topological function in class space

$V_c : \{[c]\}$ and denoted by $\gamma_{m_s}[c]$. The above geometry of induced gauge field is illustrated in Fig. 1.

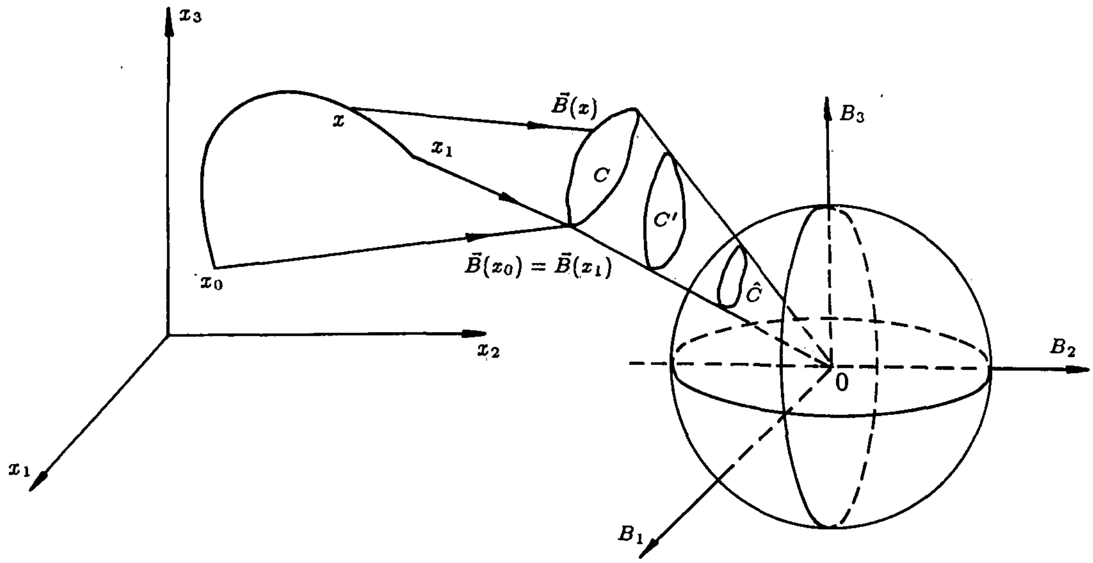

Fig. 1

IV. Observable Effects of Induced Gauge Field

Like the A-B phase factor of a usual gauge potential, $\gamma_{m_s}(c)$ is observable in experiments.

We consider a double-slit experiment slightly differing from that proposed by Berry first. A beam of particles with spin s initially polarised in state $|m_s[B(x_0)]\rangle$ at position x_0 at time $t=0$, splits two beams. One of which passes through a constant magnetic field $\vec{B} = \vec{B}(x_0)$, while the other passes through such an inhomogeneous magnetic field $\vec{B}(x)$ that $|\vec{B}(x)| = |\vec{B}(x_0)|$ and the B-O approximation holds. After time T, the two beams combined in a detector at a position x_1 such that $\vec{B}(x_1) = \vec{B}(x_0)$, which have two wave functions respectively

$$\begin{aligned} |\psi_1(t)\rangle &= \exp\left[-iE_{m_s\vec{k}}\frac{T}{\hbar}\right]\exp[ik_\mu x^\mu]\exp[i\gamma_{m_s}[c]]|m_s[\vec{B}(x_1)]\rangle\ , \\ |\psi_2(t)\rangle &= \exp\left[-iE_{m_s\vec{k}}\frac{T}{\hbar}\right]\exp[ik_\mu x^\mu]|m_s[\vec{B}(x_0)]\rangle\ . \end{aligned} \tag{20}$$

Then, we obtain from Eqs. (20) the predicted intensity contrast of particles

$$I = ||\psi_1\rangle + |\psi_2\rangle|^2 = I_0\cos^2\left[\frac{1}{2}\gamma_{m_s}[c]\right]\ . \tag{21}$$

This manifests an observable effect of induced gauge field.

Finally, we would like to point out that the B-D experiment is only a specific case of the above discussions with spin 1/2 and a certain magnetic field

$$\vec{B}(x) = B\left(\sin\theta\cos\frac{2\pi x_3}{L},\ \sin\theta\sin\frac{2\pi x_3}{L},\ \cos\theta\right)\ , \tag{22}$$

where θ = const. What is observed in the B–D experiment is the polarization of neutrons through $\vec{B}(x)$ for $x_3 = L$ at $t = T$, our discussions give the wave function of neutron

$$\begin{aligned}\psi(T,L) &= \Big\{\cos\frac{\theta}{2}\cdot\exp\Big[iE^{[0]}_{\vec{k}/2}\cdot\frac{T}{\hbar}\Big]\exp[i\gamma_{1/2}[c]]\;\Big|\;\frac{1}{2},\frac{1}{2}[\vec{B}(L)]\Big\rangle \\ &\quad+\sin\frac{\theta}{2}\exp\Big[iE^{[0]}_{-\vec{k}/2}\cdot\frac{T}{\hbar}\Big]\exp[i\gamma_{-1/2}[c]]\;\Big|\;\frac{1}{2},-\frac{1}{2}[\vec{B}(L)]\Big\rangle\Big\} \\ &\quad\cdot(2\pi)^{-3/2}\exp[ik_\mu x^\mu] \\ &\equiv a(T)\;\Big|\;\frac{1}{2},\frac{1}{2}\Big\rangle + b(T)\;\Big|\;\frac{1}{2},-\frac{1}{2}\Big\rangle\end{aligned} \tag{23}$$

for the neutron beam being initially in the state $|+1/2\rangle$ and thereby we obtain the polarization of neutron along the x_3-axis

$$\begin{aligned}p_3 &= |a(T)|^2 - |b(T)|^2 = 1 - 2\sin^2[\omega_0 T + \gamma_{1/2}[c]]\,, \\ \omega_0 &= \frac{1}{2}gB\,.\end{aligned} \tag{24}$$

V. Non-Adiabatic Effects

If the magnetic field is not uniform enough to neglect the perturbation $\hat{O}$ in Eq. (7), we, at last need to consider the lowest order approximation resulting in non–adiabatic effects, i.e. the second order approximation.

According to the general discussion in Sec. II, we have effective equation about the space component

$$\hat{H}_{m_s}\Phi_{m_s}(x) + \sum_{m'_s\neq m_s}\hat{O}_{m_s m'_s}\Phi_{m'_s}(x) = E\Phi_{m_s}(x)\,. \tag{25}$$

By direct computation, we have

$$\begin{cases}\hat{O}(m,m) = \dfrac{\pi^2\hbar^2}{ML^2}\sin^2\theta[s(s+1)-m_s^2]\,, \\ \hat{O}(m,m\pm 1) = -\dfrac{\hbar^2}{2M}f_\mp(s,m\pm 1)\vec{F}_\mp\cdot[2\nabla + i(2m\pm 1)\cos\theta\,\nabla\phi]\,, \\ \hat{O}(m,m\pm 2) = -\dfrac{\hbar^2}{2M}f_\mp(s,m\pm 2)f_\mp(s,m\pm 1)\vec{F}_\mp\cdot\vec{F}_\mp\,, \\ \hat{O}(m,m') = 0\,, \qquad m'\neq m,\quad m\pm 1,\quad m\pm 2\,,\end{cases} \tag{26}$$

where

$$\begin{aligned}f_\pm(s,m) &= [s(s+1) - m(m\pm 1)]^2\,, \\ \vec{F}_\mp(x) &= \frac{1}{2}[\pm\nabla\theta + i\sin\theta\,\nabla\phi]\,.\end{aligned} \tag{27}$$

For a certain magnetic field, we obtain the second order approximation solutions

$$\begin{aligned}\psi^{[1]}_{m s k} &= \epsilon(+1)\psi^{[0]}_{m_s+1,\vec{k}-\vec{k}_A}(x) + \epsilon(-1)\psi^{[0]}_{m_s-1,\vec{k}+\vec{k}_A}(x) \\ &\quad+\epsilon(+2)\psi^{[0]}_{m_s+2,\vec{k}-2\vec{k}_A}(x) + \epsilon(-2)\psi^{[0]}_{m_s-2,\vec{k}+2\vec{k}_A}(x)\,,\end{aligned} \tag{28}$$

where

$$\epsilon(\pm 1) = \frac{\frac{\pi\hbar^2}{ML^2}[(3m_s + 1/2)2\pi\cos\theta + k_3L]f_\pm(s,m_s)}{\hbar\omega_0 + \vec{k}_A\cdot(\vec{k}_A \mp 2\vec{k})\cdot\hbar^2/2M}\,,$$
$$\epsilon(\pm 2) = \frac{\frac{\pi^2\hbar^2}{ML^2}f_\pm(s,m)f_\pm(s,m\pm 1)}{\hbar\omega_0 + 2\vec{k}_A\cdot[\vec{k}_A \mp \vec{k}]\cdot\hbar^2/2M} \tag{29}$$

are first-order small quantities and can be neglected under the adiabatic condition

$$\frac{\hbar}{\omega_0 ML^2} \ll 1\,, \qquad \frac{\hbar k_3}{ML\omega_0} \ll 1\,, \tag{30}$$

which imply that $\vec{B}(x) = \vec{B}(x_3)$ is uniform and strong (for large L and $\omega_0 = gB$ respectively) and the velocity along z-axis ($v_z = \hbar k_z$) is small enough. This time, the B-O approximation works well.

From the second approximate solution (28), we see that after the particles pass through $\vec{B}(x)$ from x_0 to x_1, there exist the transitions from $|m_s[B(x_0)]\rangle$ to $|m_{s'}[B(x)]\rangle$, ($m'_s = m_s \pm 1$, $m_s \pm 2$) with the probabilities

$$p(m_s \longrightarrow m'_s) \propto |\epsilon(\pm 1, \pm 2)|^2\,.$$

These transitions are manifestations of non-adiabatic correction in experiments.

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