Generalizing Born-Oppenheimer approximations and observable effects of an induced gauge field

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By extending the Born-Oppenheimer approximation improved by Wilczek *et al.* to deal with separation of the spin and space coordinates of a particle in an external field, we generally discuss the direct effects of an induced gauge field and the higher-order corrections to the problem. It is shown that Bitter and Dubbers's experiment about Berry's phase is directly explained as an effect of the induced gauge potential in terms of the first-order approximation in this paper. The higher-order effects appearing in this experiment are also pointed out when the adiabatic conditions are broken.

The discovery of Berry's phase is not only a breakthrough in the older theory of quantum adiabatic approximations,[1] but also provides us with new insights in many physical phenomena, as, for instance, the chiral anomaly and quantum Hall effect (for reviews see Ref. 2). The existence of Berry's phase has been verified in certain experiments. A typical one was more recently seen in Ref. 3. At present, the concept of Berry's phase has developed in some different directions; an important one is the introduction of the induced gauge field by Wilczek *et al.*[4]

It is found that for a quantum (molecular) system with two sets of variables, a fast (electric) one and a slow (nuclear) one, after resolving the dynamics of fast variables to the first-order approximation, Born-Oppenheimer (BO) approximation, the left effective Hamiltonian governing the slow variables involves an external vector potential $\mathbf{A}_n$ induced by the fast variables. This magneticlike potential $\mathbf{A}_n$ is called the induced gauge potential or Berry's connection. Here, we naturally ask whether there is an experiment testing the direct physical effects of the induced gauge field. This question is answered under a general condition in this paper.[2]

We first generalize the improved BO approximation with nonzero $\mathbf{A}_n$ to deal with separation of the spin part and the space part of a neutral particle in an inhomogeneous external field and obtain the higher-order corrections to the problem when the adiabatic conditions are broken. The presented method is parallel to the high-order adiabatic approximation method (HOAAM) proposed by one of the authors (C.P.S.),[5] in which the slow variables, as parameters, are under experimental control. Then, we show that the results of an experiment carried out by Bitter and Dubbers[6] (BD experiment) are just the direct manifestations of the Aharonov-Bohm phase of the induced gauge potential in the laboratory frame of reference, which were previously understood as the effects of Berry's phase in a moving frame of reference (in an inhomogeneous magnetic field, the neutrons on their flight see a varying magnetic field and then have a time-dependent adiabatic Hamiltonian).[6] The nonadiabatic effects in this experiment are also pointed out and a quantitative prediction is given when the adiabatic conditions are violated.

I. GENERALIZED BO APPROXIMATION

The full Hamiltonian of a neutral particle with spin $\hat{S}$ is

$$\hat{H}=\frac{\hat{p}^2}{2M}+V(\mathbf{x})+\hat{H}_s[\mathbf{B}_i(\mathbf{x}),\hat{S}]\ , \tag{1}$$

where the spin part and the space part interact with each other through an inhomogeneous external field $B_i(\mathbf{x})$ ($\mathbf{i}=1,2,\ldots,k$). Let $\hat{H}_s=\hat{H}_s[B_i(\mathbf{x}),\hat{S}]$ have nondegenerate eigenfunctions $\chi_n\equiv\chi_n(\mathbf{x},S)$ ($n=1,2,\ldots,N$) and corresponding eigenvalues $\varepsilon_n\equiv\varepsilon_n(\mathbf{x})$ for fixed but arbitrary $\mathbf{x}$. The full wave function $\mathbf{\Phi}$ of $\hat{H}$ is expanded as

$$\tilde{\Phi}=\sum_{n=1}^{N}\Phi(\mathbf{x},n)\chi_n(\mathbf{x},S)\ . \tag{2}$$

Substituting (2) into the Schrödinger equation $\hat{H}\tilde{\Phi}=E\tilde{\Phi}$, we obtain effective equations about the space components $\Phi(n)\equiv\Phi(n,\mathbf{x})$:

$$\hat{H}(n)\Phi(n)+F(n)\Phi(n)+\sum_{m\neq n}\hat{O}(n,m)\Phi(m)=E\Phi(n)\ , \tag{3}$$

where

$$\hat{H}(n)=-\frac{\hbar^2}{2M}[\nabla-i\,\mathbf{A}(n)]^2+V(\mathbf{x})+\varepsilon_n(\mathbf{x})\ , \tag{4a}$$

$$\mathbf{A}(n)=i\langle\chi_n|\nabla\chi_n\rangle\ , \tag{4b}$$

$$F(n)=-\frac{\hbar^2}{2M}\sum_{m\neq n}\langle\chi_n|\nabla\chi_m\rangle\langle\chi_m|\nabla\chi_n\rangle\ , \tag{4c}$$

$$\hat{O}(n,m)=-\frac{\hbar^2}{2M}(2\langle\chi_n|\nabla\chi_m\rangle\nabla+\langle\chi_n|\nabla^2|\chi_m\rangle)\ . \tag{4d}$$

It can be seen from (4) that when the external field B_i is completely homogeneous, both terms of $F(n)$ and $\hat{O}(m,n)$ vanish, and the spin and space components completely separate from each other. Therefore, from the point of view of physics, when the external field slightly depends on $\mathbf{x}$, the terms of $F(n)$ and $\hat{O}(m,n)$ in (3) are very small and can be regarded as a perturbation. In order to use the standard perturbation theory to solve (3) with a more homogeneous external field, we rewrite (3) in matrix-value form as

$$(\mathcal{H}_0+\epsilon\mathcal{W})\Phi=E\Phi\ , \tag{5}$$

where ϵ is a perturbation parameter induced for calculation and is finally taken to be 1; Φ, $\mathcal{H}_0$, and $\mathcal{W}$ are, respectively, defined as

$$\Phi=\begin{bmatrix}\phi(1)\\ \phi(2)\\ \vdots\\ \phi(n)\end{bmatrix},\quad \mathcal{H}_0=\begin{bmatrix}\hat{H}(1) & 0 & \cdots & 0\\ 0 & \hat{H}(2) & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & \cdots & \hat{H}(N)\end{bmatrix}, \tag{6}$$

$$\mathcal{W}=\begin{bmatrix}F(1) & \hat{O}(1,2) & \hat{O}(1,3) & \cdots & \hat{O}(1,N)\\ \hat{O}(2,1) & F(2) & \hat{O}(2,3) & \cdots & \hat{O}(2,N)\\ \hat{O}(3,1) & \hat{O}(3,2) & F(3) & \cdots & \hat{O}(3,N)\\ \vdots & & & & \vdots\\ \hat{O}(N,1) & \hat{O}(N,2) & \hat{O}(N,3) & \cdots & F(N)\end{bmatrix}.$$

By making use of time-independent perturbation theory, we successively obtain each order approximate solutions of (3) or (5): the first-order approximation solutions

$$\tilde{\Phi}_k^{[0]}(1)=\begin{bmatrix}\Phi_k^{[0]}(1)\\ 0\\ \vdots\\ 0\end{bmatrix},\quad \tilde{\Phi}_k^{[0]}(2)=\begin{bmatrix}0\\ \Phi_k^{[0]}(2)\\ \vdots\\ 0\end{bmatrix},\ldots,$$

$$\tilde{\Phi}_k^{[0]}(N)=\begin{bmatrix}0\\ 0\\ \vdots\\ \Phi_k^{[0]}(N)\end{bmatrix}. \tag{7}$$

are given by

$$\hat{H}(n)\Phi_k^{[0]}(n)=E_k^{[0]}(n)\Phi_k^{[0]}(n) \tag{8}$$

or

$$\left[-\frac{\hbar^2}{2M}[\nabla-i\,\mathbf{A}(n)]^2+V(\mathbf{x})+\varepsilon_n(\mathbf{x})\right]\Phi_k^{[0]}(n)=E_k^{[0]}(n)\Phi_k^{[0]}(n)\ , \tag{9}$$

which can be checked to satisfy $\mathcal{H}_0\tilde{\Phi}_k^{[0]}(n)=E_k^{[0]}(n)\tilde{\Phi}_k^{[0]}(n)$; from these first-order approximate solutions $\tilde{\Phi}_k^{[0]}(n)$'s the second-order corrections are obtained as

$$E_k^{[1]}(n)=F(n)\ ,$$

$$\Phi_k^{[1]}(n)=\sum_{k',n'\neq k,n}\frac{\langle\Phi_{k'}^{[0]}(n')|\hat{O}(n',n)|\Phi_k^{[0]}(n)\rangle}{E_{k'}^{[0]}(n')-E_k^{[0]}(n)}\tilde{\Phi}_{k'}^{[0]}(n')\ . \tag{10}$$

It can be seen from (10) that the second-order corrections can be neglected and we can take the BO approximate solutions (7) accordingly when the BO (or adiabatic) conditions

$$\left|\frac{\langle\phi_{k'}^{[0]}(n')|\hat{O}(n',n)|\Phi_k^{[0]}(n)\rangle}{E_{k'}^{[0]}(n')-E_k^{[0]}(n)}\right|\ll 1,\quad k',n'\neq k,n \tag{11}$$

are satisfied. The higher-order approximate solutions are also obtained by perturbation theory.

II. BD EXPERIMENT AND OBSERVABLE EFFECTS OF INDUCED GAUGE FIELD

In the BD experiment, the Hamiltonian of a neutron in a static helical magnetic field

$$\mathbf{B}\equiv\mathbf{B}(z)=B\left[\sin\theta\left[\cos\frac{2\pi z}{L}\mathbf{e}_x+\sin\frac{2\pi z}{L}\mathbf{e}_y\right]+\cos\theta\mathbf{e}_z\right] \tag{12}$$

is

$$\hat{H}\equiv\hat{H}(z)=\frac{\hat{p}^2}{2M}+g\hat{S}\cdot\mathbf{B}(z)\equiv\frac{\hat{p}^2}{2M}+\hat{H}_s \tag{13}$$

and for given z its interacting Hamiltonian $\hat{H}_s$ has nondegenerate eigenfunctions

$$\chi_1 \equiv \chi_1[\mathbf{B}(z)] = \begin{bmatrix} \cos\frac{\theta}{2}\exp\left[-\frac{2\pi z i}{L}\right] \\ \sin\frac{\theta}{2} \end{bmatrix},$$
$$\chi_2 \equiv \chi_2[\mathbf{B}(z)] \equiv \begin{bmatrix} \sin\frac{\theta}{2}\exp\left[-\frac{2\pi z i}{L}\right] \\ -\cos\frac{\theta}{2} \end{bmatrix}, \quad (14)$$

and corresponding eigenvalues $\varepsilon_1 = \hbar\omega_0 \equiv \frac{1}{2}gB\hbar$ and $\varepsilon_2 = -\hbar\omega_0$.

According to the above general discussion, we obtain the solutions of the BO approximate equations

$$-\frac{\hbar^2}{2M}[\nabla - i\,\mathbf{A}(n)]^2\Phi_{\mathbf{k}}^{[0]}(n) + (-1)^{n+1}\hbar\omega_0\Phi_{\mathbf{k}}^{[0]}(n) = E_{\mathbf{k}}^{[0]}(n)\Phi_{\mathbf{k}}^{[0]}(n), \quad n = 1,2 \quad (15)$$

as

$$\Phi_{\mathbf{k}}^{[0]}(n) = (2\pi)^{-3/2}\exp\left[i\int A_\mu(n)dx^\mu\right]\exp(i\,\mathbf{k}\cdot\mathbf{x}),$$
$$E_{\mathbf{k}}^{[0]}(n) = \frac{\hbar^2|\mathbf{k}|^2}{2M} + (-1)^{n+1}\hbar\omega_0, \quad (16)$$

where the induced gauge potentials are explicitly written as

$$\mathbf{A}(n) = i\langle\chi_n|\nabla\chi_n\rangle = \begin{cases} \frac{2\pi}{L}\cos^2\frac{\theta}{2}\mathbf{e}_z & \text{for } n=1, \\ \frac{2\pi}{L}\sin^2\frac{\theta}{2}\mathbf{e}_z & \text{for } n=2. \end{cases} \quad (17)$$

When a neutron reaches $z = L$ after time T, the interacting Hamiltonian $\hat{H}_s(\mathbf{B}(z))$ is subjected to a cycle evolution in a loop $C:\{B(z)|B(0)=B(L)\}$ in parameter space $\tilde{V}:\{\mathbf{B}\}$. The Aharonov-Bohm phases of the induced gauge potentials $\mathbf{A}(1)$ and $\mathbf{A}(2)$ can be regarded as loop phases in $\tilde{V}$, i.e.,

$$\int A_\mu^{(n)}dx^\mu = \int_0^L A_z(n)dz = \oint_c\left\langle\chi_n\left|\frac{\partial}{\partial B_i}\chi_n\right.\right\rangle dB_i = \mathcal{V}_n(c), \quad n=1,2. \quad (18)$$

Because these phases are independent of the parametrization way of the loop C, they are pure geometrical. In the meanwhile, the wave function of the neutron is

$$\Psi(t,L) = \left\{\cos\frac{\theta}{2}\exp[iE_{\mathbf{k}}^{[0]}(1)T/\hbar]\exp[i\mathcal{V}_1(c)]|\chi_1[\mathbf{B}(L)]\rangle + \sin\frac{\theta}{2}\exp[iE_{\mathbf{k}}^{[0]}(2)T/\hbar]\exp[i\mathcal{V}_2(c)]|\chi_2[\mathbf{B}(L)]\rangle\right\}(2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{x})$$
$$\equiv a(T)|+\tfrac{1}{2}\rangle + b(T)|\tfrac{1}{2}\rangle \quad (19)$$

for the neutron beam initially in the state $|+\frac{1}{2}\rangle$, which gives the polarization of neutron along the z axis:

$$\mathbb{P}_z = |a(T)|^2 - |b(T)|^2 = 1 - 2\sin^2\theta\sin^2[\omega_0 T + \mathcal{V}_1(c)], \quad (20)$$

where the additional topological phase shift $\mathcal{V}_1(c)$ is just what was observed in BD experiment. In our opinion, this result shows the direct observable effect of induced gauge field in the laboratory frame of reference.

III. NONADIABATIC EFFECTS IN THE BD EXPERIMENT

In the following, we will use the general result in Sec. II to discuss the nonadiabatic effects appearing in the BD experiment when the conditions of BO approximation are violated. For the concrete problem in the above section, it is easy to obtain

$$F(1) = F(2) = \frac{\pi^2\hbar^2}{2ML^2}\sin^2\theta,$$
$$\hat{O}(1,2) = \hat{O}(2,1) = \frac{\pi\hbar^2}{ML^2}\sin\theta\left[iL\frac{\partial}{\partial z} + \pi\right], \quad (21)$$

and the corresponding effective equation

$$\left[\begin{bmatrix} \hat{H}(1) & 0 \\ 0 & \hat{H}(2) \end{bmatrix} + \epsilon\begin{bmatrix} F(1) & \hat{O}(1,2) \\ \hat{O}(2,1) & F(2) \end{bmatrix}\right]\begin{bmatrix} \Phi(1) \\ \Phi(2) \end{bmatrix} = E\begin{bmatrix} \Phi(1) \\ \Phi(2) \end{bmatrix}. \quad (22)$$

The first- and the second-order approximate solutions are, respectively,

$$\tilde{\Phi}_{\mathbf{k}}^{[0]}(1)=\begin{bmatrix}\Phi_{\mathbf{k}}^{[0]}(1)\\0\end{bmatrix},\quad \tilde{\Phi}_{\mathbf{k}}^{[0]}(2)=\begin{bmatrix}0\\\Phi_{\mathbf{k}}^{[0]}(2)\end{bmatrix}, \tag{23}$$

and

$$\begin{aligned}\tilde{\Phi}_{\mathbf{k}}(1)&=\tilde{\Phi}_{\mathbf{k}}^{[0]}(1)+\tilde{\Phi}_{\mathbf{k}}^{[1]}(1)\equiv\tilde{\Phi}_{\mathbf{k}}^{[0]}(1)+\epsilon_{+}\tilde{\Phi}_{\mathbf{k}'}^{[0]}(2)\\&\equiv\Phi_{\mathbf{k}}^{[0]}(1)+\frac{\pi\hbar^2(\pi\cos\theta+kzL)}{2\hbar^2(k_zL+\pi\cos\theta)\pi\cos\theta-2\hbar\omega_0ML^2}\tilde{\Phi}_{\mathbf{k}'}^{[0]}(2),\quad \mathbf{k}'=\mathbf{k}+\mathbf{A}(1)-\mathbf{A}(2)\,,\\\tilde{\Phi}_{\mathbf{k}}(2)&=\tilde{\Phi}_{\mathbf{k}}^{[0]}(2)+\tilde{\Phi}_{\mathbf{k}}^{[1]}(2)\equiv\tilde{\Phi}_{\mathbf{k}}^{[0]}(2)+\epsilon_{-}\tilde{\Phi}_{\mathbf{k}''}^{[0]}(1)\\&=\tilde{\Phi}_{\mathbf{k}}^{[0]}(2)+\frac{\pi\hbar^2(\pi\cos\theta-kzL)}{2\hbar^2(k_zL-\pi\cos\theta)\phi\cos\theta+2\hbar\omega_0ML^2}\tilde{\Phi}_{\mathbf{k}''}^{[0]}(1),\quad \mathbf{k}''=\mathbf{k}+\mathbf{A}(2)-\mathbf{A}(1)\,.\end{aligned} \tag{24}$$

From (24), one observes that when the conditions of the BO approximation

$$\frac{\hbar}{\omega_0M_L^2}\ll 1,\quad \frac{\hbar k_z}{ML\omega_0}\ll 1 \tag{25}$$

are satisfied, i.e., $\mathbf{B}(z)$ is homogeneous and strong enough (for large L and $\omega_0=\frac{1}{2}gB$) respectively) and the velocity of the neutron along the z axis ($v_z=\hbar k_z/M$) is small enough, the second corrections $\Phi_{\mathbf{k}}^{[1]}(n)$ can be neglected. In this case, we only take the BO approximations (23), otherwise the second corrections are taken to give a nonadiabatic effect in the polarization of a neutron

$$\mathbb{P}_z^1=\mathbb{P}_z+4\{\alpha\cos\theta\cos^2[\omega_0T+\mathcal{V}_1(c)]+\beta\sin\theta\sin^2[\omega_0T+\mathcal{V}_1(c)]\}\,, \tag{26}$$

where $\alpha=\frac{1}{2}\sin\theta(\epsilon_{+}-\epsilon_{-})$ and $\beta=\epsilon_{+}\cos^2\theta/2+\epsilon_{-}\sin^2\theta/2$ are small. It is expected that the second term of (26) representing the nonadiabatic effect can be experimentally verified.

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