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The monopole, pure gauge and Born–Oppenheimer equation

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Abstract. The modified Born–Oppenheimer equation arising from Berry's phase is studied extensively in two physical systems. One is the spin-$\frac{1}{2}$ neutral particle in the spherically symmetric magnetic field, the other is the electron in the cylindrically symmetric magnetic field. The results show the significant topological effects in simple quantum systems.

1. Introduction

Berry's phase [1] appears naturally in time varying systems where external parameters are added, but for systems with compound freedoms we may use the modified Born–Oppenheimer equation (MBOE) arising from Berry's phase. Typical examples are the diatoms [2–4].

In this paper, we study the MBOE through two simple physical systems, namely the spin-$\frac{1}{2}$ particle moving in a magnetic field. The dynamics for the spin system has been discussed in various cases [5–9]. Here we explore the two other cases with emphasis on the physical effects from topological origination. Since these systems have both configurational and internal freedoms, the most efficient way to study them is by using the MBOE. We review it first.

Consider a Hamiltonian

$$H = H_0(\boldsymbol{P}, \boldsymbol{X}) + h(\boldsymbol{X}, \boldsymbol{p}, \boldsymbol{r}) \tag{1}$$

where H_0 describes the slow variable $\boldsymbol{X}$ and h the fast variable $\boldsymbol{r}$, and $\boldsymbol{P}$ and $\boldsymbol{p}$ are the canonical momenta corresponding to $\boldsymbol{X}$ and $\boldsymbol{r}$. The wavefunction can be written as

$$\Psi(\boldsymbol{X}, \boldsymbol{r}) = \sum_m \psi_m(\boldsymbol{X})\chi_m(\boldsymbol{X}, \boldsymbol{r}) \tag{2}$$

where $\chi_m(\boldsymbol{X}, \boldsymbol{r})$ is the instantaneous eigenfunction for h with fixed $\boldsymbol{X}$. Considering

$$H_0(\boldsymbol{P}, \boldsymbol{X}) = \frac{1}{2M}\boldsymbol{P}^2 + V(\boldsymbol{x}) \tag{3}$$

where the fast variable $\boldsymbol{r}$ may be a configurational or internal variable, an extensive study [2, 3] leads to the following matrix-valued Hamiltonian for Ψ_m:

$$\sum_m \left[\frac{1}{2M} \sum_l (-\mathrm{i}\delta_{nl}\nabla_X - \boldsymbol{A}_{nl})(-\mathrm{i}\delta_{lm}\nabla_X - \boldsymbol{A}_{lm}) + V(\boldsymbol{X})\delta_{mn} + \epsilon_n(\boldsymbol{X})\delta_{mn} \right] \Psi_n(\boldsymbol{X}) = E\Psi_n(\boldsymbol{X}) \tag{4}$$

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where $\boldsymbol{A}_{nl} = \mathrm{i}\langle\chi_n|\partial/\partial\boldsymbol{X}|\chi_l\rangle$ and $\epsilon_n(\boldsymbol{X})$ is the instantaneous eigenvalue for h:

$$h\chi_n(\boldsymbol{X}, \boldsymbol{r}) = \epsilon_n(\boldsymbol{X})\chi_n(\boldsymbol{X}, \boldsymbol{r}). \tag{5}$$

In the following we study equation (4) in two systems.

2. Neutrons in a spherically symmetric magnetic field

The model is given as [7]

$$H = H_1 + H_2$$

$$H_1 = \frac{1}{2M}\boldsymbol{P}^2 + V(\boldsymbol{r}) \tag{6}$$

$$H_2 = \beta\boldsymbol{n}\sigma \tag{7}$$

which describes a neutron moving in the magnetic field along the direction $\boldsymbol{n} = \boldsymbol{r}/r$. This system has been discussed in [7] using an algebraic method, but the whole dynamics remains unsolved explicitly. We will study it using (4) and give a complete solution in the strong field limit.

In spherical coordinates, we have $\boldsymbol{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, thus the instantaneous eigenstates of (7) read

$$\chi_+(\boldsymbol{n}) = \begin{pmatrix}\cos(\theta/2)\mathrm{e}^{-\mathrm{i}\varphi/2}\\ \sin(\theta/2)\mathrm{e}^{-\mathrm{i}\varphi/2}\end{pmatrix} \qquad \chi_-(\boldsymbol{n}) = \begin{pmatrix}-\sin(\theta/2)\mathrm{e}^{-\mathrm{i}\varphi/2}\\ \cos(\theta/2)\mathrm{e}^{\mathrm{i}\varphi/2}\end{pmatrix} \tag{8}$$

with the eigenvalues $\pm\beta$ respectively. Then Berry's connection 1-form is defined as $A_{ij} = \langle\chi_i|\partial/\partial\boldsymbol{X}|\chi_j\rangle\mathrm{d}\boldsymbol{X}$, from which one gets

$$A_{++\varphi} = \frac{\cos\theta}{2r\sin\theta}$$

$$A_{+-\varphi} = -\frac{1}{2r} \qquad A_{+-\theta} = \frac{-\mathrm{i}}{2r} \qquad A_{-+\varphi} = -\frac{1}{2r} \qquad A_{-+\theta} = \frac{\mathrm{i}}{2r}$$

$$A_{--\varphi} = -\frac{\cos\theta}{2r\sin\theta}. \tag{9}$$

Unfortunately there is a singularity of A_{ij} at $\theta = 0$ or π. This is unacceptable for such a spherically symmetric system. To see this, we mention that the state in quantum mechanics can differ by an arbitrary phase; therefore we take the following gauge transformation $\chi'_\pm(\boldsymbol{n}) = \mathrm{e}^{-\mathrm{i}\varphi/2}\chi_\pm(n)$ and correspondingly

$$A'_{++\varphi} = \frac{1+\cos\theta}{2r\sin\theta} \qquad A'_{--\theta} = \frac{1-\cos\theta}{2r\sin\theta} \tag{10}$$

with $A'_{-+} = A_{-+}$, $A'_{+-} = A_{+-}$. It should be noted that $A'_{++\varphi}$ at $\theta = 0$ and $A'_{--\varphi}$ at $\theta = \pi$ have singularities.

Of course we can take the gauge transformation $\chi''_\mp(\boldsymbol{n}) = \mathrm{e}^{\mathrm{i}\varphi/2}\chi_\pm(\boldsymbol{n})$ and obtain

$$A''_{++\varphi} = \frac{-1+\cos\theta}{2r\sin\theta} \qquad A''_{--\varphi} = -\frac{1+\cos\theta}{2r\sin\theta} \tag{11}$$

with $A''_{-+} = A_{-+}$, $A''_{+-} = A_{+-}$. We again find that $A''_{++\varphi}$ at $\theta = \pi$ and $A''_{--\varphi}$ at $\theta = 0$ have singularities.

However, it is impossible to avoid such a problem. We have to solve it by using the language of a fibre bundle, because Berry's connection induces a monopole here. However, the wavefunction around a monopole should be treated as a section [10]. As a matter of fact, the singularities in (9)–(11) are superficial, the reason being that the quantum axis violates the $U(1)$ symmetry in quantum mechanics. We find that (9) is just Schwinger's potential for the monopole, and (10) and (11) are Wu–Yang monopole potential.

Before further discussion, we need to know the curvature for the Berry's connection; the matrix-valued connection 1-form reads

$$A = A_\varphi \sigma^\varphi + A_\theta \sigma^\theta = \tfrac{1}{2}\cos\theta \mathrm{d}\varphi\sigma_3 - \tfrac{1}{2}\sin\theta \mathrm{d}\varphi\sigma_1 + \tfrac{1}{2}\sigma_2 \mathrm{d}\theta \tag{12}$$

where σ^φ, σ^θ are the coordinate 1-forms as $\sigma^\varphi = r\sin\theta \mathrm{d}\varphi$, $\sigma^\theta = r\mathrm{d}\theta$. Choosing Schwinger's potential here without affecting the physical results, one can deduce the curvature from $F = \mathrm{d}A + \mathrm{i}A \wedge A$:

$$F = -\cos\theta \mathrm{d}\theta \wedge \mathrm{d}\varphi\sigma_1 - \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\varphi\sigma_3. \tag{13}$$

However, the curvature 2-form in spherical coordinates reads: $F = F_{\theta\varphi}\sigma^\theta \wedge \sigma^\varphi = F_{\theta\varphi} r^2 \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\varphi$, hence

$$F_{\theta\varphi} = -\frac{\cos\theta}{r^2\sin\theta}\sigma_1 - \frac{1}{r^2}\sigma_3 \tag{14}$$

with the components

$$\begin{aligned} F_{++\theta\varphi} &= -F_{--\theta\varphi} = -F_{++\varphi\theta} = F_{--\varphi\theta} = -\frac{1}{r^2} \\ F_{+-\theta\varphi} &= F_{-+\theta\varphi} = -F_{+-\varphi\theta} = -F_{-+\varphi\theta} = -\frac{1}{r^2}\cot\theta. \end{aligned} \tag{15}$$

We notice that Berry's connection is usually non-Abelian without adiabatic approximation.

Using (12), if the wavefunction for the whole system is written as $\Psi(t) = \Psi_+(t)\chi_+ + \Psi_-(t)\chi_-$, we have from (4)

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix}\Psi_+(t)\\ \Psi_-(t)\end{pmatrix} = \begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--}\end{pmatrix}\begin{pmatrix}\Psi_+(t)\\ \Psi_-(t)\end{pmatrix} \tag{16}$$

where the H_{ij} read as

$$\begin{aligned} H_{++} &= \frac{1}{2M}(\boldsymbol{P} - \boldsymbol{A}_{++})^2 + \frac{1}{2M}\boldsymbol{A}_{+-}\boldsymbol{A}_{-+} + V(\boldsymbol{r}) + \beta \\ H_{--} &= \frac{1}{2M}(\boldsymbol{P} - \boldsymbol{A}_{--})^2 + \frac{1}{2M}\boldsymbol{A}_{+-}\boldsymbol{A}_{-+} + V(\boldsymbol{r}) - \beta \\ H_{+-} &= -\frac{1}{2M}(\boldsymbol{P} - \boldsymbol{A}_{++})\boldsymbol{A}_{+-} - \frac{1}{2M}\boldsymbol{A}_{+-}(\boldsymbol{P} - \boldsymbol{A}_{--}) \\ H_{-+} &= -\frac{1}{2M}(\boldsymbol{P} - \boldsymbol{A}_{--})\boldsymbol{A}_{-+} - \frac{1}{2M}\boldsymbol{A}_{-+}(\boldsymbol{P} - \boldsymbol{A}_{++}). \end{aligned} \tag{17}$$

We see that Berry's phase provides not only a vector potential but also a scalar potential $\boldsymbol{A}_{+-}\boldsymbol{A}_{-+}$. The former has already appeared in the literature, whereas the latter was explained in [7, 4, 11]. This term is of the order of $\hbar^2$, which is meaningful for the lower excited states just below our considerations.

To solve (16) is never easy. For a strong enough field β and particles with heavy mass we can use the Born–Oppenheimer approximation for the lower excited states, where the off-diagonal terms in (16) are treated as perturbations, namely we neglect the transition between Ψ_+ and Ψ_-. We are ready to solve Ψ_+ as well as Ψ_-.

In the case of the monopole potential, the wavefunction has been solved in [12] as a section of fibre bundle. We give the result here; the details may be found in [12]:

$$\Psi_+(t) = R(r)Y_{-\frac{1}{2},l,m}\mathrm{e}^{-\mathrm{i}(E+\beta)t} \tag{18}$$

where $Y_{-\frac{1}{2},l,m}$ are the monopole harmonics with

$$l = \tfrac{1}{2}, \tfrac{3}{2}, \tfrac{5}{2} \cdots \qquad m = -l, -l+1, \ldots, l \tag{19}$$

and $R(r)$ satisfies

$$\left[-\frac{1}{2Mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1) + \frac{1}{4}}{2Mr^2} + V(r) - E \right] R(r) = 0. \tag{20}$$

For any potential $V(r)$, the solution of (18) can easily be obtained and thus the problem is completely solved. To see the high-order effects, we can treat (16) by perturbation.

In summary, we have found the non-Abelian gauge structure sections as a fibre bundle in this simple system, with the dynamics completely solved. We see from (19) that the angular momentum is quantized in half-integers, which shares a similarity with the isospin–spin transformation in gauge theory [13]. The spectrum from (20) is nonlinearly arranged, at least for the lower excited states, which is just the condition for the adiabatic approximation. All of these originate fundamentally from non-trivial topological structure. We mention that both (7) and (17) show the singular character of the origin in the coordinate frame. From (7) the direction of the magnetic field at the origin is not well defined, while from (17) the effective vector potential should be defined separately in the two parts of the whole space. The result of this is that we can only obtain sections instead of an ordinary wavefunction.

Another interesting fact is that our result cannot degenerate into the case without the spherically symmetric magnetic field. No matter how small the magnitude of the field, the monopole does not change in any respect; meanwhile the angular momentum is quantized in half-integers because of the monopole. All of these results reflect exactly the topological origination of the problem.

3. Electrons in a cylindrically symmetric magnetic field

In this section we consider another system

$$H = \frac{1}{2m} \left(\boldsymbol{P} + \frac{e}{c} \boldsymbol{A} \right)^2 + \mu_B \sigma \boldsymbol{B} \tag{21}$$

which describes an electron moving in a magnetic field. For an uniform field, the system has been solved in [9], but for an arbitrary field it has not yet been solved satisfactorily [14].

In our case, we study the electron in the plane with a magnetic vortex [15] and a perpendicular magnetic field. In azimuthal coordinates, we have $\boldsymbol{B} = (-B\sin\theta, B\cos\theta, \Delta)$, and the vector potential reads

$$\boldsymbol{A} = \tfrac{1}{2} \boldsymbol{B} \times \boldsymbol{r} = \tfrac{1}{2} \Delta r \boldsymbol{e}_\theta - \tfrac{1}{2} B r \boldsymbol{e}_z. \tag{22}$$

Defining $\tan\xi = B/\Delta$, such that $\beta = \sqrt{\Delta^2 + B^2} = \Delta \csc\xi$, we have the eigenstates

$$\sigma \boldsymbol{B} |\chi_\pm\rangle = \pm\beta |\chi_\pm\rangle \tag{23}$$

$$|\chi_+\rangle = \begin{pmatrix} \cos\frac{1}{2}\xi \,\mathrm{e}^{-\mathrm{i}\theta/2 - \mathrm{i}\pi/4} \\ \sin\frac{1}{2}\xi \,\mathrm{e}^{\mathrm{i}\theta/2 + \mathrm{i}\pi/4} \end{pmatrix} \qquad |\chi_-\rangle = \begin{pmatrix} -\sin\frac{1}{2}\xi \,\mathrm{e}^{-\mathrm{i}\theta/2 - \mathrm{i}\pi/4} \\ \cos\frac{1}{2}\xi \,\mathrm{e}^{\mathrm{i}\theta/2 + \mathrm{i}\pi/4} \end{pmatrix}. \tag{24}$$

From (24) we obtain the Berry's connection

$$\begin{aligned} A_{++\theta} &= \frac{1}{2r}\cos\xi \qquad A_{+-\theta} = -\frac{1}{2r}\sin\xi \\ A_{-+\theta} &= -\frac{1}{2r}\sin\xi \qquad A_{--\theta} = -\frac{1}{2r}\cos\xi. \end{aligned} \tag{25}$$

Obviously, it is a pure gauge, i.e. $F = \mathrm{d}A + \mathrm{i}A \wedge A = 0$. Using the same algorithm as in the last section, we have the MBOE:

$$\sum_m \left[\frac{1}{2M} \sum_l \left(\delta_{nl} \left(-\mathrm{i}\nabla_{\boldsymbol{X}} + \frac{e}{c}\boldsymbol{A} \right) - \boldsymbol{A}_{nl} \right) \times \left(\delta_{lm} \left(-\mathrm{i}\nabla_{\boldsymbol{X}} + \frac{e}{c}\boldsymbol{A} \right) - \boldsymbol{A}_{lm} \right) + \epsilon_n(\boldsymbol{X})\delta_{mn} \right] \Psi_m(\boldsymbol{X}) = E\Psi_n(\boldsymbol{X}). \tag{26}$$

We can rewrite the above equation in the matrix-valued form

$$\mathrm{i}\frac{\partial}{\partial t} \begin{pmatrix} \Psi_+(t) \\ \Psi_-(t) \end{pmatrix} = \begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--} \end{pmatrix} \begin{pmatrix} \Psi_+(t) \\ \Psi_-(t) \end{pmatrix} \tag{27}$$

where the elements read

$$\begin{aligned}
H_{++} &= \frac{1}{2M}\left(\boldsymbol{P} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{++} \right)^2 + \frac{1}{2M}\boldsymbol{A}_{+-}\boldsymbol{A}_{-+} + \mu_B \beta \\
H_{--} &= \frac{1}{2M}\left(\boldsymbol{P} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{--} \right)^2 + \frac{1}{2M}\boldsymbol{A}_{+-}\boldsymbol{A}_{-+} - \mu_B \beta \\
H_{+-} &= -\frac{1}{2M}\left(\boldsymbol{P} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{++} \right)\boldsymbol{A}_{+-} - \frac{1}{2M}\boldsymbol{A}_{+-}\left(\boldsymbol{P} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{--} \right) \\
H_{-+} &= -\frac{1}{2M}\left(\boldsymbol{P} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{-+} \right)\boldsymbol{A}_{-+} - \frac{1}{2M}\boldsymbol{A}_{-+}\left(\boldsymbol{A} + \frac{e}{c}\boldsymbol{A} - \boldsymbol{A}_{++} \right).
\end{aligned} \tag{28}$$

In the case of a strong field, and if we only restrict ourselves to the lower excited states, we can solve (27) using the Born–Oppenheimer approximation, i.e. we neglect the off-diagonal terms in (27), hence we are able to solve (28) for Ψ_+ and Ψ_- at zero order. From (28) we have ($e = c = \hbar = 1$)

$$H_{++} = -\frac{1}{2M}\nabla^2 + \frac{1}{2M}\left(\Delta - \frac{1}{r^2}\cos\xi \right) P_\theta + \frac{1}{8M}\beta^2 r^2 + \frac{1}{8Mr^2} + \beta - \frac{\Delta\cos\xi}{4M}. \tag{29}$$

The wavefunction for H_{++} can be written as

$$\Psi_+(t) = \sum_n \mathrm{e}^{-\mathrm{i}(E_n+\beta-\Delta\cos\xi/4M)t} f_n(r)\mathrm{e}^{\mathrm{i}n\theta} \tag{30}$$

where $f_n(r)$ satisfies

$$f_n'' + \frac{1}{r}f_n' - \frac{1}{4}\beta^2 r^2 - \frac{n^2 - n\cos\xi + \frac{1}{4}}{r^2} f_n + 2ME_n' f_n = 0 \tag{31}$$

with the eigenvalue

$$E_n' = E_n - \frac{n\Delta}{2M}. \tag{32}$$

If we set $\nu_n = \sqrt{n^2 - n\cos\xi + \frac{1}{4}}$, then the solution of (31) is

$$f_n(r) = r^{\nu_n}\mathrm{e}^{-\frac{1}{4}\beta r^2} F\left(-\frac{ME_n'}{\beta} + \frac{1}{2}(\nu_n + 1), \frac{4\nu_n + 3}{2}, \beta r^2 \right). \tag{33}$$

Here F is the confluent hypergeometric function. The asymptotic condition requires the quantized condition for the energy, namely

$$-\frac{ME_n'}{\beta} + \frac{1}{2}(\nu_n + 1) = -n_r \qquad n_r = 0, 1, 2, \ldots. \tag{34}$$

Since we are discussing the spin-up state, the total energy spectrum should be

$$\begin{aligned} E_{n_r,n} &= E_n + \beta - \frac{\Delta\cos\xi}{4M} \\ &= E'_n + \frac{n\Delta}{2M} + \beta - \frac{\Delta\cos\xi}{4M} \\ &= \frac{1}{2M}(2n_r + \nu_n + 1)\beta + \frac{\Delta}{4M}(2n - \cos\xi) + \beta. \end{aligned} \tag{35}$$

Up until now we have solved the problem in the adiabatic limit. The higher-order effects can be derived from (28) by perturbation, which is outside our present research.

We note that Berry's connection in this system is a pure gauge. It is well known that a pure gauge can be eliminated by a gauge transformation in the case of trivial topology, without affecting any physical results. However, we see that the pure gauge affects the angular momentum and the energy here because of the non-trivial topology. Our system is restricted on the plane and the origin of the coordinates frame is a singularity, when the pure gauge cannot be eliminated continuously.

As a remark, we point out that the adiabatic approximation is the projection of the total wavefunction to the spin-polarized subspace of the Hilbert space. Finally, the problem becomes somewhat like a Landau level problem, and it is no surprise that we get a series of bound states.

4. Discussion

The approach here is less beautiful in mathematical structure than the algebraic approach of [7], for it is heavily reliant on the wavefunction, but it is clearer in its geometric and physical origination. Furthermore, the $U(1)$ monopole appeared in the $SU(2)$ representation in [7], whereas here it appears in the $U(1)$ form by violating the $SU(2)$ Berry's connection. A direct result is that we can solve the eigenequation, but it seems difficult to solve the matrix-valued Hamiltonian in [7] if we still want to preserve a clearly physical picture.

The model in section 3 seems novel; however, in two-dimensional condensed matter systems, if we consider the effect from an inhomogeneous magnetic field, our results may have some application.

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