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BORN–OPPENHEIMER REVISITED

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An algebraic approach to solving degenerate perturbation theory is exhibited. This approach is used to solve the canonical Berry phase problem in the Born–Oppenheimer approximation, as well as the analogous classical problem. The slow variables need not commute. Non-abelian phases and field theory anomalies are treated as examples. A non-adiabatic extension is suggested.

1. Introduction

The Born–Oppenheimer approximation [1] can be used whenever the hamiltonian of a fast system depends on the coordinates of a slow system. In some textbooks, the problem is solved by freezing the coordinates of the slow system and solving the hamiltonian of the fast system; then the energy of the fast system enters the effective hamiltonian for the slow system as a potential energy term. This solution was found by Mead and Truhlar [2] to be insufficient: a vector potential must be inserted to adjust for the separation of the system into two parts. Berry [3] derived the general form of this vector potential. Even when the vector potential is included, however, errors and unjustified approximations are sometimes made. We have found a conceptually simple and direct approach to solving the Born–Oppenheimer approximation. We treat the problem via degenerate perturbation theory and solve it by modifying a subset of the operators, without introducing trial wave functions. In this approach, no geometrical tools are needed. The application of degenerate perturbation theory leads to an inhomogeneous set of linear equations, the solution of which contains the desired vector potential.

We present the algebraic method in sect. 2 of this paper. Sect. 3 extends the method to classical mechanics. A non-abelian example is given in sect. 4, and an application to field theory is worked out in sect. 5. Sect. 6 shows that the slow variables need not commute. Our last example, in sect. 7, suggests how to treat the non-adiabatic case along these lines.

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2. The algebraic method

The approach is quite general, but for the sake of clarity, we begin with a simple example exhibiting Berry's phase [3]*. The model consists of a spin-$\frac{1}{2}$ particle, $\boldsymbol{\sigma}$, which sits in a strong magnetic field, $\mathscr{B}$, pointing in the direction $\hat{\boldsymbol{n}}$. While Berry treated the direction as a slow-moving parameter, we will take a setting [4] appropriate to the Born–Oppenheimer approximation [1]. In this setting $\hat{\boldsymbol{n}}$ is a dynamical quantity representing the direction of a second, massive particle.

The complete hamiltonian can be divided into two parts, a fast one $\mathscr{H}_1$ and a slow one $\mathscr{H}_2$:

$$\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2, \tag{1}$$

where

$$\mathscr{H}_1 = \mathscr{B}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} = \mathscr{B}\frac{\boldsymbol{r}\cdot\boldsymbol{\sigma}}{r}, \qquad \mathscr{H}_2 = \frac{\boldsymbol{P}^2}{2M}, \tag{2}$$

and the momentum $\boldsymbol{P}$ is conjugate to $\boldsymbol{r}$. If $\mathscr{B}M$ is large enough, we can treat the problem in degenerate perturbation theory, where $\mathscr{H}_1$ is taken to be the degenerate hamiltonian and $\mathscr{H}_2$ the perturbation. Following the procedure of degenerate perturbation theory, we start by finding the eigenvalues of $\mathscr{H}_1$, which are $\pm\mathscr{B}$. The eigenvectors with the same eigenvalue form a subspace. We can project onto the two subspaces with projection operators

$$\Pi_{\pm} = \int (|\boldsymbol{r}, \pm\rangle\langle\boldsymbol{r}, \pm|)\,\mathrm{d}\boldsymbol{r} = \frac{1 \pm \hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}}{2}. \tag{3}$$

Here $|\boldsymbol{r}, +\rangle$ (or $|\boldsymbol{r}, -\rangle$) represents an eigenstate of both operators $\boldsymbol{r}$ and $\boldsymbol{r}\cdot\boldsymbol{\sigma}$, sharp in $\boldsymbol{r}$ and (anti-)polarized along $\boldsymbol{r}$. As $\boldsymbol{r}$ has a continuum of eigenvalues, the two subspaces are infinitely degenerate. The next step in solving the degenerate perturbation problem is to diagonalize the perturbation in the subspaces, projecting with the operators Π_i, $i = \pm$. Since $\boldsymbol{P}$ does not commute with Π_i, we should expand the perturbation as follows**:

$$\Pi_i\boldsymbol{P}^2\Pi_i = \Pi_i\boldsymbol{P}\Pi_+\boldsymbol{P}\Pi_i + \Pi_i\boldsymbol{P}\Pi_-\boldsymbol{P}\Pi_i. \tag{4}$$

This expression can be simplified by decomposing $\boldsymbol{P}$ into two parts: one part, $\boldsymbol{P} - \boldsymbol{A}$, acts only within a subspace, while $\boldsymbol{A}$ causes transitions between Π_+ and Π_-:

$$[\boldsymbol{P} - \boldsymbol{A}, \Pi_i] = 0. \tag{5}$$

* Berry's phase is obtained from the vector potential by integration along a loop in the slow-variable space.

** Usually, the approximations $\Pi_i\boldsymbol{P}^2\Pi_i = \boldsymbol{P}^2\Pi_i$ or $\Pi_i\boldsymbol{P}^2\Pi_i = (\Pi_i\boldsymbol{P}\Pi_i)^2$ are made.

There is some ambiguity in A which can be removed by requiring

$$\Pi_i A \Pi_i = 0. \tag{6}$$

Indeed, since $P - A$ is the diagonal part of P, we have in the general case

$$P - A = \sum \Pi_i P \Pi_i, \tag{7}$$

where the sum is over all subspaces i, and so for any number of levels

$$A = P - \sum \Pi_i P \Pi_i = \tfrac{1}{2} \sum [\Pi_i, [\Pi_i, P]]. \tag{8}$$

Inserting eq. (3) into eq. (8), we obtain $A = (\hat{n} \times \sigma)/2r$. Suppose that we are searching for solutions in the subspace of Π_+ only; the effective hamiltonian to be solved is then

$$\begin{aligned} \frac{1}{2M} \Pi_+ P^2 \Pi_+ &= \frac{1}{2M} \Pi_+ (P - A + A)^2 \Pi_+ \\ &= \frac{1}{2M} \Pi_+ (P - A) \Pi_+ (P - A) \Pi_+ + \frac{1}{2M} \Pi_+ A \Pi_- A \Pi_+ \\ &= \frac{1}{2M} (P - A)^2 \Pi_+ + \frac{1}{2M} \Pi_+ A^2 \Pi_+ . \end{aligned} \tag{9}$$

Within the subspace of Π_+, the hamiltonian becomes

$$\frac{1}{2M} \left(P - \frac{\hat{n} \times \sigma}{2r} \right)^2 + \frac{1}{4Mr^2} . \tag{10}$$

The second term is usually not mentioned, but is derived in the second paper of ref. [3]. The first term describes a particle moving in an SU(2) vector potential; the field is

$$B_l = \tfrac{1}{2} \epsilon_{ijk} F_{jk} = \tfrac{1}{2} \epsilon_{ijk} \left(\partial_{[j} A_{k]} - i [A_j, A_k] \right) = -\frac{\hat{n}}{2r^2} (\sigma \cdot \hat{n}) , \tag{11}$$

with $\sigma \cdot \hat{n} = 1$; hence $B = -\hat{n}/2r^2$. By solving a set of equations on the relevant operators we have obtained the effective magnetic monopole found by Berry [3]. It is amusing that the U(1) monopole appears here in a non-abelian representation; it has no string and is singular only at $r = 0$.

Eqs. (5) and (6) are general conditions for determining A, and eq. (8) always provides a solution*. In practice, it is not always convenient to obtain explicit expressions for the projection operators, but they are often not needed, as we show below. The technique is efficient for two-level systems, since the projection operators can be immediately written in terms of the hamiltonian. Moreover, our result for B_i immediately extends to all spins, with $\sigma/2$ replaced by the matrices for any other spin representation. One can check that the commutation relation (5) does not depend on a particular representation, and the definition (8) of A in terms of the hamiltonian always yields vanishing matrix elements between degenerate states. Once eq. (5) is verified as an algebraic identity, the form of A is guaranteed to be independent of the representation.

This derivation of A and its algebraic definition are our main results; however, A itself has appeared in the literature before. In Messiah [5] it generates a "rotating axis representation" of eigenstates. A is not of Berry's form of the vector potential, but it generalizes the operator J defined by Stone and Goff [6, 7] in their derivation of Berry's phase and its application to anomalies. It may seem strange that Berry's phase, which is relevant to the case of no level mixing, can be generated by an A which does nothing but mix levels. Although A connects subspaces with different energies, the field strength can be written [6]

$$F_{ij} = -i\left[P_i - A_i, P_j - A_j\right], \tag{12}$$

and the operators $P_i - A_i$, $P_j - A_j$ operate within each degenerate subspace (by definition). Therefore F_{ij} is also diagonal in the degenerate subspaces. To compute field strengths it is often convenient to use a short cut [6]: the commutator of A_i and A_j is

$$\left[A_i, A_j\right] = \left[P_i - \sum \Pi_m P_i \Pi_m, P_j - \sum \Pi_n P_j \Pi_n\right], \tag{13}$$

and if we look only at the diagonal elements of the commutator, we find

$$\begin{aligned} \sum \Pi_n \left[A_i, A_j\right] \Pi_n &= -\left[\sum \Pi_m P_i \Pi_m, \sum \Pi_n P_j \Pi_n\right] \\ &= -\left[P_i - A_i, P_j - A_j\right] = -iF_{ij}. \end{aligned} \tag{14}$$

It is enough to compute either $\sum \Pi_n [A_i, A_j] \Pi_n$ or $\sum \Pi_n (\partial_i A_j - \partial_j A_i) \Pi_n$; the other part is obtained from this formula. The field strength computed this way coincides with Berry's formula [3].

* If only one of the degenerate subspaces is of interest, then eq. (8) can be replaced by a simpler formula: $A = [\Pi, [\Pi, P]]$, where Π projects onto that subspace. Again $\Pi P^2 \Pi = (P - A)^2 \Pi + \Pi A^2 \Pi$ as in eq. (9).

To see the connection with Berry's phase, note that $0 = \langle m|\Pi_m(P-A)\Pi_n|n\rangle = \langle m|P-A|n\rangle$ for $m \neq n$. Then A is seen to transport states:

$$i\langle m|A|n\rangle = \langle m|\partial|n\rangle .$$

The right-hand side is just the component of $\partial|n\rangle$ along $|m\rangle$. The requirement that A have vanishing diagonal elements implies parallel transport of the phase of the state $|n\rangle$. If we now regard the slow variables as slowly changing external parameters, then A generates changes in a state $|n\rangle$ induced by its dependence on the slow parameters. Thus $i\,\Delta r^i \Delta r^j \langle n|[A^i, A^j]|n\rangle = \Delta r^i \Delta r^j \langle n|F_{ij}|n\rangle$ is the Berry phase acquired by the state when the parameters r make a slow infinitesimal loop $\Delta r^i \Delta r^j$.

3. The classical analogue

Berry's phase is known to have a classical analogue, called Hannay's angle [8]. A Hannay angle can arise in systems with periodic motion, which may be described in terms of action-angle variables. For such systems, the classical adiabatic theorem [9] states that the action is an adiabatic invariant of the motion. Thus, the classical action plays a role analogous to the quantum number of an energy eigenstate. Our algebraic method can be extended to the classical case and effectively shows the parallel with the quantum case [10]. The classical hamiltonian will consist of two parts: $\mathscr{H}_1$, describing fast, quasi-periodic motion regulated by slow variables, and $\mathscr{H}_2$, which involves only those slow variables. For a fixed value of the slow variables, the fast variables in $\mathscr{H}_1$ can be replaced by action-angle variables $\mathscr{I}$, ϕ. Consider our previous example in a classical version [11]. The fast hamiltonian $\mathscr{H}_1 \equiv \mathscr{B} r \cdot S/r$ depends on fast variables S_1, S_2, and S_3 whose Poisson bracket relations

$$\{S_i, S_j\} = \epsilon^{ijk} S_k \tag{15}$$

imply precession around the r-axis with frequency $\mathscr{B}$. The action $\mathscr{I}$ is $r \cdot S/r = \hat{n} \cdot S$ while the frequency $\mathrm{d}\phi/\mathrm{d}t$ is $\mathscr{B}$, so $\mathscr{H}_1$ is $\mathscr{B}\mathscr{I}$. The slow hamiltonian $\mathscr{H}_2$ is $P^2/2M$ and the condition corresponding to eq. (5) takes the form

$$\{P - A, \mathscr{I}\} = \{P - A, \hat{n} \cdot S\} = 0. \tag{16}$$

To fix A we need a condition analogous to eq. (6). Eq. (6) can be interpreted as the requirement that the expectation value of A vanish in all the subspaces, i.e. that A should have no diagonal entries. The analogous statement here is that A should vanish in averaging over the angle variable ϕ. A can be expanded in a Fourier series in ϕ, and ϕ causes $\mathscr{I}$ to shift since $\{\phi, \mathscr{I}\} = 1$. The averaging removes all the ϕ-dependence from A, leaving a constant term which we require to vanish.

To solve the first condition (16), we can take $\mathscr{H}_1$ as the instantaneous hamiltonian and look for a constant of the motion of the form $P-A$. We find that $A=(\hat{n}\times S)/r$ satisfies the condition. Furthermore, A is perpendicular to r and precesses around it, so its average value in the averaging over ϕ is zero. Thus it fulfills the second condition as well. Finally, we get the adiabatic form of $\mathscr{H}_2$:

$$\langle\mathscr{H}_2\rangle=\frac{1}{2M}\langle P^2\rangle=\frac{1}{2M}\langle(P-A+A)^2\rangle=\frac{1}{2M}(P-A)^2+\frac{1}{2M}A^2. \quad (17)$$

Note that although the average value of A vanishes, A^2 is independent of ϕ and must be included in the adiabatic hamiltonian as a scalar potential. The vector potential A in $(P-A)/M$, which is the velocity operator, induces a modification of the Poisson brackets among the velocities, as if a monopole of strength $\mathscr{I}$ were present [11]. If the slow variables are treated as external parameters, the effect of A is seen in Hannay's angle: an addition to ϕ when the external parameters change slowly in a loop [8]. When the Poisson brackets among the components of $P-A$ do not depend on $\mathscr{I}$, Hannay's angle is zero [8]. However it may be noted that, even in this case, the vector potential A appears in the effective classical hamiltonian, $\mathscr{H}_1+\mathscr{H}_2$, for the slow variables treated dynamically.

Thus we have the following correspondence between the classical and quantum cases: there is an adiabatic invariant (action $\mathscr{I}$ or quantum level m) of the fast hamiltonian $\mathscr{H}_1$, but the slow hamiltonian $\mathscr{H}_2$ induces translations both within a subspace (trajectory of constant $\mathscr{I}$ or m) and out of it. Imposition of the adiabatic limit induces vector and scalar potentials in the slow variables, which are fixed by the requirement that A should contain only the non-adiabatic (ϕ-dependent or off-diagonal) part.

4. A non-abelian example

We have seen that the algebraic approach naturally yields a non-abelian representation of the monopole vector potential. Genuinely non-abelian phases [12] also arise naturally. As an example, consider the following hamiltonian:

$$\mathscr{H}=\frac{P^2}{2M}+\mathscr{B}(\hat{n}\cdot S)^2, \quad (18)$$

where S represents a spin-$\frac{3}{2}$ particle. We want to find an A that satisfies conditions (5) and (6). Of course, choosing $A=(\hat{n}\times S)/r$ insures that $P-A$ will commute with $(\hat{n}\cdot S)^2$, but this A no longer satisfies eq. (6); it connects states that now are degenerate. The correct A, obtained from eq. (8), is

$$A=\tfrac{1}{4}\left[(\hat{n}\cdot S)^2,\left[(\hat{n}\cdot S)^2,P\right]\right]=\frac{4(\hat{n}\cdot S)\hat{n}\times S(\hat{n}\cdot S)+\hat{n}\times S}{4r}. \tag{19}$$

It equals $A=(\hat{n}\times S)/r$ except that matrix elements connecting degenerate states are zero. To compute the field strength it is helpful to use the short cut described above in eq. (14). It is easiest to compute $(\partial_i A_j-\partial_j A_i)$ which happens to be diagonal, and

$$F_{ij}\equiv\partial_i A_j-\partial_j A_i-i\left[A_i,A_j\right]=\tfrac{1}{2}(\partial_i A_j-\partial_j A_i), \tag{20}$$

so that

$$B_i=\tfrac{1}{2}\epsilon_{ijk}F_{jk}=\frac{n_i(\hat{n}\cdot S)}{2r^2}\left[2S^2-\tfrac{1}{2}-4(\hat{n}\cdot S)^2\right]. \tag{21}$$

For states with $\hat{n}\cdot S=\pm\frac{3}{2}$, B is the same as in sect. 2; it is abelian, despite the degeneracy of these two states. For the states $\hat{n}\cdot S=\pm\frac{1}{2}$, B is

$$B=3\frac{\hat{n}(\hat{n}\cdot S)}{r^2} \tag{22}$$

and is multiplied by -3 compared with the previous result. Hence for these states B contains a truly non-abelian contribution. (Since we require A to have vanishing matrix elements within a degenerate subspace, it is not easy to see from A alone whether the field is truly non-abelian.) The present example does not immediately generalize to higher spin representations, however. The requirement $[P-A,(\hat{n}\cdot S)^2]=0$ is satisfied in the spin-$\frac{3}{2}$ representation but it is not an algebraic identity. The underlying reason is the appearance of squares of generators, which lead to the enveloping algebra of SU(2).

5. Anomalies in field theory

As a further application of the algebraic approach, we turn to field theory. Berry's phase has been fruitfully applied to the understanding of anomalies [6, 7, 13]. Let us see how this works in the case of Weyl fermions in 1 + 1 dimensions. The fermions will be governed by a fast hamiltonian, $\mathscr{H}_1$, that depends upon a gauge field for which the kinetic hamiltonian is $\mathscr{H}_2$:

$$\mathscr{H}_1=\int :\psi^\dagger(-i\partial-A)\psi:\mathrm{d}x,\qquad \mathscr{H}_2=e^2\int E^2\,\mathrm{d}x. \tag{23}$$

Here $\psi(x)$ is a one-component chiral fermion field, $A(x)$ is a gauge field, and

$E(x)$ is its conjugate momentum, $E(x) = -i\partial/\partial A(x)$. Space is taken to be compact, with x running from 0 to 2π. (So the spectrum of $\mathscr{H}_1$ is discrete.) The coupling e is arbitrary, and for purposes of the adiabatic approximation it can be assumed small. In the adiabatic approximation, transitions among the eigenstates of $\mathscr{H}_1$ are suppressed, although $E(x)$ causes transitions among these eigenstates. Here we have no simple way to write down projection operators for the eigenstates, so our strategy will be a little different. We will look for a part $\mathscr{A}(x)$ to subtract from $E(x)$ so that $E - \mathscr{A}$ will commute with $\mathscr{H}_1$. Afterwards we will check that $\mathscr{A}$ does not connect degenerate states. It is helpful to use Fourier transforms:

$$A(x) = \sum A_k \mathrm{e}^{ikx}, \qquad E(x) = \frac{1}{2\pi}\sum E_k \mathrm{e}^{ikx}, \tag{24}$$

with $[A_p, E_q] = i\delta_{p,-q}$ and $E_k^\dagger = E_{-k}$, $A_k^\dagger = A_{-k}$. We analyze ψ in terms of the eigenfunctions of $-i\partial - A(x)$ which obey periodic boundary conditions:

$$\psi = (2\pi)^{-1/2}\sum a_k u_k, \qquad u_k(x) \equiv \exp\left\{ikx - iA_0 x + i\int_0^x A(x')\,\mathrm{d}x'\right\}, \tag{25}$$

with $a_j^\dagger a_k + a_k a_j^\dagger = \delta_{jk}$. Choosing these eigenfunctions for the expansion of $\psi(x)$ is analogous to diagonalizing $\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}$ in our earlier example, since the fast hamiltonian becomes

$$\mathscr{H}_1 = \sum :a_k^\dagger a_k:(k - A_0). \tag{26}$$

In fact A_0 can be dropped from $\mathscr{H}_1$: the total charge on a circle must be zero. (This constraint must be imposed with the choice of the hamiltonian gauge [14].) The vacuum $|0\rangle$, defined by $a_k|0\rangle = 0$ for $k - A_0 > 0$ and $a_k^\dagger|0\rangle = 0$ for $k - A_0 < 0$, is an eigenstate of $\mathscr{H}_1$, as are all other states obtained from it by pair creation. The creation operators $a_k^\dagger$ depend implicitly on $A(x)$, and since $[E(x), \psi(y)] = 0$ we find

$$0 = \left[E_j, \sum a_m u_m\right] = -i\sum\left(\frac{\partial a_m}{\partial A_j}u_m + a_m\frac{\partial u_m}{\partial A_j}\right), \tag{27}$$

so that

$$\left[E_j, a_k\right] = i\sum a_m \int u_k^* \frac{\partial}{\partial A_{-j}} u_m\,\mathrm{d}x = \frac{i}{j}(a_k - a_{k+j}). \tag{28}$$

Similarly, $[E_j, a_k^\dagger] = -(i/j)(a_k^\dagger - a_{k-j}^\dagger)$. Therefore the commutator of E_j and $\mathscr{H}_1$ is

$$\left[E_j, \mathscr{H}_1\right] = -i\sum a_{q-j}^\dagger a_q \equiv -iJ(j). \tag{29}$$

We know that the induced vector potential to be added to E_j must cause transitions among the eigenstates of $\mathscr{H}_1$, so we can expect it to include terms of the form $a_j^\dagger a_k$ for $j \neq k$. We find

$$\left[a_j^\dagger a_k, \mathscr{H}_1\right] = (j-k) a_j^\dagger a_k, \tag{30}$$

so that

$$\mathscr{A}_j = iJ(j)/j \tag{31}$$

is exactly what must be subtracted from E_j. As required, the expectation value of $\mathscr{A}_j$ in any degenerate subspace is zero.

The combination $E_j - iJ(j)/j$ is, up to a factor ij, the Fourier component of $\partial_x E(x) + \psi^\dagger(x)\psi(x)$, the generator of gauge transformations. Do these gauge generators have anomalous commutation relations? This question must be answered with respect to Tomonaga [6, 15] states, those built from the vacuum $|0\rangle$. With respect to Tomonaga states, the infinite sum of terms in $J(j) = \sum a_{q-j}^\dagger a_q$ can be restricted to a finite sum over $-L \leqslant q \leqslant L$; here L is an arbitrarily large number such that all levels for $q < -L$ are filled, all levels for $q > L$ are empty. The expectation value of a commutator becomes

$$\left[E_j - \frac{iJ(j)}{j}, E_k - \frac{iJ(k)}{k}\right] = \frac{1}{jk}\delta_{j,-k} \sum \left(a_{q-j}^\dagger a_{q-j} - a_q^\dagger a_q\right). \tag{32}$$

In the sum $-L \leqslant q \leqslant L$ most of the terms cancel. Terms with $q \approx L$ annihilate Tomonaga states, so the only contribution comes from $q \approx -L$ and gives the result $\delta_{j,-k}/k$. (As noted by Stone and Goff [6] the purely fermionic part of the commutator is the same as the overall commutator except for a minus sign.) For the gauge generators, this result implies

$$\left[\partial_x E(x) + \psi^\dagger(x)\psi(x), \partial_y E(y) + \psi^\dagger(y)\psi(y)\right] = \frac{i}{2\pi}\frac{\partial}{\partial x}\delta(x-y), \tag{33}$$

which is the familiar Schwinger term. The Schwinger term can be interpreted as a breakdown of gauge invariance on the states of our model, because a small loop in the space of gauge orbits, corresponding to this commutator, does not return a state to itself but leaves it with a Berry phase [6, 7, 13].

6. Non-commuting slow variables

Moving to a new example, let us examine the motion of a particle in a strong magnetic field [16]. The scaled hamiltonian can be written in the form

$$\mathscr{H} = \tfrac{1}{2}\Omega\left[\left(p_x - \tfrac{1}{2}y\right)^2 + \left(p_y + \tfrac{1}{2}x\right)^2\right], \tag{34}$$

where Ω is the Larmor frequency. By defining [17]

$$P = p_x - \tfrac{1}{2}y, \qquad Q = p_y + \tfrac{1}{2}x, \qquad [Q, P] = i, \tag{35}$$

we have the hamiltonian of a harmonic oscillator:

$$\mathscr{H} = \tfrac{1}{2}\Omega(P^2 + Q^2). \tag{36}$$

The eigenstates of this hamiltonian are the Landau levels, which have infinite degeneracy, depending on the localization of the state. The coordinates which specify the localization are non-commuting; so this example differs from the previous one, in which the degeneracy was indexed by the commuting components of $\boldsymbol{r}$. To this hamiltonian we add a perturbation, $\mathscr{V}(x, y)$. This potential should be projected onto a subspace of $\mathscr{H}$, for example via the ground state projector Π_g. To find an A_x and A_y which will accomplish this projection for us, we should solve the double set of equations

$$\begin{cases} [x - A_x, \Pi_g] = [y - A_y, \Pi_g] = 0, \\ \Pi_g A_x \Pi_g = \Pi_g A_y \Pi_g = 0. \end{cases} \tag{37}$$

The solution is

$$A_x = Q, \qquad A_y = -P. \tag{38}$$

The effect of A is not a magnetic monopole or flux but a redefinition of the coordinates from x and y, which commute, to

$$x' = \tfrac{1}{2}x - p_y, \qquad y' = \tfrac{1}{2}y + p_x$$

with the commutation relation $[x', y'] = i$. If the perturbation is

$$\mathscr{V} = x^2 + y^2, \tag{39}$$

we end up with a hamiltonian for a harmonic oscillator

$$\Pi_g \mathscr{V} \Pi_g = (x')^2 + (y')^2 + 1, \tag{40}$$

and if it is

$$\mathscr{V} = \cos(\beta x), \tag{41}$$

we have a hamiltonian which causes a jump in the y'-direction:

$$\Pi_g \mathscr{V} \Pi_g = \exp\left(-\tfrac{1}{4}\beta^2\right)\cos(\beta x'). \tag{42}$$

Note that even powers of A contribute. This result is not contained in the usual formulation of the Born–Oppenheimer approximation, since the coordinates indexing the degeneracy do not commute and therefore cannot be treated as parameters in the usual sense.

7. Beyond the adiabatic assumption

The condition imposed by eq. (6) – no transitions among eigenstates of the fast hamiltonian $\mathscr{H}_1$ – is precisely the adiabatic approximation. However, the vector potential can appear outside of this approximation. The general behavior was discussed in more detail in ref. [20]. The non-adiabatic role of the vector potential appears if we take a simplified version of the problem of sect. 2 and solve it exactly. The hamiltonian is

$$\mathscr{H} = \mathscr{B}(\sigma_x \cos\phi + \sigma_y \sin\phi) + P_\phi^2/2I, \tag{43}$$

where the slow particle is constrained to move along a ring in the x–y plane. Once again, we find a combination $P_\phi + \frac{1}{2}\sigma_z$ which commutes with the first (fast) term in $\mathscr{H}$. But this time we leave the off-diagonal terms in $\mathscr{H}$, so that the exact hamiltonian is

$$\mathscr{H} = \mathscr{B}(\sigma_x \cos\phi + \sigma_y \sin\phi) + \left(P_\phi + \tfrac{1}{2}\sigma_z\right)^2/2I - P_\phi\sigma_z/2I + \text{constant}. \tag{44}$$

We use a single-valued unitary transformation $U = \exp\{i(\sigma_z + 1)\phi/2\}$ to rotate the frame of reference, so that

$$\mathscr{H} = \mathscr{B}\sigma_x + P_{\phi'}^2/2I - \sigma_z P_{\phi'}/2I + \text{constant}, \tag{45}$$

where we define $P_{\phi'} \equiv P_\phi - \frac{1}{2}$. This modification of P_ϕ corresponds to a singular line of flux of strength π along the z-axis. By diagonalizing the combination $\mathscr{B}\sigma_x - \sigma_z P_{\phi'}/2I$ we get a hamiltonian

$$\mathscr{H} = \sqrt{\mathscr{B}^2 + P_{\phi'}^2/4I^2}\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}} + P_{\phi'}^2/2I + \text{constant}, \tag{46}$$

where $\hat{\boldsymbol{n}}$ is a function of $\mathscr{B}$ and $P_{\phi'}$. Since $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}$ commutes with $P_{\phi'}$ we can replace $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}$ with one of its eigenvalues, ± 1. We now choose an approximate eigenstate of the momentum $P_{\phi'}$ such that

$$P_{\phi'} = \bar{P} + \delta P, \tag{47}$$

with $\bar{P}$ a c-number and the range of δP much smaller than $\bar{P}$. Since we are interested in having the magnetic energy comparable to the kinetic energy, in contrast to the adiabatic limit, we write

$$\alpha\mathscr{B} = \bar{P}/2I \tag{48}$$

where $\alpha \approx 1$. According to our approximation $\delta P \ll \bar{P}$,

$$\sqrt{\mathscr{B}^2 + P_{\phi'}^2/4I^2} \approx \mathscr{B}\sqrt{1+\alpha^2+\bar{P}\,\delta P/\mathscr{B}^2 2I^2} \approx \mathscr{B}\sqrt{1+\alpha^2}\left(1+\frac{\alpha^2}{(1+\alpha^2)\bar{P}}\,\delta P\right)$$

$$\approx \frac{\mathscr{B}\alpha^2}{\sqrt{1+\alpha^2}\,\bar{P}} P_{\phi'} + \text{constant}, \tag{49}$$

so the hamiltonian can be written as

$$\mathscr{H} = \frac{(P_\phi + A)^2}{2I} + \text{constant}, \tag{50}$$

where A is a magnetic flux line. The magnitude of the flux is a function of the ratio between the magnetic field and the average momentum:

$$A \equiv \frac{1}{2} \pm \frac{\alpha}{2\sqrt{1+\alpha^2}}\,. \tag{51}$$

In the adiabatic limit $\alpha \to 0$ the two spin states have the same flux, since $A = \frac{1}{2}$; for $\alpha > 0$ the two states get opposite corrections, and for $\mathscr{B}$ small ($\alpha \to \infty$) A approaches 0 or 1, both of which are equivalent to no flux. This non-adiabatic behavior looks like the effect of spin flips washing out the vector potential, and we suggest that adiabatic eigenstates can in this way be used to interpret nonadiabatic processes.

8. Summary

In conclusion, we have seen that a vector potential appears naturally when a perturbation is constrained to act within a degenerate subspace of a free hamiltonian. In calculating this vector potential there is no need to consider the intrinsic geometry of the problem; the derivation does not need a geometrical setting. The vector potential is obtained as the solution to an algebraic problem. The algebraic approach unifies many aspects of quantum and classical holonomy. It provides a correspondence between the quantum and classical adiabatic theorems; it naturally includes the non-abelian case and cases where the slow parameters do not commute. For a model field theory, the algebraic approach quickly demonstrates the connection between Berry's phase and anomalies. Finally, we have suggested a way to interpret results that arise outside of the adiabatic approximation as the effect of flipping among adiabatic eigenstates which progressively washes out the vector potential.

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