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Perturbative Induction of Vector Potentials

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Degenerate perturbation theory, without geometrical tools, directly yields vector potentials in the Born-Oppenheimer approximation. The derivation uses only the algebra of the dynamical operators, and the slow variables need not commute.

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The Born-Oppenheimer approximation[1] is a standard tool for problems in which 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. Mead and Truhlar[2] found this solution to be insufficient: A vector potential must be inserted to adjust for the separation of the system into two parts. A general form for this vector potential was derived by Berry.[3] Even with the vector potential 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.

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 $\mathcal{B}$ pointing in the direction $\hat{\mathbf{n}}$. 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 $\hat{\mathbf{n}}$ is a dynamical quantity representing the direction of a second, massive particle.

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

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

where

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

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

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

Here $|\mathbf{r},+\rangle$ ($|\mathbf{r},-\rangle$) represents an eigenstate of both operators $\mathbf{r}$ and $\mathbf{r}\cdot\boldsymbol{\sigma}$, sharp in $\mathbf{r}$ and (anti)polarized along $\mathbf{r}$. As $\mathbf{r}$ 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 $\mathbf{P}$ does not commute with Π_i, we should expand the perturbation as follows:[5]

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

This expression is awkward because $\mathbf{P}$ has a part that

causes transitions between subspaces. A way to simplify it is to decompose $\mathbf{P}$ into two parts: One part, $\mathbf{P}-\mathbf{A}$, acts only within a subspace, while $\mathbf{A}$ causes transitions between Π_+ and Π_-:

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

There is some ambiguity in $\mathbf{A}$ which can be removed by requiring

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

Indeed, since $\mathbf{P}-\mathbf{A}$ is the diagonal part of $\mathbf{P}$, we have, in general,

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

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

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

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

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

Within the subspace of Π_+, the Hamiltonian becomes

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

The second term is usually not mentioned. The first term describes a particle moving in an SU(2) vector potential; the field is

$$\begin{aligned}B_i&=\tfrac{1}{2}\epsilon_{ijk}F_{jk}=\tfrac{1}{2}\epsilon_{ijk}(\partial_{[j}A_{k]}-i[A_j,A_k])\\&=-\frac{\hat{\mathbf{n}}}{2r^2}(\boldsymbol{\sigma}\cdot\mathbf{n}),\end{aligned} \tag{11}$$

with $\boldsymbol{\sigma}\cdot\mathbf{n}=1$; hence $\mathbf{B}=-\hat{\mathbf{n}}/2r^2$. 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 $\mathbf{r}=0$.

Although we have found the solution for a simple example, the algebraic approach is quite general. In particular, Eqs. (5) and (6) are general conditions for determining $\mathbf{A}$, and Eq. (8) always provides a solution.[6] 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. For two-level systems the method is efficient, 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 (5) is verified as an algebraic identity, the form of $\mathbf{A}$ is guaranteed to be independent of the representation.

This derivation of $\mathbf{A}$ and its algebraic definition are our main results; however, $\mathbf{A}$ itself has appeared in the literature before. In the work of Messiah[7] it generates a "rotating-axis representation" of eigenstates. $\mathbf{A}$ is not Berry's form of the vector potential, but it generalizes the operator $\mathbf{J}$ defined by Stone and Goff[8,9] in their discussion of Berry's phase and anomalies. It may seem strange that Berry's phase, which is relevant to the case of no level mixing, can be generated by an $\mathbf{A}$ which does nothing but mix levels. Although $\mathbf{A}$ connects subspaces with different energies, the field strength can be written[8]

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

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:[8] The commutator of A_i and A_j is

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

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

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

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

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

$$i\langle m|\mathbf{A}|n\rangle=\langle m|\partial|n\rangle. \tag{15}$$

The right-hand side is just the component of $\partial|n\rangle$ along $|m\rangle$. The requirement that $\mathbf{A}$ 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 $\mathbf{A}$ 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 $\mathbf{r}$ make a slow infinitesimal loop $\Delta r^i \Delta r^j$.

Moving to a new example, let us examine the motion of a particle in a strong magnetic field.[10] The scaled Hamiltonian can be written in the form

$$\mathcal{H} = \tfrac{1}{2}\Omega[(p_x - \tfrac{1}{2}y)^2 + (p_y + \tfrac{1}{2}x)^2], \quad (16)$$

where Ω is the Larmor frequency. By defining[11]

$$P = p_x - \tfrac{1}{2}y, \quad Q = p_y + \tfrac{1}{2}x, \text{ and } [Q,P] = i, \quad (17)$$

we have the Hamiltonian of a harmonic oscillator:

$$\mathcal{H} = \tfrac{1}{2}\Omega(P^2 + Q^2). \quad (18)$$

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 noncommuting; so this example differs from the previous one, in which the degeneracy was indexed by the commuting components of $\mathbf{r}$. To this Hamiltonian we add a perturbation, $\mathcal{V}(x,y)$. This potential should be projected onto a subspace of $\mathcal{H}$, for example, via the ground-state projector Π_g. Here, rather than writing down projection operators for the eigenstates, our strategy will be a little different. We will look for a part $\mathbf{A}$ to subtract from x and y, such that $x - A_x$ and $y - A_y$ will commute with $\mathcal{H}$. Afterwards we will check that $\mathbf{A}$ does not connect states within a degenerate subspace. To find the A_x and A_y which accomplish this projection for us, we solve the double set of equations

$$[x - A_x, \Pi_g] = [y - A_y, \Pi_g] = 0, \quad \Pi_g A_x \Pi_g = \Pi_g A_y \Pi_g = 0. \quad (19)$$

The solution is

$$A_x = Q \text{ and } A_y = -P. \quad (20)$$

It is easy to check that the projection $\Pi_g \mathbf{A} \Pi_g$ vanishes, as desired, because Q and P are sums of raising and lowering operators. The effect of $\mathbf{A}$ is not a magnetic monopole or flux but a redefinition of the coordinates from x and y, which commute, to

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

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

$$\mathcal{V} = x^2 + y^2, \quad (21)$$

we end up with a Hamiltonian for a harmonic oscillator

$$\mathcal{V} = (x')^2 + (y')^2 + 1, \quad (22)$$

and if it is

$$\mathcal{V} = \cos(\beta x), \quad (23)$$

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

$$\mathcal{V} = \exp(-\beta^2/4)\cos(\beta x'). \quad (24)$$

Note that even powers of $\mathbf{A}$ 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.

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 simply diagonalizes the perturbation within degenerate subspaces, and then the vector potential is obtained as the solution to an algebraic problem. The solution has been given explicitly in terms of projection operators onto the subspaces. The condition imposed by Eq. (6) —no transitions among eigenstates of the fast Hamiltonian $\mathcal{H}_1$— is precisely the adiabatic approximation. However, the appearance of a vector potential need not be limited to this approximation.[12] An extension of the algebraic approach to the nonadiabatic regime is indicated in a longer version[13] of the present work, which contains further examples of the algebraic method, including non-Abelian phases, anomalies in field theory, and the classical version of the Born-Oppenheimer approximation and Hannay's angle.[14]

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[5]Usually the approximations $\Pi_i \mathbf{P}^2 \Pi_i = \mathbf{P}^2 \Pi_i$ or $\Pi_i \mathbf{P}^2 \Pi_i = (\Pi_i \mathbf{P} \Pi_i)^2$ are made.

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

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