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Short Communication

WKB calculation of quantum adiabatic phases and nonadiabatic corrections

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Résumé. — Berry a découvert que les fonctions d’onde peuvent acquérir — en plus de la phase dynamique habituelle — un facteur de phase géométrique, pendant un cycle adiabatique de période T. Les phases dynamique et de Berry sont ici identifiées comme les deux premiers termes d’un développement WKB systématique en puissance de \( \varepsilon = 1/T \). Nous donnons ainsi une méthode simple pour le calcul des phases adiabatiques et pour l’inclusion cohérente de corrections non adiabatiques.

Abstract. — Berry discovered that wave functions may acquire a geometrical phase factor, in addition to the usual dynamical phase, during an adiabatic cycle with period T. The dynamical and Berry phases are here recognized as the first two terms in a systematic WKB expansion in powers of \( \varepsilon = 1/T \). We thus provide a simple method for the calculation of adiabatic phases and for a consistent inclusion of nonadiabatic corrections.

Following the original discovery of Berry [1, 2] quantum adiabatic phases have become the subject of intense theoretical as well as experimental investigations. In a recent paper [3] Bouchiat provided a group-theoretical derivation of the Berry phase and suggested that the same method could be used for the computation of nonadiabatic corrections. An alternative approach is discussed here based on the realization that the usual dynamical and Berry phases are the first two terms in a suitable WKB expansion. Nonadiabatic corrections are then computed systematically by including higher-order terms in the WKB series.

For definiteness we consider the precession of a spin \( S \) in a time-dependent magnetic field; i. e. we assume a Hamiltonian of the form

\[
H = -(B.S),
\]

\[
B = B(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta).
\]  

(1)

The field is conveniently parametrized by spherical coordinates with respect to a fixed reference frame \( XYZ \), as is indicated in figure 1 which follows the conventions of reference [3]. Both the magnitude \( B \) and the direction of the field (angles \( \theta \) and \( \phi \)) are arbitrary periodic functions of time with period \( T \). As long as the Hamiltonian is linear in the spin operators, a solution for arbitrary spin \( s \) may be obtained from the spin-\( \frac{1}{2} \) solution by elementary quadratures [4-7]. We

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shall thus restrict our attention to a spin-$\frac{1}{2}$ system. A general spin-$\frac{1}{2}$ state will be represented as

$$\psi = C_1 |\uparrow> + C_2 |\downarrow> \quad (2)$$

where $|\uparrow>$ and $|\downarrow>$ are states quantized along the fixed $z$-direction, or as

$$\psi = \Gamma_1 |+> + \Gamma_2 |->$$

$$\Gamma_1 = \cos \frac{\theta_0}{2} C_1 + \sin \frac{\theta_0}{2} C_2, \quad (3)$$

$$\Gamma_2 = -\sin \frac{\theta_0}{2} C_1 + \cos \frac{\theta_0}{2} C_2,$$

where $|\pm>$ are states quantized along the direction of the initial magnetic field $B_0$. Representation (2) will be used during the intermediate steps of the calculation while (3) will lead to a more transparent physical interpretation.

Fig. 1.— Conventions concerning the time evolution of the magnetic field. Note that the field is contained in the $XZ$ plane at $t = 0$.

The original result of Berry can be simply stated as follows. Suppose that the initial state of the system is $|\pm>$ and the field is adiabatically varied to complete a full cycle. The final state is then given by $\exp(\pm i\gamma)|\pm>$ with

$$\gamma \approx \frac{1}{2} \left[ \int_0^T B(t) dt - \int_0^T (1 - \cos \theta) \phi dt \right]. \quad (4)$$

The first term in (4) is the expected dynamical phase whereas the second term is the Berry phase which is equal to the solid angle that the contour $C$ subtends at the origin of the reference frame.

The preceding approximate result is valid as long as the period $T$ is large compared with the period of spin precession ($BT >> 1$), but must be corrected to account for finite-$T$ effects which may include transitions between spin states. In this respect, it is useful to realize that the Berry phase is a subleading correction to the dynamical phase which suggests that equation (4) contains only the first two terms of a systematic expansion. What is not clear, however, is whether a phase such as (4) is physically meaningful in the presence of transitions. Nonetheless the issue of nonadiabatic corrections is obviously legitimate and can be best handled by a WKB expansion in powers of the small parameter $\epsilon = 1/T$. In such a context, nonadiabatic corrections to equation (4) will become natural and will be supplemented by a prescription for the calculation of transition probabilities. Needless to say, the WKB method will also provide a direct means for the calculation of the Berry phase itself.

The time evolution of state (2) is governed by the system of first-order linear equations.

$$\dot{C}_1 = \frac{i}{2} (aC_1 + b^* C_2), \quad \dot{C}_2 = \frac{i}{2} (bC_1 - aC_2),$$

$$a \equiv B \cos \theta, \quad b \equiv B \sin \theta e^{i\phi}. \quad (5)$$

Eliminating $C_2$ we arrive at a second-order equation for $C_1$:

$$\ddot{C}_1 = \frac{b^*}{b} \dot{C}_1 + \frac{1}{2} \left[ i \left( \dot{a} - \frac{\dot{b}^*}{b} \right) - \frac{1}{2} (a^2 + b^* b) \right] C_1,$$

$$C_2 = -\frac{1}{b^*} \left( aC_1 + 2i \dot{C}_1 \right). \quad (6)$$

In order to implement the WKB expansion we introduce the scaled time variable $\tau = t/T = \epsilon t$, so $\epsilon = 1/T$, and we denote the derivative with respect to $\tau$ by a prime. For the moment we concentrate on the equation for $C_1$ which is written as

$$\epsilon^2 \left( C''_1 - \Gamma C'_1 \right) + \left( \frac{1}{4} B^2 - i\epsilon \Delta \right) C_1 = 0,$$

$$B^2 = a^2 + b^* b, \quad \Gamma = \frac{b^*}{b^*}, \quad (7)$$

$$\Delta = \frac{1}{2} \left( a' - \frac{b'^*}{b^*} \right).$$

We follow the usual WKB procedure and represent $C_1$ as an exponential:

$$C_1 = \exp(F/\epsilon), \quad F = F_0 + \epsilon F_1 + \epsilon^2 F_2 + \cdots \quad (8)$$

Substituting (8) into (7) gives

$$F'' + \frac{1}{4} B^2 + \epsilon (F'' - \Gamma F' - i\Delta) = 0 \quad (9)$$
or
\[
F''_2 + \frac{1}{4} B^2 = 0,
\]
\[
F'_0 - i \Delta + 2 F'_1 F'_0 = 0,
\]
\[
F'_1 - i \Delta + F''_1 + 2 F'_0 F'_1 = 0, \ldots,
\]
which is a typical system of recursive WKB equations [8] that can be used to determine the functions \( F_0, F_1, F_2 \cdot \cdot \cdot \).

The first two equations in (10) yield
\[
F'_0 = \pm \frac{i}{2} B,
\]
\[
F'_1 = -\frac{1}{2} (1 \mp \cos \theta) \left( i \phi' \pm \frac{\theta'}{\sin \theta} \right),
\]
where we have restored the original spherical variables for the magnetic field. If our intention were only to compute the Berry phase, equations (11) would have already accomplished the task. Deferring for the moment a discussion of the choice of sign in (11), we note that integrating the first equation provides the usual dynamical phase in (4). The second equation in (11) leads to the Berry phase because the real part of \( F'_1 \) is a total time derivative whose contribution vanishes upon integration around a complete cycle. Of course the real part of \( F'_1 \) is important at intermediate times as well as for the computing of the next correction \( F_2 \). The latter is determined from the third equation in (11). After some algebra we find that
\[
F'_2 = \pm \frac{i}{4B} \left( \phi'^2 + \sin^2 \theta \phi'^2 \right) - \frac{1}{2} \left( \frac{F'_1}{B} \right). \tag{12}
\]

We observe again that the real part of \( F'_2 \), contained in the second term of (12), is a total time derivative. As a rule, the real parts of all higher-order terms are total derivatives.

A complete calculation of physical quantities entails an explicit construction of both amplitudes \( C_1 \) and \( C_2 \) and a specification of integration constants according to definite initial conditions. First we must deal with the sign ambiguity in equations (11) and (12). Let us retain the symbol \( F \) for the solution corresponding to the upper sign and introduce the symbol \( G \) for the solution with the lower sign. Both \( F \) and \( G \) satisfy the differential equation (9). Thus a general solution for \( C_1 \) is a linear superposition of the form
\[
C_1 = \mu \exp(F/\epsilon) + \nu \exp(G/\epsilon) \tag{13}
\]
where \( \mu \) and \( \nu \) are arbitrary complex constants. To complete this construction, we determine \( C_2 \) from the second equation in (6) using as input \( C_1 \) from (13):
\[
C_2 = -\frac{1}{\epsilon^*} \left[ \mu(a + 2iF') \exp(F/\epsilon) + \nu(a + 2iG') \exp(G/\epsilon) \right]. \tag{14}
\]

Because we have introduced the arbitrary constants \( \mu \) and \( \nu \), we may fix the integration constants in \( F \) and \( G \) so that \( F(0) = 0 = G(0) \). This convention, together with our earlier observation that the real parts of \( F'' \) and \( G' \) are total derivatives, implies that \( F \) and \( G \) are purely imaginary at \( r = t/T = 1 \) or \( t = T \). We summarize these findings in
\[
F(0) = 0 = G(0), \quad \frac{1}{\epsilon} F(T) = i \gamma = -\frac{1}{\epsilon} G(T), \tag{15}
\]
where \( \gamma \) is a real constant calculated by integrating equations (11) and (12) over a complete cycle:
\[
\gamma = \frac{1}{2} \left[ \int_0^T B(t) dt - \int_0^T (1 - \cos \theta) \phi \ dt \right. \nonumber \\
\left. + \frac{1}{2} \int_0^T (\dot{\theta}^2 + \sin^2 \theta \phi^2) \frac{dt}{B(t)} + \ldots \right]. \tag{16}
\]

Here we have returned to the original time variable \( t \). Equation (16) is a generalization of equation (4) including the first nonadiabatic correction. It is now clear that the Berry phase is the only term in the WKB expansion with purely geometrical origin.

Of course the phase (16) is not entirely meaningful until a prescription is given for the computation of transition probabilities. These are now important because of the inclusion of nonadiabatic corrections. At this point we must explicitly specify the initial conditions. We consider the time evolution of a spin state which at \( t = 0 \) points in the direction of the initial field \( B_0 \). It is therefore prudent to use the spin basis (3) and impose the initial conditions \( \Gamma_1(0) = 1 \) and \( \Gamma_2(0) = 0 \). Recall that \( \theta_{(0)} = \theta_0 = \theta(T) \) and \( \phi(0) = 0 = \phi(T) \) in view of our conventions in figure 1.

Expressing \( \Gamma_1 \) and \( \Gamma_2 \) in terms of \( C_1 \) and \( C_2 \) we write
\[ I_1 = \mu(\alpha + \beta M)\exp(F/\epsilon) + \nu(\alpha + \beta N)\exp(G/\epsilon) \]
\[ I_2 = \mu(-\beta + \alpha M)\exp(F/\epsilon) + \nu(-\beta + \alpha N)\exp(G/\epsilon) \]  
(17)

where we use the notational abbreviations

\[ \alpha = \cos \frac{\theta_0}{2}, \beta = \sin \frac{\theta_0}{2}, \]
\[ M = -\frac{1}{b^*}(a + 2iF') = -\frac{1}{b^*}[a + 2i(F'_0 + \epsilon F'_1 + \ldots)], \]
\[ N = -\frac{1}{b^*}(a + 2iG') = -\frac{1}{b^*}[a + 2i(G'_0 + \epsilon G'_1 + \ldots)]. \]  
(18)

At \( t = 0 \) the exponentials in (17) become unity, in view of (15), and the initial conditions \( I_1(0) = 1 \) and \( I_2(0) = 0 \) are enforced if the constants \( \mu \) and \( \nu \) are chosen as

\[ \mu = \frac{\alpha N(0) - \beta}{N(0) - M(0)}, \quad \nu = \frac{\alpha M(0) - \beta}{M(0) - N(0)}. \]  
(19)

We shall further restrict our attention to the amplitudes resulting after a complete cycle. Then we may set \( F/\epsilon = i\gamma \) and \( G/\epsilon = -i\gamma \) in (17) and write

\[ I_1 = \gamma_{11}e^{i\gamma} + \gamma_{12}e^{-i\gamma}, \]
\[ I_2 = \gamma_{21}e^{i\gamma} + \gamma_{22}e^{-i\gamma}, \]  
(20)

where the phase \( \gamma \) is computed from (16) and the coefficients \( \gamma_{ij} \) are extracted from (17) using as input the WKB solution and taking into account simplifications due to periodicity, e.g., \( M(T) = M(0) \) and \( N(T) = N(0) \).

In order to obtain expressions for the coefficients \( \gamma_{ij} \) which are as explicit as is the phase \( \gamma \) in (16) we proceed as follows. The zeroth order contribution is calculated by setting \( F'_0 = \frac{1}{2}B \) and \( G'_0 = -\frac{1}{2}B \) in (18) and by dropping higher-order terms. We thus find that \( M(0) = (\tan \frac{\theta_0}{2})e^{i\phi} \) and \( N = -\left(\cot \frac{\theta_0}{2}\right)e^{i\phi} \) which must be evaluated at \( t = 0 \) to obtain the constants in (19) and at \( t = T \) for a subsequent evaluation of the coefficients in (17). Because \( \theta(0) = \theta_0 = \theta(T) \) and \( \phi(0) = 0 = \phi(T) \), we find that \( M(0) = \beta/\alpha = M(T) \) and \( N(0) = -\alpha/\beta = N(T) \) using the notation of (18). Hence \( \mu = \alpha, \nu = 0 \) and \( \gamma_{11} = 1, \gamma_{12} = \gamma_{21} = \gamma_{22} = 0 \). This is the expected result indicating that transitions do not occur in leading order and the wavefunction simply acquires a phase \( \gamma \). However there is an important question here concerning the number of terms that must be included in (16). Putting it differently, the question is whether or not the subleading or Berry phase can be included consistently with absence of transitions. As we shall see shortly, the transition probability is of order \( \epsilon^2 \), so the Berry phase can be consistently included to leading order. More generally, if \( n \) terms are retained in the WKB series of the phase \( \gamma \), it is sufficient to calculate \( n-1 \) terms in the expansion of the \( \gamma_{ij} \).

Therefore, to exploit all three terms in the expansion of \( \gamma \) displayed in (16), one should only include the next-to-leading contribution to the \( \gamma_{ij} \). We thus keep in (18) terms proportional to \( F'_1 \) and \( G'_1 \) and proceed with a consistent expansion in \( \epsilon \). The required input is given by equations (11). A reasonably straightforward calculation yields the simple result

\[ \gamma_{11} = 1 - \frac{1}{4B^2}\left(\dot{\theta}^2 + \sin^2\theta \dot{\phi}^2\right), \]
\[ \gamma_{12} = \frac{1}{4B^2}\left(\dot{\theta}^2 + \sin^2\theta \dot{\phi}^2\right), \]
\[ \gamma_{21} = \frac{i}{2B}\left(\dot{\theta} + i \sin \theta \dot{\phi}\right), \]
\[ \gamma_{22} = -\frac{i}{2B}\left(\dot{\theta} + i \sin \theta \dot{\phi}\right). \]  
(21)

Note that we have restored the original time variable, using a dot instead of a prime for differentiation and suppressing the parameter \( \epsilon \). The relative orders of magnitude are made apparent in (16) and (21) by the corresponding powers of \( 1/B \). We have also suppressed a subscript in (21) which would indicate that the functions involved must be evaluated at \( t = 0 \) or \( t = T \). The final result applies for any choice of origin on the contour \( C \). The amplitudes \( \gamma_{ij} \) are defined by the instantaneous values of the field at the origin while the history of the cycle is coded in the phase \( \gamma \). However the latter is no longer an overall phase because of the inclusion of a nonadiabatic corrections.

Equations (16) and (21) inserted in (20) complete our WKB solution including the first nonadiabatic correction. Perhaps we should add that the unitarity relation \( |I_1|^2 + |I_2|^2 = 1 \) can be verified explicitly to within higher-order corrections, as is usual in perturbative calculations, and that the probability for spin flip after
a complete cycle is given by

\[ |I_2|^2 = \frac{1}{B^2} \left( \dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2 \right) \sin^2 \gamma = \frac{1}{B^2} \left( \frac{dn}{dt} \right)^2 \sin^2 \gamma, \tag{22} \]

where \( n = B/B \) is the unit vector along the magnetic field. It is also amusing to apply the preceding general results for a specific choice of the field for which an exact solution has been known for 50 years \([4,5]\) and contained the Berry phase. A field of constant magnitude \( B \) precesses around the \( z \)-axis at constant angle \( \theta \) with constant frequency \( \omega (\phi = -\omega t) \). Inserting this information in (16) and (21) we obtain

\[ \gamma = \frac{\pi}{\xi} \left[ 1 + (1 - \cos \theta) \xi + \frac{1}{2} \sin^2 \theta \xi^2 \right] \]

\[ \gamma_{11} = 1 - \frac{1}{4} \sin^2 \theta \xi^2, \]

\[ \gamma_{12} = \frac{1}{4} \sin^2 \theta \xi^2, \]

\[ \gamma_{21} = -\gamma_{22} = \frac{1}{2} \sin \theta \xi \]

where \( \xi = \omega/B \) is a dimensionless counterpart of the small parameter \( \epsilon \). The exact solution gives

\[ \gamma = \frac{\pi}{\xi} (\xi + R), \]

\[ R \equiv \left( 1 - 2 \xi \cos \theta + \xi^2 \right)^{1/2}, \]

\[ \gamma_{11} = \frac{1}{2} \left[ 1 - \frac{1}{R} (1 - \xi \cos \theta) \right], \]

\[ \gamma_{12} = \frac{1}{2} \left[ 1 - \frac{1}{R} (1 - \xi \cos \theta) \right], \]

\[ \gamma_{21} = -\gamma_{22} = \frac{\xi \sin \theta}{2R}, \]

and reproduces (23) after expansion in powers of \( \xi \). This concludes our explicit demonstration and we close with some general remarks:

(i) the integrand in the first term of (16) is manifestly invariant under rotations while the Berry phase is invariant only after the integration is performed. It is not difficult to see that under a rotation the density \( (1 - \cos \theta) \dot{\phi} \) transforms by picking up an additive total derivative which does not contribute to the integral. Actually the total derivative contains a logarithm which could produce a nonvanishing contribution if the rotation were such that the \( z \)-axis crossed the contour \( C \). However such a choice of the reference frame is obviously nongeneric, so the Berry phase is unambiguous. A related question is whether higher-order terms exhibit a similar behavior. The integrand in the third term of (16) can be made manifestly invariant by using the identity \( \dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2 = n^2 \) stated after equation (22). On the other hand, we have calculated the next correction in equation (16):

\[ \frac{1}{4} \int_0^T \left[ \sin \theta \left( \ddot{\phi} - \dot{\theta} \dot{\phi} \right) - 2 \cos \theta \left( \dot{\theta}^2 + \frac{1}{2} \sin^2 \theta \dot{\phi}^2 \right) \dot{\phi} \right] \frac{dt}{B^2(t)}, \tag{25} \]

where the integrand cannot be written in a manifestly invariant form. The preceding pattern suggests that this alternating behavior persists in higher-order terms;

(ii) an important question is whether or not the WKB method can be generalized to other systems. The answer is clearly affirmative. A generalization to arbitrary spin \( s \neq \frac{1}{2} \) is not difficult for Hamiltonians that are linear in the spin operators \([4 - 7]\). A new calculation is required for systems having quadratic anisotropies. Anisotropies can occur when \( s > \frac{1}{2} \) and these are actually encountered in nuclear quadrupole resonance \([9]\):

\[ H = - \left[ \sum_a B_a(t) \mathcal{S}_a + \sum_{ab} \Omega_{ab}(t) \mathcal{Q}_{ab} \right], \tag{26} \]

Time dependence in the anisotropy constants \( \Omega_{ab} \) may be induced by sample rotation. In practice we have to solve a system of three linear equations for \( s = 1 \), four equations for \( s = \frac{3}{2} \), and so on. On eliminating all but one variable, we arrive at a third-order equation for \( s = 1 \), a fourth-order equation for \( s = \frac{3}{2} \), etc., all of which can be solved by the WKB method except that calculations become lengthier. It should be interesting to carry out an explicit calculation for (26) in view of possible level degeneracy, which may lead to new phenomena \([10]\), and the experimental work of reference \([9]\);

(iii) finally we make a remark about our use of a WKB approximation. Ordinarily WKB is used to obtain a semiclassical approximation to a quantum theory as an expansion in powers of the parameter \( \hbar \). Here we are not expanding in \( \hbar \) but rather in inverse powers of a long-time scale which in this problem is the period \( T \). WKB as it is used here is a generic tool for studying prob-
lems that involve two or more disparate physical scales, that is, problems exhibiting adiabatic behaviour.

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Note added: The issue of nonadiabatic corrections is addressed by a different method in a recent paper of Berry [Proc. R. Soc. A 414 (1987) 31] and in some related work of Garrison quoted in the above reference. In the interim, we have carried out a detailed WKB calculation of several nonadiabatic corrections for arbitrary spin. These results apply for a wide range of slowly varying magnetic fields, which are not necessarily periodic, and will be presented in a forthcoming publication.

References