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Non-adiabatic Berry phase for periodic Hamiltonians

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Abstract. Berry's formulation of the topological phase for periodic Hamiltonians is extended to the case of non-adiabatic evolution by proper choice of initial states. This restores a full parallel with the non-adiabatic formalism of Aharonov and Anandan for periodic orbits in projective Hilbert space. The Berry phase for the novel example of a single electron in a rigidly rotating octahedral environment is calculated using both this formalism and that used previously by Aharonov and Anandan and by Page.

1. Introduction

Since the discovery by Berry of the topological phase that bears his name, two approaches have commonly been used in its investigation. In the first (Berry 1984, Cheng and Fung 1989), an instantaneous eigenstate of $H(0)$ is adiabatically evolved from $t=0$ to $t=\tilde{t}$, where the Hamiltonian is cyclic, i.e. $H(\tilde{t})=H(0)$. In the second (Aharonov and Anandan 1987, Page 1987), one considers a closed path in projective Hilbert space, rather than in parameter space, and without reference to the Hamiltonian that generates it or to any choice of initial state. At first sight these approaches seem very different, the most significant difference being the use of the adiabatic approximation in the first, Aharonov and Anandan (1987) presenting the second method as the method of choice for going beyond the adiabatic approximation.

This apparent contrast may be considered as an artefact of the choice of initial state in the adiabatic approach. It is the choice of the initial state as an instantaneous eigenstate of $H(0)$ which forces Berry to use adiabatic evolution so as to guarantee a closed path in projective Hilbert space. We relax this restriction by choosing the initial state in such a way that, although not an eigenstate at $t=0$, it returns to itself (to within a phase) at time $\tilde{t}$, thereby ensuring a cyclic path in projective Hilbert space. Cheng and Fung (1989) also profess to link the two formulations, but insofar as these authors commit themselves to an initial state that is an eigenstate of $H(0)$, the cyclic behaviour which they discuss can arise only in the adiabatic case. We show later how a generalisation of their formulation corresponds to the present development.

Using our cyclic choice of initial state, we derive an explicit formula for the Berry phase in the case of evolution by a cyclic Hamiltonian, and discuss the region of the adiabatic limit.

2. Development

Consider a quantum mechanical system with d-dimensional Hilbert space $\mathscr{H}$ and Hamiltonian $\hat{H}$. By specifying some basis $\mathscr{B}=\{|n\rangle \,|\, n=1(1)d\}$, we may represent $\hat{H}$

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by a $d \times d$ matrix H, and a quantum state $|\phi\rangle$ by a column vector ϕ. An initial state $\phi(0)$ then evolves according to the matrix equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = -\mathrm{i}H\phi/\hbar. \tag{1}$$

In the case that H is $\tilde{t}$-periodic, i.e. $H(t+\tilde{t}) = H(t)$ for some $\tilde{t}$, and using Floquet's theorem, any fundamental matrix of the linear system of ordinary differential equations (1) has the form

$$U(t) = Z(t)\,\mathrm{e}^{\mathrm{i}Mt} \tag{2}$$

where Z and M are $d \times d$ matrices, M being constant and Z being $\tilde{t}$-periodic. (The factor i in the exponent is conventional at this point.) As the above notation suggests, we now consider exclusively the particular fundamental matrix $U(t)$ satisfying $U(0) = I$. As the time development of any initial state is then given by $\phi(t) = U(t)\phi(0)$, we see that $U(t)$ is simply the matrix representation of the time evolution operator $\hat{U}(t)$ in the basis $\mathcal{B}$, U is unitary and H and U are related by

$$\mathrm{i}\hbar\frac{\mathrm{d}U}{\mathrm{d}t} = HU. \tag{3}$$

Since $U(\tilde{t})$ is unitary and is equal to $\exp(\mathrm{i}M\tilde{t})$, M is Hermitian; since in addition $U(t)$ is unitary for all t, $Z(t)$ is unitary. $U(\tilde{t})$ has d linearly independent eigenvectors $\phi_m(0)$ with eigenvalues $\exp(\mathrm{i}\chi_m)$; χ_m is real since M is hermitian. If we choose one of the $\phi_m(0)$ as our initial state and write $\phi_m(t)$ for the evolved form $U(t)\phi_m(0)$, we get

$$\phi_m(\tilde{t}) = U(\tilde{t})\phi_m(0) = \exp(\mathrm{i}\chi_m)\phi_m(0). \tag{4}$$

Thus the initial states $\phi_m(0)$ each return to themselves after time $\tilde{t}$ (in the evolution associated with $H(t)$) up to a phase χ_m. The existence of a basis of $\mathcal{H}$ in which each basis state returns to itself up to a phase after a fixed time t' is general, depending only on the unitarity of $U(t')$ and is not dependent on the finite dimensionality of $\mathcal{H}$ nor the cyclicity of H†.

To calculate the Berry phase angle γ_m associated with the evolution of the initial state $\phi_m(0)$ we must calculate the dynamical phase δ_m given by

$$\delta_m = -\frac{1}{\hbar}\int_0^{\tilde{t}} \langle\phi_m(t)|H|\phi_m(t)\rangle\,\mathrm{d}t = -\frac{1}{\hbar}\int_0^{\tilde{t}} \langle\phi_m(0)|U^\dagger HU|\phi_m(0)\rangle\,\mathrm{d}t. \tag{5}$$

Now equations (2) and (3) give

$$U^\dagger HU = \mathrm{i}\hbar U^\dagger\frac{\mathrm{d}U}{\mathrm{d}t} \tag{6}$$

$$= \mathrm{e}^{-\mathrm{i}Mt}(\mathrm{i}\hbar Z^\dagger\dot{Z} - \hbar M)\,\mathrm{e}^{\mathrm{i}Mt}. \tag{7}$$

Since $\phi_m(0)$ is an eigenstate of $\exp(\mathrm{i}M\tilde{t})$ with eigenvalue $\exp(\mathrm{i}\chi_m)$, it is also an eigenstate of M with eigenvalue $\chi_m/\tilde{t}$. Equations (5) and (7) give

$$\langle\phi_m(t)|H|\phi_m(t)\rangle = \langle\phi_m(0)|(\mathrm{i}\hbar Z^\dagger\dot{Z} - \hbar\chi_m/\tilde{t})|\phi_m(0)\rangle \tag{8}$$

$$\delta_m = -\frac{1}{\hbar}\int_0^{\tilde{t}} \langle\phi_m(0)|\mathrm{i}\hbar Z^\dagger\dot{Z}|\phi_m(0)\rangle\,\mathrm{d}t + \chi_m. \tag{9}$$

† In a finite basis of dimension d it is obvious that there are d cyclic states, since a $d \times d$ unitary matrix has d eigenvectors.

Hence Berry's phase is given by

$$\gamma_m = \chi_m - \delta_m = \mathrm{i}\int_0^{\tilde{t}} \langle m(t)|\dot{m}(t)\rangle \,\mathrm{d}t \tag{10}$$

where $|m(t)\rangle \equiv Z|\phi_m(0)\rangle$.

This is of similar form to equation (2.21) of Cheng and Fung (1989), and similarities can be traced in Berry (1984). Cheng and Fung take the eigenstate $|n(0)\rangle$ of $H(0)$ as the initial state, and decompose U as $\boldsymbol{U}\mathbb{R}$, $\mathbb{R}$ being chosen to be diagonal in the basis $|n(0)\rangle$ so as to facilitate the calculation of U; $|n(0)\rangle$ evolves into $|n(t)\rangle$ under $\boldsymbol{U}$. They distinguish between the (invariant) topological phase angle γ_T and the (partially conventional, as also discussed by Giavarini *et al* 1989) Berry phase angle γ_B in their problem: $\gamma_T = \gamma_B + \alpha$.

To extend their formulation to include the evolution of cyclic initial states, we need only to choose $\mathbb{R}$ to be diagonal in the new basis $|\{\phi_n(0)\}\rangle$; the relationships between the phases of the evolved states are $|\phi_n(\tilde{t})\rangle = \exp(\mathrm{i}[\gamma_D + \gamma_B])|n(\tilde{t})\rangle$, $|n(\tilde{t})\rangle = \mathrm{e}^{\mathrm{i}\alpha}|n(0)\rangle$, where the dynamical phase angle is γ_D. If now the breakdown between $\boldsymbol{U}$ and $\mathbb{R}$ is constrained as in equation (2) ($\boldsymbol{U} \to \boldsymbol{Z}, \mathbb{R} \to \mathrm{e}^{\mathrm{i}Mt}$), then $\alpha = 0$, and the Berry phase is the topological phase.

Differentiating equation (2) with respect to time, using equation (3), and substituting $t = 0$, we find

$$M = -H(0)/\hbar + \mathrm{i}\dot{Z}(0) \tag{11}$$

which gives a simple method of calculating M as well as the possibility of a perturbative approach to its calculation for the case of almost adiabatic evolution (Berry 1987).

3. Examples

3.1. Time-independent case

When H is time independent, $U = \exp(-\mathrm{i}Ht/\hbar)$ and we may take $M = -H/\hbar$, $Z = I$. The initial states are eigenstates of H and the Berry phase vanishes.

3.2. Adiabatic evolution

In the original example of Berry (1984), $H = H(\boldsymbol{R}(t))$, where $\boldsymbol{R}(t)$ is a closed path C in some parameter space: $\boldsymbol{R}(t) = \boldsymbol{R}(0)$. By the adiabatic theorem, $\phi_m(t)$ is an instantaneous eigenstate of $H(t)$ with eigenvalue $E_m(t)$:

$$H\phi_m(t) = E_m(t)\phi_m(t). \tag{12}$$

Now $\phi_m(t) = Z\,\mathrm{e}^{\mathrm{i}Mt}\phi_m(0)$, and $\phi_m(0)$ is an eigenstate of $\mathrm{e}^{\mathrm{i}Mt}$ with eigenvalue $\exp(\mathrm{i}\chi_m t/\tilde{t})$, so that

$$HZ\phi_m(0) = E_m(t)Z\phi_m(0). \tag{13}$$

Since $Z|\phi_m(0)\rangle = |m(t)\rangle$, $|m(t)\rangle$ is an instantaneous eigenfunction of H with eigenvalue $E_m(t)$. Now $|m(\tilde{t})\rangle = Z(\tilde{t})|\phi_m(0)\rangle = |\phi_m(0)\rangle = |m(0)\rangle$, so that $|m(t)\rangle$ is single valued and may be written $|m(\boldsymbol{R}(t))\rangle$. Thus $\mathrm{d}|m(t)\rangle/\mathrm{d}t = \nabla_R|m(\boldsymbol{R})\rangle\,\mathrm{d}\boldsymbol{R}/\mathrm{d}t$, and changing variable from t to $\boldsymbol{R}$, we obtain Berry's result:

$$\gamma_m = \mathrm{i}\oint \langle m(\boldsymbol{R})|\nabla_R m(\boldsymbol{R})\rangle \,\mathrm{d}\boldsymbol{R}. \tag{14}$$

3.3. Rigid rotation in a two-dimensional system

We consider a Jahn-Teller active system, with two or more quasimolecular electronic states which are degenerate when the molecule has its full symmetry, and which are coupled to a normal mode of the complex whose distortions break the degeneracy.

Mead (1980, 1983) has discussed the non-trivial 'molecular Aharonov-Bohm' phase change arising in the Born-Oppenheimer electronic wavefunctions of such a system under a cyclic excursion in the normal mode; Berry (1984) has already indicated the relevance of this work to the Berry phase. For applications of the concept of Berry phase *per se* in such systems, see O'Brien (1989) and Ham (1987).

We now consider a new way of generating a cyclic wavefunction and an allied topological phase, not as the result of a cyclic evolution of a normal coordinate, but as the result of a symmetry operation of the molecular point group G. For definiteness, we consider an octahedral molecule, and as symmetry operation O we take a $\frac{1}{2}\pi$ rotation about one of the fourfold axes, say z.

The degenerate members of any electronic level transform as partners under some irrep (unitary irreducible representation) of G, and will in general be mixed under a symmetry operation O. Because of the irreducible nature of the representation, it is only in an appropriate choice of basis, itself dependent on the choice of symmetry operation, that this mixture will become a diagonal matrix. The formulation of Aharonov and Anandan (1987) is adaptable to this problem, since there is cyclic evolution in projective Hilbert space. The analogous formulation of Berry requires the definition of a closed path in a parameter space, which must therefore be chosen not as the space $\mathcal{M}$ of all orientations of the octahedron, but the factor space $\mathcal{M}/G$ of all physically distinguishable orientations.

There are several methods for calculating the analogue to the Berry phase.

Method 1. Brute force. Let the required change in orientation be generated by rotation at constant angular velocity ω for a time $\tilde{t} = \pi/2\omega$. The Hamiltonian H is given by $H(t) = T + R(\omega t)V$, where T and V are the kinetic and potential energy operators for the original system and where $R(\theta)$ rotates coordinates by the time-dependent angle θ about the z axis. (For the relationship between rotations and the conventionality of the Berry phase, see Giavarini *et al* (1989) and references therein.) We consider the evolution of one initial state of the form

$$\psi(0) \equiv \alpha\psi_+(0) + \beta\psi_-(0) \tag{15}$$

where $\psi_\pm(t) \equiv R(\omega t)\psi_\pm(0)$ and are instantaneous eigenstates of $H(t)$ with (time-independent) eigenvalues $E_\pm$. In the SO_3-SO_2 basis $\psi_\pm(0)$ are given by $\psi_\pm(0) \equiv \mp(|2\ 2\rangle \pm |2\ -2\rangle)/\sqrt{2}$. We note that as $R(\omega t)|lm\rangle = e^{im\omega t}|lm\rangle$,

$$\psi_\pm(t) = \cos 2\omega t\psi_\pm(0) - i \sin 2\omega t\psi_\mp(0).$$

By direct substitution we may verify with some labour that the initial state (equation 15) evolves into

$$\psi(t) = \exp(-iEt/2\hbar)[\{\alpha \cos\theta t + i[-\Delta\alpha/(2\hbar\theta) + 2\omega\beta/\theta] \sin\theta t\}\psi_+(t) + \{\beta \cos\theta t + i[\Delta\beta/(2\hbar\theta) + 2\omega\alpha/\theta] \sin\theta t\}\psi_-(t)] \tag{16}$$

where $\Delta \equiv E_+ - E_-$, $E \equiv E_+ + E_-$, and $\theta \equiv [\Delta^2/(4\hbar^2) + 4\omega^2]^{1/2}$. It is easily seen that cyclic evolution is obtained for the choice

$$\frac{\beta}{\alpha} = \mp\frac{\theta}{2\omega} + \frac{\Delta}{4\hbar\omega} \tag{17}$$

up to the overall phase $e^{i\chi}$, where

$$\chi = \pi(1 \mp \theta/2\omega - E/4\hbar\omega) \tag{18}$$

for this choice the solution of equation (16) becomes

$$\psi(t) = \exp(\mp i\theta t)\exp(-iEt/2\hbar)[\alpha\psi_+(t) + \beta\psi_-(t)]. \tag{19}$$

Using the relationships $\alpha^2 = \frac{1}{2} \pm \Delta/4\hbar\theta$ and $\alpha\beta = \mp\omega/\theta$ (where α is assumed real), we may readily calculate the dynamical phase

$$\delta = -\int_0^{\tilde{t}} \langle\psi(t)|H(t)|\psi(t)\rangle \, dt/\hbar = -E\pi/(4\hbar\omega) \mp \Delta^2\pi/(8\hbar^2\theta\omega)$$

and obtain the Berry phase

$$\gamma = \pi \mp 2\pi\omega/\theta. \tag{20}$$

Method 2. Geometrical. Using the projective Hilbert space method in the terminology of Page (1987), we work in the two-dimensional Hilbert space spanned by the set $\{\psi_+(0), \psi_-(0)\}$ and with the general member $Z_+\psi_+(0) + Z_-\psi_-(0)$, with the corresponding one-dimensional projective Hilbert space parametrised by the coordinate $\lambda = Z_+/Z_-$. In terms of this coordinatisation, the Berry phase is given by $\gamma = \oint A$ where

$$A = \frac{i}{2}\frac{\bar{\lambda}\, d\lambda - \lambda\, d\bar{\lambda}}{1 + \bar{\lambda}\lambda}$$

and the integral is round the closed path C followed by the system in projective Hilbert space. In our case, and on C, we have

$$\lambda = \frac{\alpha\cos 2\omega t - i\beta\sin 2\omega t}{\beta\cos 2\omega t - i\alpha\sin 2\omega t} \qquad A(t) = -\frac{2\omega(\alpha^2 - \beta^2)\alpha\beta\cos 4\omega t\, dt}{\beta^2\cos^2\omega t + \alpha^2\sin^2\omega t}$$

and hence $\gamma = \int_0^{\tilde{t}} A(t)\, dt = \pi(1 + 2\alpha\beta)$, in agreement with equation (20).

Method 3. Cyclic. As an application of the formalism of section 2, we may use the full solution $\psi(t)$ in the $\psi_\pm(0)$ basis to write $\psi(t) = U(t)\binom{\alpha}{\beta}$, where

$$U(t) = \exp(-iEt/2\hbar)\begin{pmatrix} cc' + 2\omega ss'/\theta - i\Delta cs'/(2\hbar\theta) & -isc' + 2\omega ics'/\theta + \Delta ss'/(2\hbar\theta) \\ -isc' + 2\omega i/\theta - \Delta ss'/(2\hbar\theta) & cc' + 2\omega ss'/\theta + i\Delta cs'/(2\hbar\theta) \end{pmatrix} \tag{21}$$

where $c \equiv \cos 2\omega t$, $s \equiv \sin 2\omega t$, $c' \equiv \cos\theta t$ and $s' \equiv \sin\theta t$. We now decompose this in the form of equation (2), with Z containing the periodic time dependence and M being independent of t. Inspection suggests the $\tilde{t}$-periodic form

$$Z = \exp(-2i\omega t)\begin{pmatrix} c & -is \\ -is & c \end{pmatrix}$$

and this in turn gives the (as desired) time-independent expression

$$M = \begin{pmatrix} 2\omega - (E + \Delta)/2\hbar & 2\omega \\ 2\omega & 2\omega - (E - \Delta)/2\hbar \end{pmatrix}$$

either by using equation (11) with the form

$$H = \tfrac{1}{2}\begin{pmatrix} E + \Delta\cos 4\omega t & +i\Delta\sin 4\omega t \\ -i\Delta\sin 4\omega t & E - \Delta\cos 4\omega t \end{pmatrix}$$

or by transforming $Z^{\dagger}U$ to a basis in which it is diagonal, taking logarithms of the eigenvalues, and transforming back again. In the first method the original guess for Z is verified by constructing U from equation (2); in the second method, the diagonal form of M is $M_d = SMS^{\dagger} = \mathrm{diag}(2\omega - E/2\hbar + \theta,\ 2\omega - E/2\hbar - \theta)$, where $S \equiv \begin{pmatrix} \eta_- & \eta_+ \\ -\eta_+ & \eta_- \end{pmatrix}$, $\eta_\pm \equiv (\frac{1}{2} \pm \Delta/4\hbar\theta)^{1/2}$. These results imply agreement with our earlier calculation both in the overall phase shift of χ (equation (18)) and in the ratio β/α of eigenvector components in $\phi(0)$ of equation (17). $Z^{\dagger}\dot{Z}$ is then readily seen to be $-2i\omega\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, so that $\langle\phi(0)|Z^{\dagger}\dot{Z}|\phi(0)\rangle = -2i\omega(1 \mp 2\omega/\theta)$ and hence the Berry phase (from equation (10)) again in agreement with equation (20).

4. Discussion

The method is general, and certainly not restricted to the above application. We have an unambiguous prescription for the kind of decomposition of U envisaged by Cheng and Fung (1989), provided one uses cyclic states rather than eigenstates, which lends itself to direct calculational methods. It is necessary to determine the nature of the cyclic states, and the above method might be improved if a direct method for calculating $Z(t)$ were developed. A knowledge of Z would also (from equation (12)) help in a discussion of amost adiabatic evolution (Berry 1987).

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Note added in proof. The method described above can be combined with a similar decomposition of another fundamental matrix (Shirley 1965) to give a much simplified calculation of Z and so of the Berry phases. We report this elsewhere.

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