On geometric phases and dynamical invariants

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Abstract. A formalism is developed for calculating Berry phases for non-adiabatic time-periodic quantum systems when a dynamical invariant is known. It is found that, when the invariant is periodic and has a non-degenerate spectrum, this method allows a convenient way to obtain generalized Berry phases and the proper cyclic initial states. The method is applied to the generalized harmonic oscillator and the two-level system, where the invariant operators are explicitly constructed. Formulae for the conventional Berry's phases are readily obtained by taking the adiabatic limit of the exact results.

1. Introduction

Recently, there has been considerable interest in Berry's phase for time-periodic quantum systems, first discussed by Berry [1] in an adiabatic context and later extended to non-adiabatic and non-periodic motion [2, 3].

In a recent paper, Moore and Stedman [4] showed that by proper choice of the initial states Berry's formulation can be extended in a general way to non-adiabatic time evolution. Their treatment is based on the knowledge of the exact evolution operator $\hat{U}(t)$. Furthermore, an operator decomposition for $\hat{U}(t)$ was developed to calculate the initial states and their associated Berry phases. Some remarks can be made at this point. (i) It is well known that even for simple systems the construction of the exact evolution operator is in itself a difficult task. (ii) The decomposition for $\hat{U}(t)$ and the subsequent calculation of the Berry phase is in most cases non-trivial.

The purpose of this paper is to elucidate the intimate connection between dynamical invariants and generalized Berry phases. If an invariant operator for the system is known, then there is a convenient way to construct both the cyclic initial states and their associated Berry phases. The method avoids the use of the evolution operator $\hat{U}(t)$ and is much simpler to apply than the one suggested previously in [4].

In section 2, the formalism is developed based on the existence of a dynamical invariant, which is constructed using the dynamical Lie algebra generated by the Hamiltonian [5, 6]. Sections 3 and 4 present detailed applications to two different models: the generalized harmonic oscillator and the two-level system. In the first case, the well known (generalized) Lewis invariant [7, 8] is rederived. Finally, in section 5, the adiabatic limit is taken in order to compare our results with conventional ones.

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2. Formalism

Consider a quantum system whose Hamiltonian $\hat{H}(t)$ is T-periodic. An initial state $|\phi(0)\rangle$ will evolve as $|\phi(t)\rangle = \hat{U}(t)|\phi(0)\rangle$, where the evolution operator $\hat{U}(t)$ is the solution of the Schrödinger equation

$$i\hbar \frac{d\hat{U}(t)}{dt} = \hat{H}(t)\hat{U}(t). \tag{2.1}$$

As we have mentioned above, Moore and Stedman [4] extended Berry's formulation of the geometric phase for time-periodic Hamiltonians to the case of non-adiabatic evolution. In their formalism, the evolution operator $\hat{U}(t)$ is decomposed in a Floquet product form

$$\hat{U}(t) = \hat{Z}(t)\,e^{i\hat{M}t} \tag{2.2}$$

where $\hat{Z}(t)$ is unitary and T-periodic and $\hat{M}$ is Hermitian and constant. The initial condition $\hat{U}(0) = \hat{1}$ implies $\hat{Z}(0) = \hat{Z}(T) = \hat{1}$. This decomposition is not unique [9].

The cyclic initial states $|\phi_m(0)\rangle$ for the evolution in question are precisely the eigenstates of $\hat{M}$, as can be seen from

$$|\phi_m(T)\rangle = \hat{U}(T)|\phi_m(0)\rangle = e^{i\chi_m}|\phi_m(0)\rangle \tag{2.3}$$

i.e. each state returns to itself after a time T, up a phase χ_m. As this is the usual condition for the so-called Floquet states [10, 11] we can relate the phase χ_m to the quasi-energies ϵ_m associated with the Floquet states: $\chi_m = -\epsilon_m T/\hbar$. According to Moore and Stedman [4] the non-adiabatic geometric phases associated with the initial states $|\phi_m(0)\rangle$ are

$$\gamma_m = i \int_0^T \langle\phi_m(0)|\hat{Z}^\dagger(t)\dot{\hat{Z}}(t)|\phi_m(0)\rangle\,dt \tag{2.4}$$

where the dot denotes differentiation with respect to t.

In what follows, we assume that the system possesses a dynamical invariant $\hat{I}(t)$

$$\frac{d\hat{I}(t)}{dt} = \frac{\partial\hat{I}(t)}{\partial t} + \frac{1}{i\hbar}[\hat{I}(t),\hat{H}(t)] \equiv 0 \qquad \hat{I}^\dagger(t) = \hat{I}(t) \tag{2.5}$$

which is one of a complete set of commuting observables, so that there is a complete set of eigenstates of $\hat{I}(t)$. Furthermore, $\hat{I}(t)$ should not involve time-derivative operations. The invariants with which we treat the generalized harmonic oscillator and the two-level system satisfy these requirements. For such a system, Lewis and Riesenfeld [8] provide a way to construct the solution of the Schrödinger equation

$$|\phi(t)\rangle = \sum_{n,k} c_{nk}|\psi_{nk}(t)\rangle \qquad |\psi_{nk}(t)\rangle = e^{i\alpha_{nk}(t)}|n,k,t\rangle \tag{2.6}$$

where the c_{nk} do not depend on t. The phases $\alpha_{nk}(t)$, called Lewis phases, are determined by

$$\hbar\dot{\alpha}_{nk}(t) = \left\langle n,k,t\left|i\hbar\frac{\partial}{\partial t} - \hat{H}(t)\right|n,k,t\right\rangle \tag{2.7}$$

where $|n,k,t\rangle$ are the eigenstates of $\hat{I}(t)$ with eigenvalues λ_n. As $\hat{I}(t)$ is an invariant operator, its eigenvalues do not depend on time.

We now show how to relate the two formalisms. Assuming that the invariant $\hat{I}(t)$ is T-periodic and that its eigenvalues are non-degenerate, $|n,k,t\rangle = |n,t\rangle$, then the eigenstates of $\hat{I}(t)$ satisfy

$$|n,T\rangle = |n,0\rangle \tag{2.8}$$

and a particular Lewis and Riesenfeld solution $|\psi_n(t)\rangle$ after one period is

$$\hat{U}(T)|\psi_n(0)\rangle = |\psi_n(T)\rangle = e^{i\alpha_n(T)}|n, 0\rangle = e^{i\alpha_n(T)}|\psi_n(0)\rangle \tag{2.9}$$

(cf (2.6)). Thus, $|\psi_n(0)\rangle$ are the eigenstates of $\hat{U}(T)$ with eigenphases $\alpha_n(T)$. In other words, the Lewis and Riesenfeld solutions $|\psi_n(t)\rangle$ are the Floquet states with associated quasi-energies $\epsilon_n = -\alpha_n(T)\hbar/T$. The quasi-energy spectrum, being determined by (2.7), is in one-to-one relation with the spectrum of the invariant.

Following the procedure of Moore and Stedman, we can choose $|\psi_n(0)\rangle$ as the cyclic initial states. At this point, one can avoid the use of the evolution operator in the following way: writing $\hat{Z}(t) = \hat{U}(t)\,e^{-i\hat{M}t}$, the states $|\Psi_n(t)\rangle = \hat{Z}(t)|\psi_n(0)\rangle$ in (2.4) are

$$|\Psi_n(t)\rangle = \hat{U}(t)\,e^{-i\hat{M}t}|\psi_n(0)\rangle = e^{-i\alpha_n(T)t/T}|\psi_n(t)\rangle \tag{2.10}$$

and

$$i\langle \Psi_n(t)|\dot{\Psi}_n(t)\rangle = \alpha_n(T)/T - \dot{\alpha}_n(t) + i\langle n, t|\dot{n}, t\rangle \tag{2.11}$$

from which we obtain, by inserting into equation (2.4), the geometric phase

$$\gamma_n(T) = i\int_0^T \langle n, t|\dot{n}, t\rangle\, dt \tag{2.12}$$

for these initial states. Now, let us make some remarks. As pointed out in the introduction, the formalism of Moore and Stedman [4] is based on the assumption of the knowledge of $\hat{U}(t)$ and furthermore it is necessary to find $\hat{Z}(t)$. The problem of finding the exact evolution operator of a system is frequently a difficult task, and even if it is known the decomposition involved to obtain $\hat{Z}(t)$ is laborious. But, if an invariant can be found that satisfies the following conditions:

(i) the eigenstates $|n, t\rangle$ of $\hat{I}(t)$ are a complete set,
(ii) $\hat{I}(t)$ does not involve time-derivative operators,
(iii) the invariant $\hat{I}(t)$ is T-periodic,
(iv) its eigenvalues λ_n are non-degenerate,

the cyclic initial states are given by the particular Lewis and Riesenfeld solutions $|\psi_n(0)\rangle$, and the geometric phases can be easily calculated from (2.12) rather than from (2.4).

In what follows, we show that it is in principle possible to find such an invariant operator for systems whose Hamiltonians can be written as

$$\hat{H}(t) = \sum_{i=1}^N h_i(t)\hat{\Gamma}_i \tag{2.13}$$

where the set of operators $\{\hat{\Gamma}_1, \ldots, \hat{\Gamma}_N\}$ generates a dynamical algebra, which is closed under the action of the commutator

$$[\hat{\Gamma}_i, \hat{\Gamma}_j] = \sum_{k=1}^N C_{ij}^k\,\hat{\Gamma}_k \tag{2.14}$$

with structure constants C_{ij}^k. The $\hat{\Gamma}_i$ do not explicitly depend on time and the coefficients $h_i(t)$ are T-periodic in the case considered here.

We seek an invariant operator as a member of the algebra

$$\hat{I}(t) = \sum_{i=1}^N a_i(t)\hat{\Gamma}_i\,. \tag{2.15}$$

The invariant condition (2.5) leads to a system of linear first-order differential equations, which in matrix form reads

$$\dot{a}(t) = A(t) \cdot a(t) \tag{2.16}$$

where $a(t)$ is a N-dimensional column vector, whose components $a_k(t)$ are real because the invariant is Hermitian, and $A(t)$ is a T-periodic matrix with elements

$$A_{ik}(t) = -\frac{1}{i\hbar} \sum_j C_{ij}^k h_j(t). \tag{2.17}$$

The system of equations (2.16) are here called auxiliary equations and *any* particular solution of it may be used to construct an invariant operator of the form given by (2.15).

It is worth noting that a serious problem in dealing with equations with periodic coefficients is the lack of a general method to obtain their solutions. Each equation requires special study and whole books have been devoted to some of them [11, 12].

However, in the case of having them, $a_k(T)$ can be determined from $a_k(0)$. Then the periodicity condition on the invariant operator leads to N equations in $a_k(0)$, which means that by appropriate choice of the initial values $a_k(0)$ we can (in principle) *switch* the desired condition on the invariant to be fulfilled.

In what follows we apply the formalism to two important model systems: the generalized harmonic oscillator and the two-level system.

3. Generalized harmonic oscillator

The Hamiltonian for the generalized harmonic oscillator is

$$\hat{H}(t) = \tfrac{1}{2} [X(t) \hat{q}^2 + Y(t) (\hat{p}\hat{q} + \hat{q}\hat{p}) + Z(t) \hat{p}^2] \tag{3.1}$$

where $\hat{q}$ and $\hat{p}$ are the position and momentum operators satisfying the canonical commutation rule $[\hat{p}, \hat{q}] = i\hbar$ and $R(t) = (X(t), Y(t), Z(t))$ is a time-dependent, real-valued parameter vector. When R is fixed, $\hat{H}$ describes a harmonic oscillator with frequency $w = (XZ - Y^2)^{1/2}$, provided $XZ - Y^2 > 0$ and one can denote $w(t)$ as the instantaneous frequency.

The system (3.1) has a well known dynamical invariant, the so-called (generalized) Lewis invariant [13]

$$\hat{I}(t) = \frac{1}{2} \left\{ \frac{\hat{q}^2}{r^2} + \left[r \left(\hat{p} + \frac{Y}{Z} \hat{q} \right) - \frac{\dot{r}}{Z} \hat{q} \right]^2 \right\} \tag{3.2}$$

with $r(t) = Z^{1/2} \rho(t)$, where the auxiliary function $\rho(t)$ is a solution of the so-called Milne equation [14, 15]

$$\ddot{\rho}(t) + \Omega_h^2(t) \rho(t) = \frac{1}{\rho^3(t)} \tag{3.3}$$

with

$$\Omega_h^2(t) = w^2 + \frac{1}{2} \frac{\ddot{Z}}{Z} - \frac{3}{4} \left(\frac{\dot{Z}}{Z} \right)^2 - Z \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{Y}{Z} \right). \tag{3.4}$$

A short derivation as well as a discussion of the T-periodic solutions of (3.3) can be found in appendix A. In the most often discussed simplified case $Z = \text{constant} = 1$, and $Y = 0$, the invariant (3.2) reduces to the result derived by Lewis [7, 8].

As is usual for harmonic oscillators, we define (time-dependent) raising and lowering operators

$$\hat{a} = \frac{1}{\sqrt{2\hbar}} \left\{ \frac{\hat{q}}{r} + i\left[r\left(\hat{p} + \frac{Y}{Z}\hat{q} \right) - \frac{\dot{r}}{Z}\hat{q} \right] \right\}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar}} \left\{ \frac{\hat{q}}{r} - i\left[r\left(\hat{p} + \frac{Y}{Z}\hat{q} \right) - \frac{\dot{r}}{Z}\hat{q} \right] \right\}$$

(3.5)

so that $[\hat{a}, \hat{a}^\dagger] = \hat{1}$. Then the invariant operator can be written as $\hat{I}(t) = (\hat{a}^\dagger\hat{a} + \frac{1}{2})\hbar$ and its eigenstates are the normalized eigenstates $|n, t\rangle$ of the number operator $\hat{a}^\dagger\hat{a}$, with non-degenerate eigenvalues $\lambda_n = (n + \frac{1}{2})\hbar$, $n = 0, 1, 2, \ldots$. The relative phases of two eigenstates $|n, t\rangle$ are fixed by

$$\hat{a}|n, t\rangle = \sqrt{n}\,|n, t\rangle \qquad \hat{a}^\dagger|n, t\rangle = \sqrt{n + 1}\,|n + 1, t\rangle$$

(3.6)

except one, say the ground-state phase, which is still arbitrary. For this example it is convenient to first find the Lewis phase $\alpha_n(t)$. We need the diagonal matrix elements (see (2.7)) of $\hat{H}(t)$ and $i\hbar\,\partial/\partial t$, where the latter ones will provide the generalized Berry phases we are looking for. In what follows, we denote $|n, t\rangle = |n\rangle$ for convenience.

From (3.1) and (3.6) we obtain

$$\langle n|\,\hat{H}\,|n\rangle = \frac{1}{2}\left\{ \frac{(XZ - Y^2)}{Z}r^2 + \frac{Z}{r^2} + \frac{\dot{r}^2}{Z} \right\}(n + \tfrac{1}{2})\hbar$$

(3.7)

and, using (3.6) and taking the convenient scalar product, we find

$$\left\langle n + 1\left| \frac{\partial\hat{a}^\dagger}{\partial t} \right|n\right\rangle + (n + 1)^{1/2}\left\langle n\left| \frac{\partial}{\partial t} \right|n\right\rangle = (n + 1)^{1/2}\left\langle n + 1\left| \frac{\partial}{\partial t} \right|n + 1\right\rangle.$$

Evaluating the first term with the help of (3.5) we have

$$\left\langle n\left| \frac{\partial}{\partial t} \right|n\right\rangle = \left\langle 0\left| \frac{\partial}{\partial t} \right|0\right\rangle + n\frac{i}{2}\left\{ \frac{(XZ - Y^2)}{Z}r^2 - \frac{Z}{r^2} - \frac{\dot{r}^2}{Z} \right\}$$

(3.8)

and (2.7) thus yields

$$\alpha_n(T) = -\tfrac{1}{2}(n + \tfrac{1}{2})\int_0^T \frac{r^2 w^2 - \dot{r}^2}{Z}\,dt$$

(3.9)

where we have chosen a convenient phase, which we will call the Lewis gauge, for the ground state $|0\rangle$

$$\left\langle 0\left| \frac{\partial}{\partial t} \right|0\right\rangle = \frac{i}{4}\left(\frac{(XZ - Y^2)}{Z}r^2 - \frac{Z}{r^2} - \frac{\dot{r}^2}{Z} \right).$$

(3.10)

Then, using (3.8), (3.10) and (2.12), and assuming that a periodic or anti-periodic, real or purely imaginary solution $\rho_p(t)$ of (3.3) exists (see appendix A), the generalized Berry phase in the Lewis gauge is

$$\gamma_n(T) = -\tfrac{1}{2}(n + \tfrac{1}{2})\int_0^T \left(\frac{r_p^2 w^2 - \dot{r}_p^2}{Z} - \frac{Z}{r_p^2} \right)dt$$

(3.11)

with $r_p = Z^{1/2}\rho_p$.

4. Two-level system

For this system, the most general Hamiltonian operator can be written as

$$\hat{H}(t) = \tfrac{1}{2}[\, Z\,|1\rangle\langle 1| - Z\,|2\rangle\langle 2| + (X - iY)\,|1\rangle\langle 2| + (X + iY)\,|2\rangle\langle 1|\,] \qquad (4.1)$$

where $R(t) = (X(t), Y(t), Z(t))$ is time-dependent real vector parameter and $|1\rangle$ and $|2\rangle$ are the energy eigenstates for the $X = Y = 0$ problem, which we take as a fixed basis. In such a basis, $\hat{H}(t)$ can be represented by the matrix

$$H(t) = \tfrac{1}{2} R(t) \cdot \sigma \qquad (4.2)$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is a vector of the Pauli matrices. We need an invariant operator for this system. As $[\sigma_i, \sigma_j] = 2i\,\epsilon_{ijk}\,\sigma_k$ the Pauli matrices form a closed algebra. Thus, we can apply the ideas of section 2 to construct the invariant. Writing

$$I(t) = a(t) \cdot \sigma \qquad (4.3)$$

the real vector function $a = (a_1, a_2, a_3)$ satisfies the system (2.16) with

$$A(t) = \begin{pmatrix} 0 & -Z & Y \\ Z & 0 & -X \\ -Y & X & 0 \end{pmatrix}. \qquad (4.4)$$

In a shorter way, this equation can be written as

$$\hbar\,\dot{a} = R \wedge a. \qquad (4.5)$$

The eigenstates of $I(t)$ are

$$|\lambda\rangle = \sqrt{\frac{(\lambda + a_3)}{2\lambda}}\left[\,|1\rangle + \frac{a_1 + ia_2}{\lambda + a_3}\,|2\rangle\right] \qquad (4.6)$$

for each eigenvalue $\lambda = \pm|a|$. From (4.5) we can easily verify that $\dot{\lambda} = 0$.

Thus, from (4.1), (4.5) and (4.6), we can find the diagonal matrix elements of $H(t)$ and $i\hbar\,\partial/\partial t$, namely

$$\langle\lambda|\,H\,|\lambda\rangle = \frac{1}{2\lambda}\,R \cdot a$$

and

$$i\hbar\left\langle\lambda\left|\frac{\partial}{\partial t}\right|\lambda\right\rangle = \frac{1}{2\lambda}\frac{a_3 R \cdot a - Z\lambda^2}{\lambda + a_3}. \qquad (4.7)$$

Then, assuming a periodic solution $a_p(t)$ of the auxiliary vector equation (4.5) (see appendix B), the Lewis and the generalized Berry phases are

$$\alpha_\lambda(T) = -\frac{1}{2\hbar}\int_0^T \frac{Z\lambda + R \cdot a}{\lambda + a_3}\,dt \qquad (4.8)$$

and

$$\gamma_\lambda(T) = -\frac{1}{2\hbar}\int_0^T \frac{a_{3p} R \cdot a_p - Z\lambda^2}{\lambda + a_{3p}}\,dt. \qquad (4.9)$$

5. Adiabatic limit

In order to compare our results for the Berry phases with the conventional ones appearing in the literature, we have to consider the adiabatic limit. As usual, we write $d/dt = \varepsilon\,d/d\tau$ and expand the solution of the auxiliary equations in terms of the adiabatic parameter ε.

5.1. Harmonic oscillator

For this system, the expansion of the solution $\rho(t)$ of the auxiliary equation (3.3) is $\rho(t) = \rho_0(t) + \varepsilon\,\rho_1(t) + \varepsilon^2\,\rho_2(t) + \cdots$, which when inserted in (3.11) gives

$$\left(\frac{r^2 w^2 - \dot{r}^2}{Z} - \frac{Z}{r^2}\right) \simeq \varepsilon\, Z\left(\frac{Y}{Z}\right)' \rho_0^2 - \varepsilon^2 \left(\rho_0' + \frac{Z'}{2Z}\rho_0\right)^2 + \mathrm{O}(\varepsilon^3) + \cdots$$

where the primes denote a derivative with respect to τ and ρ_0^2 can be found from (3.3)

$$\rho_0^2 = (X Z - Y^2)^{-1/2}. \tag{5.1}$$

Thus, inserting into (3.11), the conventional (adiabatic) Berry phases are obtained up to first order in ε

$$\gamma_n(T) = -\tfrac{1}{2}\left(n + \tfrac{1}{2}\right) \int_0^T \frac{\dot{Y}Z - Y\dot{Z}}{Z(X Z - Y^2)^{1/2}}\,\mathrm{d}t \tag{5.2}$$

in agreement with the known result [16].

5.2. Two-level system

In this case, the expansions for the functions $a_i(t)$ of the auxiliary equations (4.5) are $a_i(t) = a_{i0}(t) + \varepsilon\,a_{i1}(t) + \varepsilon^2\,a_{i2}(t) + \cdots$, which when inserted into (4.9) yields

$$\frac{a_3\,R\cdot a - Z\lambda^2}{\lambda + a_3} \simeq \frac{a_{30}\,R\cdot a_0 - Z\lambda_0^2}{\lambda_0 + a_{30}\lambda_0} + \varepsilon\left\{ a_{31}\,R\cdot a_0 + a_{30}\,R\cdot a_1 \right.$$

$$\left. -2 Z\,a_0\cdot a_1 - (a_{30}\,R\cdot a_0 - Z\lambda_0^2)\left[\frac{a_0\cdot a_1}{\lambda_0^2} + \frac{a_{31} + a_0\cdot a_1/\lambda_0}{(a_{30} + \lambda_0)^2}\right] \right.$$

$$\left. \times (\lambda_0 + a_{30})^{-1}\lambda_0^{-1} \right\} + \mathrm{O}(\varepsilon^2) + \cdots \tag{5.3}$$

with $\lambda_0^2 = a_{10}^2 + a_{20}^2 + a_{30}^2$. From (4.5) we can evaluate the expansion coefficients a_{i0} and a_{i1} for $i = 1, 2, 3$. To compare with the results appearing in the literature we solve the special case of a latitude variation of the parameters $R(t)$ [17], i.e.

$$Z = B\cos\theta \qquad X = B\sin\theta\cos\omega t \qquad Y = B\sin\theta\sin\omega t \tag{5.4}$$

where B, θ and ω are real numbers. This leads to

$$a_{10} = C_1\tan\theta\cos\omega t\,\mathrm{e}^{-1/2\sin^2\theta}$$

$$a_{20} = C_1\tan\theta\sin\omega t\,\mathrm{e}^{-1/2\sin^2\theta} \tag{5.5}$$

$$a_{30} = C_1\,\mathrm{e}^{-1/2\sin^2\theta}$$

and

$$a_{11} = C_2\tan\theta\cos\omega t + \hbar\,\omega\,C_1 B^{-1}\tan\theta\sec\theta\cos\omega t$$

$$a_{21} = C_2\tan\theta\sin\omega t + \hbar\,\omega\,C_1 B^{-1}\tan\theta\sec\theta\sin\omega t \tag{5.6}$$

$$a_{31} = C_2$$

where C_1 and C_2 are real-valued constants. Thus, substituting (5.4), (5.5) and (5.6) into (5.3) we obtain to first order in ε

$$\gamma_\pm(T) = -\pi\,(1 \mp \cos\theta) \tag{5.7}$$

as was found in the adiabatic limit [17]. The $\pm$ signs correspond to the two possible signs of λ.

6. Discussion

In the present paper, we have developed a formalism for calculating generalized Berry phases when a T-periodic invariant operator is known. Two examples are worked out in detail to illustrate these ideas. The Lewis and Riesenfeld solutions are found to be the appropriate cyclic initial states and for the calculation of their associated geometric phases only the set of eigenstates of the invariant operator is needed. The simplicity of this calculation is demonstrated, in the sense that we do not need the knowledge of the evolution operator and neither make any further decomposition of it.

We have also presented—for systems whose Hamiltonian provide a closed Lie algebra— a method that in principle allows the construction of the T-periodic invariant operator. Also in this case, however, there remains the problem of the existence of a periodic solution of the auxiliary equation, which demands further investigation.

For the two-level system we have for the first time constructed a dynamical invariant, which then provided the generalized Berry phases for this system. The case of latitude variation of the parameters has been analysed in detail and it turned out that a T-periodic invariant can always be found. We have also calculated the generalized Berry phases for the generalized harmonic oscillator whenever the normalized solutions of the Hill equation (A.5) associated with (3.3) are stable.

In both cases the conventional Berry phases are obtained when the adiabatic limit is taken.

Acknowledgments

Appendix A

The invariant operator for the generalized harmonic oscillator can be found following the ideas outlined in section 2. The generators of the Lie algebra are $\{\hat{q}^2/2, (\hat{q}\hat{p}+\hat{p}\hat{q})/2, \hat{p}^2/2\}$, which is closed and the dynamical invariant

$$\hat{I}(t) = \tfrac{1}{2}\left(a_1(t)\hat{q}^2 + a_2(t)(\hat{q}\hat{p} + \hat{p}\hat{q}) + a_3(t)\,\hat{p}^2\right) \tag{A.1}$$

is determined by the coefficients $a_k(t)$, which are are real functions satisfying the linear differential equations (2.16) with

$$A(t) = \begin{pmatrix} -2Y & 2X & 0 \\ -Z & 0 & X \\ 0 & -2Z & 2Y \end{pmatrix}, \tag{A.2}$$

This system can be reduced to a single second-order equation: setting $a_3(t) = Z\rho^2(t)$, we find

$$a_2(t) = (Y - \dot{Z}/2Z)\rho^2 - \rho\dot{\rho} \tag{A.3a}$$

$$\dot{a}_1(t) = 2Xa_2(t) - 2Ya_1(t) \tag{A.3b}$$

$$a_1(t) = X\rho^2 - \dot{a}_2(t)/Z. \tag{A.3c}$$

Equating the time derivative of (A.3c) with (A.3b) and integrating, we obtain equation (3.3). In terms of $r = Z^{1/2}\rho$ the expression for the invariant is given by (2.15).

Now, the periodicity condition for the invariant, as is easily seen from the expressions for $a_k(t)$ in terms of ρ, implies periodic or anti-periodic, real or purely imaginary solutions of (3.3)

$$\rho(t + T) = \pm\rho(t) \qquad \dot\rho(t + T) = \pm\dot\rho(t) \qquad \rho(t) = \mathrm{i}^k g(t) \tag{A.4}$$

where $g(t)$ is a real function.

We now seek these solutions. The general solution of (3.3) can be written in terms of two particular independent solutions $y_1(t)$ and $y_2(t)$ of the associated Hill equation [15]

$$\ddot y + \Omega_\hbar^2 y = 0 \tag{A.5}$$

as

$$\rho(t) = [Ay_1^2(t) + By_2^2(t) + 2Cy_1(t)y_2(t)]^{1/2} \tag{A.6}$$

where A, B and C are related to the initial values $\rho(0)$ and $\dot\rho(0)$, and $AB - C^2 = W^{-2}$, the Wronskian of the two solutions $y_1(t)$ and $y_2(t)$, which can be chosen as the normalized solutions, i.e. $y_1(0) = \dot y_2(0) = 1$, $\dot y_1(0) = y_2(0) = 0$, so that $W = 1$.

As the Hill equation (A.5) has a T-periodic coefficient $\Omega_\hbar^2(t)$, the Floquet theorem provides a fundamental set of solutions [18] whose form, if $\lambda_1 \neq \lambda_2$, is

$$f_1(t) = \mathrm{e}^{\mathrm{i}\nu t} p_1(t) \qquad f_2(t) = \mathrm{e}^{-\mathrm{i}\nu t} p_2(t) \tag{A.7}$$

or, if $\lambda_1 = \lambda_2 = \pm 1$,

$$f_1(t + T) = \lambda_1 f_1(t) \qquad f_2(t + T) = \lambda_1 f_2(t) + \theta f_1(t) \tag{A.8}$$

where θ is a constant real number, and $\lambda_1 = \mathrm{e}^{\mathrm{i}\nu T}$, $\lambda_2 = \mathrm{e}^{-\mathrm{i}\nu T}$ are the roots of the characteristic equation $\lambda^2 - [y_1(T) + \dot y_2(T)] + 1 = 0$ associated with (A.5).

The roots λ_1 and λ_2 of the characteristic equation completely characterize the periodic and anti-periodic solutions of the Milne equation [15, 19]

(i) If $\lambda_1 \neq \lambda_2$, there exists a periodic solution

$$\rho_p(t) = \left\{ \frac{-y_2(T)y_1^2(t) + \dot y_1(T)y_2^2(t) + [y_1(T) - \dot y_2(T)]y_1(t)y_2(t)}{\pm\mathrm{i}\left[\left(\frac{1}{2}\left(y_1(T) + \dot y_2(T)\right)\right)^2 - 1\right]^{1/2}} \right\} \tag{A.9}$$

which is either real, or purely imaginary only if $|y_1(T) + \dot y_2(T)| < 2$, i.e. when $y_1(t)$ and $y_2(t)$ are stable (in other words: in the stability band of the corresponding Hill equation). This periodic solution is unique up to a factor i^k, $k = 0, \ldots, 3$.

(ii) If if $\lambda_1 = \lambda_2 = \pm 1$ there is *no* periodic solution provided that $\theta \neq 0$; otherwise *all* solutions are T-periodic and these solutions are real when $y_1(t)$ and $y_2(t)$ are stable, i.e. if $y_1(T) + \dot y_2(T) = \pm 2$ and $y_2(T) = \dot y_1(T) = 0$.

Appendix B

For the two-level system, we will analyse the case of latitude variation of the parameters $R(t)$, provided by equation (5.4). For this case, the auxiliary equations (4.5) are

$$\hbar\dot a_1 = B\sin\theta\sin\omega t\, a_3 - B\cos\theta\, a_2$$

$$\hbar\dot a_2 = B\cos\theta\, a_1 - B\sin\theta\cos\omega t\, a_3 \tag{B.1}$$

$$\hbar\dot a_3 = B\sin\theta\cos\omega t\, a_2 - B\sin\theta\sin\omega t\, a_1$$

with initial conditions $a_i(0) = x_{i0}$. After some manipulation, it is possible to reduce the system to a single equation in a_3:

$$\ddot{a}_3(t) + \Omega_2^2 a_3(t) = k \tag{B.2}$$

where

$$\Omega_2^2 = [(\hbar\omega - B\cos\theta)^2 + B^2\sin^2\theta]/\hbar^2$$

and

$$k = [(\hbar\omega - B\cos\theta)x_{30} - B\sin\theta\, x_{10}](\hbar\omega - B\cos\theta)/\hbar^2.$$

Thus, the general solutions for this case are

$$a_1(t) = F\,D\,G\,\cos\omega t\,\cos\Omega_2 t + x_{20}\,E\,F\,\cos\omega t\,\sin\Omega_2 t + G\,D/E\,\sin\omega t\,\sin\Omega_2 t$$

$$-x_{20}\,\sin\omega t\,\cos\Omega_2 t + [x_{10} - F\,D\,G]\cos\omega t$$

$$a_2(t) = x_{20}\,\cos\omega t\,\cos\Omega_2 t - G/E\,\cos\omega t\,\sin\Omega_2 t + F\,D\,G\,\sin\omega t\,\cos\Omega_2 t \tag{B.3}$$

$$+x_{20}\,F\,E\,\sin\omega t\,\sin\Omega_2 t + [x_{10} - F\,D\,G]\sin\omega t$$

$$a_3(t) = D\,\cos\Omega_2 t + x_{20}\,E/G\,\sin\Omega_2 t - C$$

where $C = -k/\Omega_2^2$, $D = (x_{30}+C)$, $G = B^{-1}\sin^{-1}\theta$, $E = \hbar^{-1}\Omega_2^{-1}$, and $F = \hbar\omega - B\cos\theta$ are all real numbers. At this point, we impose the periodicity condition $\hat{I}(T) = \hat{I}(0)$, which leads to $a_k(0) = a_k(T) = x_{k0}$, and so we find the appropriate initial values

$$x_{20} = -\hbar\omega B^{-1}\sin^{-1}\theta\cot\pi\Omega_2/\omega$$

$$x_{30} = [(\hbar\omega - B\cos\theta)^2 B^{-2}\sin^{-2}\theta + 1]\cot^2\pi\Omega_2/\omega + (\cot\theta - \hbar\omega B^{-1}\sin^{-1}\theta)x_{10} \tag{B.4}$$

for $\Omega_2 \neq n\omega$ and x_{10} any real number. When $\Omega_2 = n\omega$ we see by simple inspection of (B.3) that the solutions $a_k(t)$ are T-periodic, so that any real value is available for x_{k0}. Thus, the periodicity condition for the invariant operator is fulfilled.

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