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COMMENT

Berry's phase and wavefunctions for time-dependent Hamilton systems

P G L Leach†

PMMS-CNRS, 3A av de la Recherche Scientifique, F-45071 Orléans cédex 2, France

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Abstract. An alternative derivation of Berry's phase to that given by Morales is given for non-autonomous Hamiltonian systems which admit an energy-like first integral. The generality of the problems treated is greater.

In a fairly recent letter to this journal (Morales 1988), Berry's phase (Berry 1984) and Hannay's angle (Hannay 1985, Berry 1985) were calculated for the system described by the quadratic Hamiltonian:

$$H(q,p,t)=\frac{1}{2}(q,p)\begin{pmatrix}X(t) & Y(t)\\ Y(t) & Z(t)\end{pmatrix}\begin{pmatrix}q\\ p\end{pmatrix} \tag{1}$$

through an adaptation of the work of Lewis and Riesenfeld (1969) on the time-dependent harmonic oscillator with Hamiltonian:

$$H(q,p,t)=\tfrac{1}{2}\{p^2+\omega^2(t)q^2\} \tag{2}$$

and of Lewis (1967, 1968) on the behaviour of (2) in the adiabatic limit. In this comment we wish to demonstrate an alternative derivation of Morales' results. The derivation is based on earlier work on time-dependent quadratic Hamiltonians (Leach 1977a, b) and time-dependent Hamiltonians (Lewis and Leach 1982a, b, Leach *et al* 1984) which possess energy-like first integrals (or invariants; either term is taken to mean a non-trivial function of the canonical variables and time, the total time derivative of which is zero along trajectories). In addition to rederiving Morales' results for (1) by our alternative treatment we in fact obtain a more general result which clearly illustrates the nature of Berry's phase in the case of time-dependent Hamiltonians of the type mentioned above. We start with the most general Hamiltonian of $T+V$ type which possesses a first integral quadratic in the momentum. The Hamiltonian is (Lewis and Leach 1982b):

$$H(q,p,t)=\frac{1}{2}p^2-\frac{1}{2}\frac{\ddot\rho}{\rho}q^2+\frac{1}{\rho^2}V\left(\frac{q}{\rho}\right) \tag{3}$$

where $V(\cdot)$ and $\rho(t)$ are arbitrary functions of their arguments. (As usual, overdot means total differentiation with respect to time.) The associated first integral is:

$$I(q,p,t)=\frac{1}{2}(\rho q-\dot\rho q)^2+V\left(\frac{q}{\rho}\right). \tag{4}$$

† Permanent address: CAMS-CNLS, Wits 2050, South Africa.

More generally one could replace q by $q-\alpha(t)$ with suitable modifications to H and I (Lewis and Leach 1982b), but our argumentation is unchanged in its essence and the expressions derived more compact. The first thing to realise is that I is just H after a generalised canonical transformation (Munier *et al* 1981), but still expressed in terms of the old coordinates. The formal procedure is as follows. Under the linear point canonical transformation:

$$\left((q,p)\to(Q,P)\colon Q=\frac{q}{\rho},\ P=\rho p-\dot{\rho}q\right) \tag{5}$$

(3) becomes

$$\bar{H}(Q,P,t)=\frac{1}{2\rho^2}\{P^2+V(Q)\} \tag{6}$$

and, when this is followed by the time transformation:

$$\left(t\to T\colon T=\int^t \rho^{-2}(\eta)\,\mathrm{d}\eta\right) \tag{7}$$

one obtains:

$$\tilde{H}(Q,P,T)=\tfrac{1}{2}\{P^2+V(Q)\} \tag{8}$$

which is obviously I (4).

If one wishes to solve the time-dependent Schrödinger equation:

$$H\psi=\mathrm{i}\hbar\frac{\partial\psi}{\partial t} \tag{9}$$

for H (3), one simply makes use of the transformations (5) and (7) and the solution of the time-dependent Schrödinger equation for $\tilde{H}$ (8)

$$\tilde{H}\tilde{\psi}=\mathrm{i}\hbar\frac{\partial\tilde{\psi}}{\partial t}. \tag{10}$$

Hereafter we assume that $V(Q)$ is such that $\tilde{\psi}$ has discrete states. Then the solution of (10) is:

$$\tilde{\psi}_n(Q,T)=\mu_n(Q)\exp\left(-\mathrm{i}\frac{\lambda_n}{\hbar}T\right) \tag{11}$$

where $\mu_n(Q)$ is the eigenfunction of:

$$\mu_n''+\frac{2}{\hbar^2}(\lambda_n-V)\mu_n=0 \qquad \mu_n(\pm\infty)=0. \tag{12}$$

The solution of (9) is just:

$$\psi=\sum C_n\psi_n(q,t) \tag{13}$$

where

$$\psi_n(q,t)=|\rho|^{-1/2}\mu_n\left(\frac{q}{\rho}\right)\exp\left[-\mathrm{i}\frac{\lambda_n}{\hbar}T+\frac{\mathrm{i}}{2\hbar}\frac{\dot{\rho}}{\rho}q^2\right]. \tag{14}$$

Of relevance to the calculation of Berry's phase is the T-free part of (14), namely

$$\phi_n(q,t)=|\rho|^{-1/2}\mu_n\left(\frac{p}{\rho}\right)\exp\left[\frac{1}{2\hbar}\frac{\dot\rho}{\rho}q^2\right] \tag{15}$$

which, in fact, is the solution of (12) when allowance is made for the change of co-ordinates. Berry's phase is given by:

$$\begin{aligned}\gamma_n(c)&=\mathrm{i}\int_0^\tau \mathrm{d}t\left\langle\phi_n\left|\frac{\partial}{\partial t}\right|\phi_n\right\rangle\\&=-\frac{1}{2\hbar}\langle\mu_n|Q^2|\mu_n\rangle\int_0^\tau(\rho\ddot\rho-\dot\rho^2)\,\mathrm{d}t\end{aligned} \tag{16}$$

where τ is the time taken to traverse a closed loop in parameter space. This is actually a generalisation of the result to be found in Morales (1988) and has a rather interesting structure being the product of two quite distinct parts, the expectation value of Q^2 for the corresponding autonomous system and the time-dependent integral. We note that it is always the expectation value of Q^2, no matter the potential. The reason is to be found in the exponential term of (15) which is the only term which contributes to (16) and so may be said to be the source of Berry's phase in such problems.

The discussion above must be modified in the case of the Hamiltonian (1) due to the presence of the mixed terms in q and p. However, as (1) is simply a quadratic Hamiltonian, it can be readily treated by the method of time-dependent linear canonical transformations (Leach 1977a, b). In brief the Hamiltonian

$$H=\tfrac{1}{2}z^TAz \tag{17}$$

where $z^T=(\boldsymbol{q}^T,\boldsymbol{p}^T)$ and $A(t)$ is a $2n\times2n$ Hermitian matrix, is transformed to:

$$\bar H=\tfrac{1}{2}\bar z^T\bar A\bar z \tag{18}$$

by the time-dependent linear canonical transformation

$$\bar z=Sz \tag{19}$$

provided the $2n\times2n$ matrix $S(t)$ satisfies:

$$\dot S=J\bar AS-SJA \tag{20}$$

and

$$SJS^T=J \tag{21}$$

$$J=\begin{pmatrix}0_n & I_n\\ -I_n & 0_n\end{pmatrix}. \tag{22}$$

The wavefunction of the time-dependent Schrödinger equations for H and $\bar H$ are, in general, related by an integral transform, but, in the case that (19) is a point canonical transformation, this collapses to a geometric transformation of the type evident in the transition from (11) to (14) (Wolf 1979). The requirement that (19) be a point transformation amounts to the imposition of a restriction which must be compensated. It would be natural to choose $\bar A$ as the identity matrix. This is possible only if X, Y and Z satisfy a constraint. However, if one takes $\bar A$ as a function of time times the identity, the constraint becomes a differential equation for the unknown function which may subsequently be removed by a transformation of the time variable thus making the total transformation a generalised canonical transformation.

Writing S, A and $\bar{A}$ as:

$$S=\begin{pmatrix} S_1 & 0 \\ S_3 & S_4 \end{pmatrix} \qquad A=\begin{pmatrix} X & Y \\ Y & Z \end{pmatrix} \qquad \bar{A}=\rho^{-2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{23}$$

(20) and (21) become:

$$\dot{S}_1=\rho^{-2}S_3-YS_1 \tag{24}$$

$$0=\rho^{-2}S_4-ZS_1 \tag{25}$$

$$\dot{S}_3=-\rho^{-2}S_1+XS_4-YS_3 \tag{26}$$

$$\dot{S}_4=YS_4-ZS_3 \tag{27}$$

$$S_1S_4=1. \tag{28}$$

From (25) and (28):

$$S_1=(\rho Z^{1/2})^{-1} \qquad S_4=\rho Z^{1/2} \tag{29}$$

and from (24)

$$S_3=Z^{-3/2}(\rho YZ-\dot{\rho}Z-\tfrac{1}{2}\rho\dot{Z}). \tag{30}$$

Equation (27) is redundant and (26) provides the differential equation:

$$\ddot{\rho}+\left\{XZ-Y^2+\frac{\dot{Z}Y-Z\dot{Y}}{Z}+\frac{1}{2}\frac{\ddot{Z}}{Z}-\frac{3}{4}\frac{\dot{Z}^2}{Z^2}\right\}\rho=\frac{1}{\rho^3} \tag{31}$$

which, not withstanding the long coefficient of ρ, is just the Pinney equation (Pinney 1950) usually associated with time-dependent oscillator problems. The solution of the time-dependent Schrödinger equation for (1) is then of the form (13) with:

$$\psi_n(q,t)=|\rho Z^{1/2}|^{-1/2}\mu_n\left(\frac{q}{\rho Z^{1/2}}\right)\exp\left\{-\mathrm{i}(n+\tfrac{1}{2})T+\frac{\mathrm{i}q^2}{2\hbar}\left[\frac{\dot{\rho}}{\rho Z}+\frac{\dot{Z}}{2Z^2}-\frac{Y}{Z}\right]\right\} \tag{32}$$

where $\mu_n(Q)$ is the usual wavefunction for the time-dependent simple harmonic oscillator.

Berry's phase is calculated as before for (16) and the effect of the time-dependent coefficients in the Hamiltonian are seen in the time integral. We have that:

$$\gamma_n(c)=-\frac{1}{2\hbar}\langle\mu_n|Q^2|\mu_n\rangle\int_0^T\left(\rho\ddot{\rho}-\dot{\rho}^2-\frac{\rho\dot{\rho}\dot{Z}}{Z}+\frac{\rho^2\ddot{Z}}{2Z}-\frac{\rho^2\dot{Z}^2}{Z^2}-\rho^2\dot{Y}+\frac{\rho^2Y\dot{Z}}{Z}\right)\mathrm{d}t \tag{33}$$

where, since the expectation value refers to the ordinary oscillator, it may be replaced by $\hbar(n+\frac{1}{2})$.

It should be apparent from the foregoing that the same techniques can be applied to Hamiltonians of the form:

$$H(q,p,t)=\tfrac{1}{2}\{Z(t)p^2+Y(t)(qp+pq)\}+V(q,t) \tag{34}$$

which can be transformed to an invariant by a generalised canonical transformation which is point in the position.

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