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The geometric phase for chaotic unitary families

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Abstract. We consider the geometric phase for a family of quantum/classical Hamiltonians in which the effect of changing parameters is simply to induce unitary/canonical transformations. In this case the classical limit of the geometric phase is easily obtained, even when the classical motion is chaotic. The results agree with those previously obtained for general chaotic families, but may be expressed in a simpler form, not involving time integrals of correlation functions. It is also straightforward to establish some results which are problematic in the general case, for example the form of periodic orbit corrections, and the closedness of the classical 2-form. If the parameters are regarded as dynamical variables, evolving slowly so as to maintain adiabaticity, they are subject to geometric magnetism, but not, in contrast to the general case, deterministic friction and Born–Oppenheimer forces. Examples including families of translated and rotated systems are discussed.

1. Introduction

In the theory of the geometric phase (Berry 1984, Shapere and Wilczek 1989), there are a number of interesting questions related to the classical ($\hbar \to 0$) limit. This limit is best understood for integrable systems, for which Hannay (1985) found angle anholonomies along the tori of cycled integrable systems, and Berry (1984) established the semiclassical correspondence between the geometric phase and the Hannay angles.

In Robbins and Berry (1992a), hereinafter referred to as RB, we obtained the classical limit of the geometric phase 2-form for classically chaotic Hamiltonians, along with semiclassical corrections associated with periodic orbits. In Berry and Robbins (1993) we showed that the classical 2-form produces a Lorentz-like reaction force on the parameters, 'geometric magnetism', which is the antisymmetric partner of a dissipative force, 'deterministic friction', previously found by Wilkinson (1990). Whether the classical 2-form describes an anholonomy in adiabatically cycled chaotic systems is an open question.

Here we consider a special family of chaotic Hamiltonians for which the classical limit of the geometric phase is easily obtained. For these unitary/canonical families, a change in parameters amounts to a unitary/canonical transformation. For example, the parameters could describe the orientation of the system, so that changing parameters produces a spatial rotation. The intrinsic properties of the dynamics (the energy levels of the quantum system, and the actions and Liapunov exponents of the classical system) are parameter-independent. In particular, degeneracies are parameter-independent, whereas generically these act as monopole sources of the 2-form. However, in spite of this rather trivial dependence on the parameters, interesting effects appear when the parameters are varied in time.

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The paper is arranged as follows. Unitary families are introduced in section 2 and the associated 1- and 2-forms are obtained. Assuming the classical dynamics to be chaotic, we obtain (section 3 and 4) their classical limits, which for the 2-form gives a special case of the formula obtained in RB. A simple modification yields the classical limit for the integrable case. We consider next periodic corrections (section 5). These too agree with RB, although an alternative derivation avoids the analytic continuations required in the general case. In section 6 we show that the classical 2-form is closed for canonical families, and discuss possible implications for the general case. In section 7 we consider the reaction forces produced on the parameters when these are regarded as dynamical variables. To lowest order, the only reaction force is geometric magnetism. Examples are discussed in section 8.

For convenience we take parameter space $\boldsymbol{R} = (R_1, R_2, R_3)$ to be three-dimensional, and use vector notation rather than differential forms. Thus both 1-forms and 2-forms are vector fields.

2. Unitary families

Consider the family of Hamiltonians

$$\hat{h}(\boldsymbol{R}) = U(\boldsymbol{R})\hat{H}U^\dagger(\boldsymbol{R}) \tag{1}$$

unitarily related to a given Hamiltonian $\hat{H}$. The unitary operators $U(\boldsymbol{R})$ could, but need not, constitute a group representation. Assuming the energy levels of $\hat{H}$ (and therefore $\hat{h}$) to be non-degenerate, we consider the geometric phases γ_n obtained by parallel transport of the eigenstates $|n(\boldsymbol{R})\rangle = U|N\rangle$ (here $|N\rangle$ denotes the eigenstates of $\hat{H}$) round a circuit C in parameter space. As is well known, γ_n is given by the line integral of the 1-form $\boldsymbol{A}_n(\boldsymbol{R}) = \hbar\,\mathrm{Im}\,\langle n\,|\boldsymbol{\nabla} n\,\rangle$ round C, or (via Stokes' theorem) by the flux of the 2-form $\boldsymbol{V}_n(\boldsymbol{R}) = \boldsymbol{\nabla}\wedge\boldsymbol{A}_n = \hbar\,\mathrm{Im}\,\langle\boldsymbol{\nabla} n|\wedge|\boldsymbol{\nabla} n\rangle$ through a surface S bounded by C. (Note that with these conventions, the geometric phase factor is $\exp(-\mathrm{i}\gamma_n/\hbar)$.)

The 1- and 2-forms can be expressed in terms of the generators $\hat{g}(\boldsymbol{R})$ of U, defined by

$$\hat{g}(\boldsymbol{R}) \stackrel{\text{def}}{=} \mathrm{i}\hbar\boldsymbol{\nabla} U(\boldsymbol{R})U^\dagger(\boldsymbol{R}) \tag{2}$$

where $\hat{g}$ is a vector of Hermitian operators. Since

$$|\boldsymbol{\nabla} n\rangle = -\frac{\mathrm{i}}{\hbar}\hat{g}|n\rangle \tag{3}$$

it follows that

$$\boldsymbol{A}_n(\boldsymbol{R}) = \hbar\,\mathrm{Im}\,\langle n\,|\boldsymbol{\nabla} n\,\rangle = -\langle n|\hat{g}|n\rangle \tag{4}$$

$$\boldsymbol{V}_n(\boldsymbol{R}) = \hbar\,\mathrm{Im}\,\langle\boldsymbol{\nabla} n|\wedge|\boldsymbol{\nabla} n\rangle = -\frac{\mathrm{i}}{\hbar}\langle n|\hat{g}\wedge\hat{g}|n\rangle = -\frac{\mathrm{i}}{2\hbar}\langle n|[\hat{g}\wedge\hat{g}]|n\rangle\,. \tag{5}$$

Here $[\hat{g},\wedge\hat{g}]$ denotes a vector of operators whose ith component is $\sum_{jk}\epsilon_{ijk}[\hat{g}_j,\hat{g}_k]$, so that $[\hat{g},\wedge\hat{g}] = 2\hat{g}\wedge\hat{g}$.

It is useful to verify that $\boldsymbol{V}_n = \boldsymbol{\nabla}\wedge\boldsymbol{A}_n$ directly from (4) and (5). For this we need the identity

$$\boldsymbol{\nabla}\wedge\hat{g} = -\frac{\mathrm{i}}{\hbar}\hat{g}\wedge\hat{g} = -\frac{\mathrm{i}}{2\hbar}[\hat{g},\wedge\hat{g}] \tag{6}$$

obtained from the curl of (3). A similar-looking though different formula holds for the family of operators $\hat{f}(\boldsymbol{R}) \stackrel{\text{def}}{=} U\hat{F}U^{\dagger}$, namely

$$\nabla \hat{f} = -\frac{\mathrm{i}}{\hbar}[\hat{g}, \hat{f}] \tag{7}$$

where it is assumed that $\hat{F}$ has no explicit $\boldsymbol{R}$ dependence.

The gauge freedom in $\boldsymbol{A}_n$ (the fact that a gradient $\nabla\chi_n$ may be added to it) may be attributed to phase conventions in either $|n(\boldsymbol{R})\rangle$ or $U(\boldsymbol{R})$. We take the latter point of view, as it has a simple classical analogue. The unitary family $\hat{h} = U\hat{H}U^{\dagger}$ determines U up to transformations

$$U \to U\mathrm{e}^{-\mathrm{i}\hat{K}/\hbar} \tag{8}$$

where $\hat{K}(\boldsymbol{R}) = F(\hat{H}, \boldsymbol{R})$ is a (parameter-dependent) function of $\hat{H}$. Under (8),

$$\hat{g} \to \hat{g} + U\nabla\hat{K}U^{\dagger} \tag{9a}$$

$$\boldsymbol{A}_n \to \boldsymbol{A}_n - \langle n|U\nabla\hat{K}U^{\dagger}|n\rangle \tag{9b}$$

while $\boldsymbol{V}_n$ and γ_n remain unchanged.

3. Canonical families

To $\hat{H}$ there corresponds a given classical Hamiltonian $H(z)$, defined on $2N$-dimensional phase space with canonical coordinates $z = (q, p)$. We assume H is ergodic. The unitary transformations $U(\boldsymbol{R})$ correspond to a family of canonical transformations $\Phi(z, \boldsymbol{R})$, and $\hat{h}(\boldsymbol{R})$ to the family of Hamiltonians

$$h(z, \boldsymbol{R}) = H(\Phi^{-1}(z, \boldsymbol{R})) \tag{10}$$

canonically related to H.

The classical limit of $\hat{g}(\boldsymbol{R})$ gives the classical generators $\boldsymbol{g}(z, \boldsymbol{R})$, a vector of phase space functions whose 'flows' (regarding them as Hamiltonians in the equations of motion) generate the infinitesimal displacements $\Phi(z, \boldsymbol{R} + \mathrm{d}\boldsymbol{R}) - \Phi(z, \boldsymbol{R})$. More explicitly,

$$\nabla\Phi(z, \boldsymbol{R}) = \mathbf{J}\cdot\partial_z \boldsymbol{g}(\Phi(z, \boldsymbol{R}), \boldsymbol{R}) \qquad \text{where } \mathbf{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{11}$$

(In case the parameters constitute a Lie group, the generators $\boldsymbol{g}$ are related to the momentum map—see Abraham and Marsden (1978)—in a simple way.) Replacing commutators $[\cdot, \cdot]$ by Poisson brackets $\mathrm{i}\hbar\{\cdot, \cdot\}$ in (6), we have

$$\nabla \wedge \boldsymbol{g} = \tfrac{1}{2}\{\boldsymbol{g}, \wedge \boldsymbol{g}\}\,. \tag{12}$$

The classical limit of (7) follows similarily; if $f(z, \boldsymbol{R}) = F(\Phi^{-1}(z, \boldsymbol{R}))$, then

$$\nabla f = \{\boldsymbol{g}, f\}\,. \tag{13}$$

Equation (13) is used several times in what follows.

It is worth noting that the classical generators $\boldsymbol{g}$ can be determined directly from the canonical transformations Φ, without recourse to the classical limit of $\hat{g}$. This is not immediately apparent, because (11) involves $\partial_z \boldsymbol{g}$ and not $\boldsymbol{g}$ itself, and so determines $\boldsymbol{g}$ up to a z-independent but otherwise arbitrary 1-form. (This is not the gauge freedom of (9a), in which the additional 1-form is necessarily a perfect gradient.) However, as shown in the appendix, this arbitrariness can be removed (up to gauge transformations) by imposing (12) as a separate condition.

4. Classical limit

In (4) and (5), A_n and V_n are given by expectation values of $\hat{g}$ and $[\hat{g}, \wedge\hat{g}]$, both of which have well behaved classical limits. This makes it straightforward to obtain the classical limits of A_n and V_n. (In contrast, the expectation values obtained in RB involve commutators of time-evolved operators, whose classical limits diverge exponentially in time.) Assuming the classical dynamics to be ergodic (the integrable case is discussed briefly below), we take the classical limit of a typical expectation value $\langle n|\hat{f}|n\rangle$ to be the microcanonical average

$$\langle f\rangle_{ER} = \frac{1}{\partial_E\Omega}\int \mathrm{d}z\,\delta(E-h)f(z,\boldsymbol{R})\,. \tag{14}$$

Sometimes we will write simply $\langle f\rangle$, omiting the arguments. In (14), the normalization factor $\partial_E\Omega(E) \stackrel{\text{def}}{=} \int \mathrm{d}z\,\delta(E-h)$ is the phase volume on the energy shell ($h(z,\boldsymbol{R}) = E$), and its integral $\Omega(E) \stackrel{\text{def}}{=} \int \mathrm{d}z\,\Theta(E-h)$ is the phase volume contained inside the energy shell. The (canonically invariant) volume $\Omega(E)$ is of course independent of $\boldsymbol{R}$. The classical energy E and quantum number n are related by the Weyl formula

$$\Omega(E) = (2\pi\hbar)^N n \tag{15}$$

according to which each quantum state occupies a phase volume of $(2\pi\hbar)^N$. Thus from (4), (5) and (14) we obtain

$$A_n \to A^{\mathrm{c}}(E,\boldsymbol{R}) = -\langle g\rangle \tag{16}$$

$$V_n \to V^{\mathrm{c}}(E,\boldsymbol{R}) = \tfrac{1}{2}\langle\{g,\wedge g\}\rangle \tag{17}$$

the classical limits of A_n and V_n.

In RB we derived the general formula

$$V^{\mathrm{c}}(E,\boldsymbol{R}) = \frac{1}{2\partial_E\Omega}\partial_E\left(\partial_E\Omega\int_0^\infty \mathrm{d}t\,\langle(\nabla h)_t\wedge\nabla h\rangle_{E,\boldsymbol{R}}\right) \tag{18}$$

where in general f_t denotes the function f evolved along classical orbits. (More explicitly, if z_t denotes the orbit from z at time t, then $f_t(z) \stackrel{\text{def}}{=} f(z_t)$.) The integrand $\langle(\nabla h)_t\wedge\nabla h\rangle$ in (18), an antisymmetric correlation function of ∇h, is assumed to decay sufficiently fast for the t-integral to converge.

As we now show, for canonical families (17) and (18) are equivalent. From (13), $\nabla h = \{g,h\}$. But $\{g,h\}$ is the time derivative of g along trajectories of h, so that

$$\nabla h = \{g,h\} = \left.\frac{\mathrm{d}}{\mathrm{d}t}g_t\right|_{t=0} \stackrel{\text{def}}{=} \dot{g}\,. \tag{19}$$

Similarily $(\nabla h)_t = \dot{g}_t$. Substituting these into the integral in (18), we get

$$\int_0^\infty \mathrm{d}t\,\langle(\nabla h)_t\wedge\nabla h\rangle = \int_0^\infty \mathrm{d}t\,\langle\dot{g}_t\wedge\dot{g}\rangle = -\langle g\wedge\dot{g}\rangle\,. \tag{20}$$

There is no contribution from $t = \infty$ provided the dynamics is mixing; in this case $\langle g_\infty\wedge\dot{g}\rangle = \langle g\rangle\wedge\langle\dot{g}\rangle$, and

$$\langle\dot{g}\rangle = \langle\nabla h\rangle = \left.\frac{\mathrm{d}}{\mathrm{d}t}\langle g_t\rangle\right|_{t=0} = 0 \tag{21}$$

since microcanonical averages are time-invariant. With (20), (18) becomes

$$V^c(E, R) = \frac{1}{\partial_E \Omega} \partial_E \left(\partial_E \Omega \langle \dot{g} \wedge g \rangle\right) . \tag{22}$$

Using the following identity (a derivation is given in appendix A of RB)

$$\frac{1}{\partial_E \Omega} \partial_E \left(\partial_E \Omega \langle \dot{g} \wedge g \rangle\right) = \langle \{g, \wedge g\} \rangle \tag{23}$$

we see that (17) and (22) are indeed equivalent.

If the classical dynamics is integrable, then the microcanonical average of (14) should be replaced by an average over the invariant torus corresponding to the state $|n\rangle = |n_1, \ldots, n_N\rangle$. It is then straightforward to show (similar calculations can be found in RB) that the resulting expressions for the 1- and 2-forms (torus averages of g and $\{g, \wedge g\}$ respectively) are equivalent to the more familiar formulas of Hannay (1985) and Berry (1985).

Let us consider the classical limit of the gauge transformation (8). The canonical family $h = H \circ \Phi^{-1}$ (here $\circ$ denotes composition of functions) determines Φ up to transformations of the form

$$\Phi \to \Phi \circ \Sigma \tag{24}$$

where $\Sigma(z, R)$ is the time-one flow of $K(z, R) = F(H(z), R)$; since K is a function of H, Σ commutes with the flow of H. Then $\nabla\Sigma = (\mathbf{J} \cdot \partial_z \nabla K) \circ \Sigma$, and one can show (the canonical property of Φ is used explicitly) that under (24),

$$g \to g + \nabla \mathrm{K} \circ \Phi^{-1} \tag{25a}$$

$$A^c \to A^c - \langle (\nabla K) \circ \Phi^{-1} \rangle \tag{25b}$$

and V^c is unchanged.

5. Periodic orbit corrections

As the Weyl formula (15) describes the smooth behaviour of the density of states $\sum_n \delta(E - E_n)$, so too the classical 2-form V^c describes the smooth behaviour of the spectral 2-form

$$D(E, R) = \sum_n \delta(E - E_n) V_n . \tag{26}$$

In RB we obtained the following semiclassical approximation for D, in which fluctuations are described by a sum over classical periodic orbits, just as for the density of states:

$$D \to D^c(E, R) = \frac{\partial_E \Omega}{(2\pi\hbar)^N} V^c + \frac{1}{\pi\hbar} \sum_j K_j V_j^c . \tag{27}$$

Here

$$K_j(E, R) = \frac{T_j}{|M_j - I|^{1/2}} \cos\left(S_j/\hbar - \frac{1}{2}\mu_j \pi\right) \tag{28}$$

are the oscillatory amplitudes of the Gutzwiller trace formula (Gutzwiller 1990) which depend on the orbits' actions S_j, periods T_j, stabilities $|M_j - I|$ and Maslov indices μ_j. V_j^c is a 2-form associated with periodic orbits and is defined as follows. If $z_j(\theta, S, \boldsymbol{R}) \stackrel{\mathrm{def}}{=} (q_j, p_j)(\theta, S, \boldsymbol{R})$ denotes the periodic orbit as a function of the scaled time $\theta = 2\pi t/T_j$, action S and parameters $\boldsymbol{R}$, then

$$V_j^c(E, \boldsymbol{R}) = \tfrac{1}{2}\left\langle \nabla z_j \cdot \mathbf{J} \cdot \wedge \nabla z_j \right\rangle_{jE\boldsymbol{R}} = \left\langle \nabla q_j \cdot \wedge \nabla p_j \right\rangle_{jE\boldsymbol{R}} \tag{29}$$

where $\langle \cdots \rangle_{jE\boldsymbol{R}}$ (or simply $\langle \cdots \rangle_j$, omitting other arguments) denotes the orbit average $1/2\pi \oint \mathrm{d}\theta(\cdots)$. (Note that the 'dot product' in the second member in (29) is taken over $2N$ phase space dimensions, while in the third member it is taken over N degrees of freedom.) *The orbit 2-form V_j^c is entirely analogous to the Hannay 2-form for one-freedom integrable* systems, with periodic orbits taking the place of one-dimensional tori.

The derivation of the spectral 2-form (27) in the general case is not straightforward. The difficulties are connected with the exponential divergence in time of the quantity $\{(\nabla h)_t, \wedge \nabla h\}$, whose microcanonical average appears in the derivation of V^c, and whose periodic orbit average appears in the derivation of V_j^c. While microcanonical averaging removes this divergence, periodic orbit averaging does not, and we must appeal to an explicit analytical continuation, as described in appendix K of RB. However, for unitary families there exists a more direct derivation of (27). Like the derivation of (17), it follows from (5), in which V_n is expressed as the expectation value of an operator with a well behaved classical limit.

For classically chaotic Hamiltonians, a spectral-weighted expectation value such as $\mathrm{Tr}[\hat{F}\delta(E - \hat{h})] = \sum_n \delta(E - E_n)\langle n|\hat{F}|n\rangle$ is given semiclassically by

$$\frac{\partial_E \Omega}{(2\pi\hbar)^N}\langle F\rangle + \sum_j K_j \langle F\rangle_j \tag{30}$$

i.e. by the microcanonical average of F, weighted by the smooth density of states, plus periodic orbit corrections; this result follows from the semiclassical approximation of the spectral operator $\delta(E - \hat{h})$ of Berry (1989). Then from (26), (5) and (30), the spectral 2-form is given semiclassically by

$$\boldsymbol{D}^c = \frac{\partial_E \Omega}{(2\pi\hbar)^N} \boldsymbol{V}^c + \frac{1}{\pi\hbar} \sum_j \frac{1}{2} K_j \langle \{g, \wedge g\} \rangle_j\ . \tag{31}$$

To establish the agreement of (31) with the general result (27), we need to show the equivalence of their orbit 2-forms. That is, we must show that

$$V_j^c \stackrel{\mathrm{def}}{=} \tfrac{1}{2}\left\langle \nabla z_j \cdot \mathbf{J} \cdot \wedge \nabla z_j \right\rangle_j = \tfrac{1}{2}\langle \{g, \wedge g\} \rangle_j\ . \tag{32}$$

To proceed, note that the periodic orbits $z_j = (q_j, p_j)$ of h depend simply on parameters *through the canonical transformation* Φ; *explicitly*,

$$z_j(\theta, S, \boldsymbol{R}) = \Phi(Z_j(\theta, S), \boldsymbol{R}) \tag{33}$$

where $Z_j(\theta, S)$ denote the corresponding periodic orbits of H. From (11),

$$\nabla z_j = \nabla \Phi(Z_j, \boldsymbol{R}) = \mathbf{J} \cdot \partial_z g(z_j). \tag{34}$$

Therefore

$$\tfrac{1}{2}\nabla z_j \cdot \mathbf{J} \cdot \wedge \nabla z_j = \tfrac{1}{2}\partial_z g(z_j) \cdot \mathbf{J}^{\mathrm{T}}\mathbf{J} \cdot \wedge \partial_z g(z_j) = \tfrac{1}{2}\{g, \wedge g\}(z_j) \tag{35}$$

since $\mathbf{J}^{\mathrm{T}}\mathbf{J} = I$, and (32) follows.

6. Closedness of the classical 2-form

For canonical families

$$\boldsymbol{V}^{\mathrm{c}} = \nabla \wedge \boldsymbol{A}^{\mathrm{c}} = -\nabla \wedge \langle \boldsymbol{g} \rangle \tag{36}$$

so that $\boldsymbol{V}^{\mathrm{c}}$ is closed ($\nabla \cdot \boldsymbol{V}^{\mathrm{c}} = 0$). To verify (36), we differentiate the microcanonical average (14) to obtain

$$-\nabla \wedge \langle \boldsymbol{g} \rangle = -\langle \nabla \wedge \boldsymbol{g} \rangle + \frac{1}{\partial_E \Omega} \partial_E \left(\partial_E \Omega \langle \nabla h \wedge \boldsymbol{g} \rangle \right) \tag{37}$$

and using (12) and (23) obtain

$$-\nabla \wedge \langle \boldsymbol{g} \rangle = -\tfrac{1}{2} \langle \{ \boldsymbol{g}, \wedge \boldsymbol{g} \} \rangle + \langle \{ \boldsymbol{g}, \wedge \boldsymbol{g} \} \rangle = \tfrac{1}{2} \langle \{ \boldsymbol{g}, \wedge \boldsymbol{g} \} \rangle = \boldsymbol{V}^{\mathrm{c}} . \tag{38}$$

For general systems it is an open question as to whether $\boldsymbol{V}^{\mathrm{c}}$ is closed. Closedness is not necessarily inherited from quantum mechanics, because $\nabla \cdot \boldsymbol{V}_n$ has monopole-like singularities (of charge $\pm 2\pi$) at points $\boldsymbol{R}_*$ where the energy level $E_n(\boldsymbol{R}_*)$ is degenerate (Berry 1984). Thus $\nabla \cdot \boldsymbol{V}^{\mathrm{c}}(E, \boldsymbol{R})$ describes a smoothed monopole distribution, and vanishes if and only if this is neutral on a classical scale. Related to this question is the fact that at present we know of no general formula for the classical 1-form $\boldsymbol{A}^{\mathrm{c}}$. In RB we gave a formal argument showing $\boldsymbol{V}^{\mathrm{c}}$ is closed, but with subsequent consideration this argument no longer seems satisfactory. There is a formal generalization of the derivation (37) which is more promising, but it remains to be seen whether it will lead to a conclusive result.

Let us point out two questions concerning purely classical mechanics which depend on whether $\boldsymbol{V}^{\mathrm{c}}$ is closed in the general case. The first concerns the existence of an analogue of the Hannay angle for chaotic systems. Leaving aside the question of its proper definition, we would expect this 'chaotic angle' to be, in analogy with the integrable case, the flux of $\boldsymbol{V}^{\mathrm{c}}$ through a surface S bounded by an adiabatic cycle C. In order for this flux to depend solely on C, it is necessary that $\boldsymbol{V}^{\mathrm{c}}$ be closed. The second point concerns the geometric magnetism acting on slow classical systems coupled to fast chaotic ones; closedness would mean the geometric magnetic field is free of monopoles.

7. Geometric magnetism without dissipation

As in Berry and Robbins (1993), we now regard the parameters $\boldsymbol{R}$ as dynamical variables in their own right, coupled to an ensemble $\rho(z, t)$ of 'fast' systems. The equations of motion are

$$\epsilon \dot{\rho} = \{ \rho, h \} \tag{39a}$$

$$\ddot{\boldsymbol{R}} = -\int \mathrm{d}z \, \rho \nabla h \tag{39b}$$

where ϵ is a small parameter which insures that $\boldsymbol{R}$ evolves slowly relative to ρ. Within an adiabatic treatment of the reaction forces on the slow system (the fast ensemble is taken to be microcanonical to lowest order), there appears a 'classical Born–Oppenheimer' force

$-\langle\nabla h\rangle_{ER}$ at zeroth order, and at first order a velocity-dependent force $-\epsilon\mathrm{K}\cdot\dot{R}$, where the tensor K is given by

$$K_{ij}(E,R)=\frac{1}{\partial_E\Omega}\partial_E\left[\partial_E\Omega\int_0^\infty \mathrm{d}t\left\langle\widetilde{(\partial_i h)_t}\widetilde{\partial_j h}\right\rangle_{ER}\right]$$

$$\text{where}\quad \partial_i\stackrel{\mathrm{def}}{=}\partial/\partial R_i\quad\text{and}\quad \widetilde{f}(z,E,R)\stackrel{\mathrm{def}}{=}f-\langle f\rangle_{ER}\,. \tag{40}$$

The classical 2-form V^c is recognized as the antisymmetric part of K; it produces the Lorentz-like force $-\dot{R}\wedge V^c$ called geometric magnetism. The symmetric part produces a dissipative force, deterministic friction, found by Wilkinson (1990). (See also Ott (1979) and Brown *et al* (1987).) Jarzynski (1993) has shown that there is also in general a velocity-*independent* force at first order, which may be expressed as the gradient of a memory-dependent potential.

As we now show, deterministic friction vanishes for canonical families. (For the case of translations and rotations, a related result was obtained by Jarzynski (1992).) First, (21) implies that $\widetilde{\partial_i h}=\partial_i h$. Proceeding as in (20),

$$\int_0^\infty \mathrm{d}t\left\langle(\partial_i h)_t\partial_j h\right\rangle=\int_0^\infty \mathrm{d}t\left\langle(\dot{g_i})_t\dot{g}_j\right\rangle=-\left\langle g_i\dot{g}_j\right\rangle \tag{41}$$

so that

$$K_{ij}=-\frac{1}{\partial_E\Omega}\partial_E\left(\partial_E\Omega\left\langle g_i\dot{g}_j\right\rangle\right). \tag{42}$$

But $\left\langle g_i\dot{g}_j\right\rangle+\left\langle\dot{g}_i g_j\right\rangle=\mathrm{d}\left\langle g_i g_j\right\rangle/\mathrm{d}t$, and $\mathrm{d}\left\langle g_i g_j\right\rangle/\mathrm{d}t=0$ (time invariance of microcanonical averages.) Thus $\left\langle g_i\dot{g}_j\right\rangle$ and K_{ij} are antisymmetric.

Equation (21) implies that the classical Born–Oppenheimer force $\langle\nabla h\rangle$ also vanishes for canonical families, and therefore so does Jarzynski's force. Thus, to lowest order in ϵ,

$$\ddot{R}=-\epsilon\dot{R}\wedge V^c\,. \tag{43}$$

For canonical families, the only force acting on the slow system up to second order is geometric magnetism.

It is also interesting to consider 'half-classical mechanics' (Berry and Robbins 1993), in which the fast system is quantum mechanical and is described by a density operator $\hat{\rho}$. The equations of motion are then (cf (39))

$$\epsilon\dot{\hat{\rho}}=[\hat{\rho},\hat{h}] \tag{44a}$$

$$\ddot{R}=-\mathrm{Tr}[\hat{\rho}\nabla\hat{h}]\,. \tag{44b}$$

Within an adiabatic treatment of the reaction forces (taking the fast system to be in an eigenstate), there appears the Born–Oppenheimer force $-\nabla E_n(R)$ at zeroth order, and geometric magnetism $-\dot{R}\wedge V_n$ at first order. There is no friction in 'half-classical mechanics', an example of a quantum-classical discordance (see also Robbins and Berry (1992b)). Suppose now that $\hat{h}(R)$ is a unitary family. Then the Born–Oppenheimer force vanishes (the energy levels are independent of parameters). Thus for unitary families, as for canonical families, the only reaction force up to second order is geometric magnetism.

8. Examples

Consider first the trivial case of translational families of three-dimensional systems, for which $h(\boldsymbol{r}, \boldsymbol{p}, \boldsymbol{R}) = H(\boldsymbol{r} - \boldsymbol{R}, \boldsymbol{p})$. In this case $g(\boldsymbol{r}, \boldsymbol{p}, \boldsymbol{R}) = \boldsymbol{p}$ (momentum is the generator of translations), and since $\{p_i, p_j\} = 0$, $\boldsymbol{V}^{\mathrm{c}}$ vanishes. Analogous considerations hold for the quantum case, so that V_n vanishes too. The situation may be more interesting when there are external magnetic fields. Then the translated vector potential $\boldsymbol{a}(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{r} - \boldsymbol{R})$ can be shifted by an $\boldsymbol{R}$-dependent gauge term $\nabla_{\boldsymbol{r}}\chi(\boldsymbol{r}, \boldsymbol{R})$, which alters the dynamics (if $\boldsymbol{R}$ is changing in time) and changes the 2-form. A general discussion of the magnetic gauge-dependence of the 2-form is given by Mondragon and Berry (1989). In the special case where $\boldsymbol{B}$ is uniform and the gauge is chosen to make $\boldsymbol{a}(\boldsymbol{r})$ independent of $\boldsymbol{R}$, Jarzynski (personal communication) has shown that $\boldsymbol{V}^{\mathrm{c}} = \boldsymbol{V}_n = \boldsymbol{B}$. A related discussion of geometric magnetism on the nuclei of atoms moving through a magnetic field is given by Li and Mead (1992).

Another simple case involves rotated families, for which $h(\boldsymbol{r}, \boldsymbol{p}, \boldsymbol{R}) = H(\mathcal{R}\cdot\boldsymbol{r}, \mathcal{R}\cdot\boldsymbol{p})$; here $\mathcal{R}(\boldsymbol{R})$ is a parameterization of the three-dimensional rotations. The generators $\boldsymbol{g}$ of rotations correspond to components of angular momentum $\boldsymbol{l} = \boldsymbol{r} \wedge \boldsymbol{p}$ in the following manner. If $\delta\boldsymbol{R}(\boldsymbol{\omega})$ produces an infinitesimal rotation about the axis $\boldsymbol{\omega}/||\boldsymbol{\omega}||$ by an angle $||\boldsymbol{\omega}||$ (so that $(\mathcal{R}(\boldsymbol{R}+\delta\boldsymbol{R}) - \mathcal{R}(\boldsymbol{R}))\cdot\boldsymbol{r} = \boldsymbol{\omega}\wedge(\mathcal{R}(\boldsymbol{R})\cdot\boldsymbol{r})$), then $\langle\boldsymbol{g}\rangle\cdot\delta\boldsymbol{R} = \langle\boldsymbol{l}\rangle\cdot\boldsymbol{\omega}$, so that

$$\boldsymbol{A}^{\mathrm{c}}(E, \boldsymbol{R})\cdot\delta\boldsymbol{R} = -\langle\boldsymbol{l}\rangle_{E\boldsymbol{R}}\cdot\boldsymbol{\omega} = -(\mathcal{R}(\boldsymbol{R})\cdot\langle\boldsymbol{L}\rangle_E)\cdot\boldsymbol{\omega}\,. \tag{44}$$

Here $\langle\boldsymbol{L}\rangle_E$ is the microcanonically-averaged angular momentum of the given Hamiltonian H. Similarily,

$$\boldsymbol{V}^{\mathrm{c}}(E, \boldsymbol{R})\cdot(\delta\boldsymbol{R}_1\wedge\delta\boldsymbol{R}_2) = \langle\boldsymbol{l}\rangle_{E\boldsymbol{R}}\cdot(\boldsymbol{\omega}_1\wedge\boldsymbol{\omega}_2) = (\mathcal{R}(\boldsymbol{R})\cdot\langle\boldsymbol{L}\rangle_E)\cdot(\boldsymbol{\omega}_1\wedge\boldsymbol{\omega}_2)\,. \tag{45}$$

Thus non-vanishing 1- and 2-forms require non-zero expectation values of angular momentum. Analogous results hold for the quantum case. While we have been considering ergodic systems, (45) applies to certain integrable systems such as the Foucault pendulum, and it should be straightforward to generalize to three-dimensional systems with an axis of symmetry, such as the double pendulum and the heavy asymmetric top.

Let us consider in more detail the restricted case of rotations in two dimensions. For definitiveness consider a planar billiard (a particle $\boldsymbol{r} = (x, y)$ confined to a domain and specularly reflected at the boundary) in a uniform magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ and a tangential electric field $\boldsymbol{E}(\boldsymbol{r}) = -\nabla\Phi(\boldsymbol{r})$. (A particular significance of the electric field is explained below.) The Hamiltonian is then

$$H(\boldsymbol{r}, \boldsymbol{p}) = \tfrac{1}{2}(\boldsymbol{p} - \boldsymbol{A})^2 + \Phi + V \tag{46}$$

where $\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{B}\wedge\boldsymbol{r}$, and $V(\boldsymbol{r})$ vanishes inside the billiard and is infinite outside; we assume H is ergodic. Rotating about $\hat{\boldsymbol{z}}$ we obtain the family $h(\boldsymbol{r}, \boldsymbol{p}, \phi) = H(\mathcal{R}_z(\phi)\cdot\boldsymbol{r}, \mathcal{R}_z(\phi)\cdot\boldsymbol{p})$. Parameter space is the one-dimensional circle $[0 \leqslant \phi \leqslant 2\pi]$, so that the 2-form vanishes trivially. However, the (scalar) 1-form A^{c} does not vanish; its integral round the circle (equal to $2\pi A^{\mathrm{c}}$, since A^{c} is independent of ϕ) corresponds to the geometric phase accompanying a 2π-rotation of the billiard. From (44), $A^{\mathrm{c}}(E) = -\langle l_z\rangle_E = -\langle\boldsymbol{r}\wedge\boldsymbol{p}\rangle_E$. Noting that $\boldsymbol{p} = \boldsymbol{v} + \frac{1}{2}\boldsymbol{B}\wedge\boldsymbol{r}$ and $\langle\boldsymbol{r}\wedge\boldsymbol{v}\rangle_E = 0$ by symmetry, we get

$$A^{\mathrm{c}}(E) = \tfrac{1}{2}B[r^2]_E \tag{47}$$

where $[f(\boldsymbol{r})]_E$ denotes the normalized coordinate-space average of f over the energetically accessible region ($\Phi(\boldsymbol{r}) < E$) of the billiard.

The system (46) provides a simple example for studying a possible chaos analogue of the Hannay angle. This should manifest itself as a time shift along the trajectories of the adiabatically rotated billiard. In analogy with the integrable case, we would expect it to be proportional to $\mathrm{d}A^c/\mathrm{d}E$. Thus the potential Φ is necessary for A^c to have a non-trivial energy dependence.

9. Discussion

Unitary/canonical families provide simple examples of the classical limit of the geometric phase for chaotic systems. In this case it is easy to show the classical 2-form is closed, and the alternative derivation of the periodic orbit corrections lends support to the formal general derivation given in RB. Certain characteristic features of the general case are absent, for example degeneracies and monopoles, and deterministic friction and Born–Oppenheimer forces—for unitary/canoncial families, the only reaction force to first order is geometric magnetism.

For canonical families it may be possible to define a chaos analogue of the Hannay angle, and the billiard of section 8 provides a good example for numerical experiment. It is hoped further study may suggest how to define this chaos analogue in the general case, or alternatively may illustrate the impossibility of doing so.

We conclude with some speculations motivated by the above. For a general parameterized family, the quantum/classical Hamiltonians are not unitarily/canonically related. But perhaps there is a unitary/canonical transformation which makes them look 'as similar as possible'. We might expect the geometric phase and its classical limit to have simple (and manifestly closed) expressions in terms of the infinitesimal generators of these transformations. On the quantum side, we have at hand the unitary transformation $U(\boldsymbol{R})$ which maps the eigenstates of $\hat{H} \stackrel{\mathrm{def}}{=} \hat{h}(\boldsymbol{R}_0)$, a given Hamiltonian chosen arbitrarily from the family, to those of $\hat{h}(\boldsymbol{R})$. Is there a classical analogue? One interesting possibility concerns families of Anosov Hamiltonians, for which there exists a transformation mapping the orbits of $H(z) \stackrel{\mathrm{def}}{=} h(z, \boldsymbol{R}_0)$ into orbits of $h(z, \boldsymbol{R})$ (Arnold and Avez 1989). In general this transformation is not canonical, and indeed may not be differentiable. However, the correspondence may be worth pursuing.

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Appendix

The definition of the classical generators,

$$\nabla\Phi(z, \boldsymbol{R}) = \mathbf{J} \cdot \partial_z \boldsymbol{g}(\Phi(z, \boldsymbol{R}), \boldsymbol{R}) \tag{A.1}$$

determines $\boldsymbol{g}$ up to a z-independent vector field (i.e. a parameter-dependent shift in the zero 'energies' of the 'Hamiltonians' $\boldsymbol{g}$.) We would like to remove this arbitrariness. Since $\nabla \wedge \nabla\Phi = 0$, (A.1) implies

$$\nabla \wedge \partial_z \boldsymbol{g} = \tfrac{1}{2}\partial_z \{\boldsymbol{g}, \wedge \boldsymbol{g}\}\,. \tag{A.2}$$

We try to fix g uniquely by imposing the z-antiderivative of (A.2),

$$\nabla \wedge g = \tfrac{1}{2}\{g, \wedge g\}. \tag{A.3}$$

(We remark that if the parameters constitute a Lie group, then (A.2), when reformulated in terms of the momentum map, describes a Lie algebra homomorphism at the level of vector fields; and (A.3), at the level of Hamiltonians. If (A.3) is satisfied globally, the group action Φ is said to be co-adjoint equivariant—Abraham and Marsden 1978.)

To show that (A.3) can be satisfied, first suppose g_0 satisfies (A1) but not (A3), and let

$$\alpha = \nabla \wedge g_0 - \tfrac{1}{2}\{g_0, \wedge g_0\}. \tag{A4}$$

From (A.2), α depends only on $\boldsymbol{R}$, so that $\{\alpha, f\}$ vanishes for arbitrary f. Then

$$\begin{aligned}\nabla\cdot\alpha &= -\tfrac{1}{2}\nabla\cdot\{g_0, \wedge g_0\} = \{g_0, \cdot\nabla\wedge g_0\} = \{g_0, \cdot(\tfrac{1}{2}\{g_0, \wedge g_0\} + \alpha)\} = \tfrac{1}{2}\{g_0, \cdot\{g_0, \wedge g_0\}\} \\ &= \tfrac{1}{2}\sum_{ijk} \epsilon_{ijk}\{g_{0i}, \{g_{0j}, g_{0k}\}\} = 0 \end{aligned} \tag{A5}$$

where the last equality follows from the Jacobi identity for Poisson brackets. Since $\nabla\cdot\alpha = 0$, α is given (locally at least) by $\nabla \wedge \beta$. Letting $g = g_0 + \beta$, one verifies that g satisfies (A.3).

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