The geometric phase for chaotic systems†

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The geometric phase acquired by the eigenstates of cycled quantum systems is given by the flux of a two-form through a surface in the system's parameter space. We obtain the classical limit of this two-form in a form applicable to systems whose classical dynamics is chaotic. For integrable systems the expression is equivalent to the Hannay two-form. We discuss various properties of the classical two-form, derive semiclassical corrections to it (associated with classical periodic orbits), and consider implications for the semiclassical density of degeneracies.

1. Introduction

Since its discovery (Berry 1984), considerable attention has been devoted to the geometric phase γ_n acquired by the eigenstates $|n\rangle$ of quantum systems $\hat{H}(R)$ whose parameters R are taken through a cycle C. According to one of a number of equivalent expressions,

$$\gamma_n = -\frac{1}{\hbar}\int_S V_n, \tag{1.1}$$

where S is a surface in parameter space bounded by C, and

$$V_n = -\mathrm{i}\hbar\langle \mathrm{d}n|\wedge|\mathrm{d}n\rangle \tag{1.2}$$

is the two-form whose flux through S is the geometric phase. There exist several extensive reviews of the geometric phase (see, for example, Shapere & Wilczek 1989). (Note: multiplying by $-\mathrm{i}$ in (2) is equivalent to taking the imaginary part, and the factor of $\hbar$ introduced will render V_n $\hbar$-independent in the classical limit.)

Given V_n, a quantum mechanical quantity of geometric origin, it is natural to ask what it corresponds to classically. For integrable systems this question was answered by Hannay (1985), who discovered a classical anholonomy for cycled integrable systems, analogous to the geometric phase. Hannay's two-form was subsequently shown to correspond to V_n in the classical limit (Berry 1985).

More generally, the correspondence principle, couched in geometrical language, asserts that in the classical limit, the spectral invariants of quantum systems correspond to the invariant manifolds of classical systems. For integrable systems the invariant manifolds are tori, and this correspondence is embodied in the torus wave functions and quantization conditions (Berry 1983) which form the basis for the semiclassical analysis of Berry (1985). The invariant manifolds of chaotic systems are the energy shells and the isolated periodic orbits contained therein. Semiclassical quantization conditions in terms of these are fundamentally more difficult than for the integrable case; the quest for such conditions lies at the heart of *quantum chaology* (see, for example, Gutzwiller 1990; Berry 1991; Keating 1991).

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As Hannay's two-form is associated with invariant tori, one would expect the classical two-form for chaotic systems to be associated with the energy shell and periodic orbits. A theory along these lines, along with some of the difficulties encountered, was previously discussed informally in Berry (1990). Here we present a complete account of the classical limit of the two-form in a form applicable to chaotic systems.

Before proceeding, let us mention an interesting though quite distinct extension of the Hannay two-form due to Montgomery (1988) and Golin *et al.* (1989). These authors consider classical hamiltonian systems with parameter-dependent continuous symmetries (though not necessarily integrable), and establish the existence of a unique (hamiltonian) connection, i.e. a prescription for lifting curves from parameter space to phase space (with certain additional properties). Crudely speaking, the connection describes the geometrical component of motion in the 'ignorable' coordinates (i.e. those conjugate to the momenta which generate the symmetries); in the integrable case these momenta are the actions, and the connection determines the geometrical component of the angle evolution, namely the Hannay angles.

Here we are considering a different problem; our concern is the intrinsic anholonomy, defined quantally but so far not classically, associated with ergodic hamiltonians with no symmetries at all. One might attempt to apply the preceding formalism to such systems, by regarding the dynamics itself as the symmetry, but the associated connection is ill defined, as the expressions for it diverge exponentially.

The paper is organized as follows. We introduce a time-dependent formalism for the quantum two-form (§2), from which its classical limit, our principal result, follows directly (§3). The cases of anticanonical symmetries and additional constants of the motion (in particular, integrable systems) are considered (§4), along with some specific examples (§5). We then develop an alternative formalism for both the quantum and classical two-forms (§6), which is used to establish formally that the two-form is closed (§7). Finally, we calculate the periodic orbit contributions to the two-form (§8) and its derivative, the density of degeneracies (§9). In the interest of maintaining continuity, the derivations of some results have been placed in Appendixes. Throughout we use the notation of differential forms; Arnold (1978) provides a good general reference.

2. Time-dependent quantum formalism

(*a*) *Derivation*

For chaotic systems, the classical limit of (1.2) is not directly accessible, because (and in contrast to integrable systems), semiclassical eigenstates are not known. As is customary in quantum chaology, we proceed by expressing the spectral property of interest (in this case, V_n) within a time-dependent formalism. Taking the classical limit is then a straightforward matter.

We start with the equation (Berry 1984)

$$V_n = -\mathrm{i}\hbar \sum_{m \neq n} \frac{\langle n|\mathrm{d}\hat{H}|m\rangle \wedge \langle m|\mathrm{d}\hat{H}|n\rangle}{(E_n - E_m)^2}. \tag{2.1}$$

Here, as elsewhere, d is the exterior derivative with respect to parameters R. Throughout the paper the R dependences are usually left implicit, though occasionally in the interest of clarity they are indicated explicitly.

The energy denominator in (2.1) may be expressed as a time integral;

$$(E_n - E_m)^{-2} = -\frac{1}{\hbar^2} \lim_{\epsilon \to 0} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\epsilon t}\, t \cos \omega_{nm} t, \tag{2.2}$$

where $\omega_{nm} = (E_n - E_m)/\hbar$. (Usually the convergence factor $\lim_{\epsilon \to 0} \exp(-\epsilon t)$ is left implicit.) The oscillations $\cos \omega_{nm} t$ may then be incorporated into time-dependent matrix elements, as in

$$\cos \omega_{nm} t \langle n | \mathrm{d}\hat{H} | m \rangle \wedge \langle m | \mathrm{d}\hat{H} | n \rangle$$
$$= \tfrac{1}{2}(\langle n | (\mathrm{d}\hat{H})_t | m \rangle \wedge \langle m | \mathrm{d}\hat{H} | n \rangle + \langle n | \mathrm{d}\hat{H} | m \rangle \wedge \langle m | (\mathrm{d}\hat{H})_t | n \rangle). \tag{2.3}$$

Here $(\mathrm{d}\hat{H})_t = U^\dagger(t)\,(\mathrm{d}\hat{H})\,U(t)$ is the time-evolved operator, in which $U(t)$ is the evolution operator at fixed R, namely

$$U(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}. \tag{2.4}$$

With the substitution of (2.3) and (2.2) into (2.1), the restriction $m \neq n$ on the sum is no longer necessary, and $\Sigma_m |m\rangle\langle m|$ gives the identity. Therefore

$$V_n = \frac{\mathrm{i}}{2\hbar} \int_0^\infty \mathrm{d}t\, t \langle n | (\mathrm{d}\hat{H})_t \wedge \mathrm{d}\hat{H} + \mathrm{d}\hat{H} \wedge (\mathrm{d}\hat{H})_t | n \rangle. \tag{2.5}$$

The sum of operators appearing in (2.5) is actually a commutator, i.e.

$$(\mathrm{d}\hat{H})_t \wedge \mathrm{d}\hat{H} + \mathrm{d}\hat{H} \wedge (\mathrm{d}\hat{H})_t = [(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}]. \tag{2.6}$$

At first this might appear surprising, since the commutator of two scalar operators is antisymmetric in its arguments. However, the commutator of operator one-forms is symmetric, the two antisymmetries cancelling as it were. To clarify this point, let us consider (as we often will in what follows) the 'reference' area element $\square_R$ in parameter space drawn in figure 1*a*, spanned by infinitesimal displacements r_1 and r_2 from R. The flux through $\square_R$ of $\mathrm{d}\hat{A} \wedge \mathrm{d}\hat{B} + \mathrm{d}\hat{B} \wedge \mathrm{d}\hat{A}$, as computed from the usual rules for two-forms, is

$$(\hat{A}_1 \hat{B}_2 - \hat{A}_2 \hat{B}_1) + (\hat{B}_1 \hat{A}_2 - \hat{B}_2 \hat{A}_1) \tag{2.7}$$

(here $\hat{A}_i \stackrel{\mathrm{def}}{=} \mathrm{d}\hat{A} \cdot r_i$ and similarly for $\hat{B}$), whereas the flux of $[\hat{A}, \wedge \hat{B}]$ through $\square_R$ is $[\hat{A}_1, \hat{B}_2] - [\hat{A}_2, \hat{B}_1]$, or

$$(\hat{A}_1 \hat{B}_2 - \hat{B}_2 \hat{A}_1) - (\hat{A}_2 \hat{B}_1 - \hat{B}_1 \hat{A}_2). \tag{2.8}$$

Clearly (2.7) and (2.8) are the same.

Substituting (2.6) into (2.5) we obtain

$$V_n = \frac{\mathrm{i}}{2\hbar} \int_0^\infty \mathrm{d}t\, t \langle n | [(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}] | n \rangle, \tag{2.9}$$

our principal formula for the quantum two-form. We may write it in a form more symmetrical with respect to time. Since expectation values of eigenstates are time invariant, $\langle n | (\mathrm{d}\hat{H})_t \wedge \mathrm{d}\hat{H} | n \rangle = \langle n | \mathrm{d}\hat{H} \wedge (\mathrm{d}\hat{H})_{-t} | n \rangle$. Therefore

$$V_n = \frac{\mathrm{i}}{4\hbar} \int_0^\infty \mathrm{d}t\, t \langle n | [(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}] | n \rangle. \tag{2.10}$$

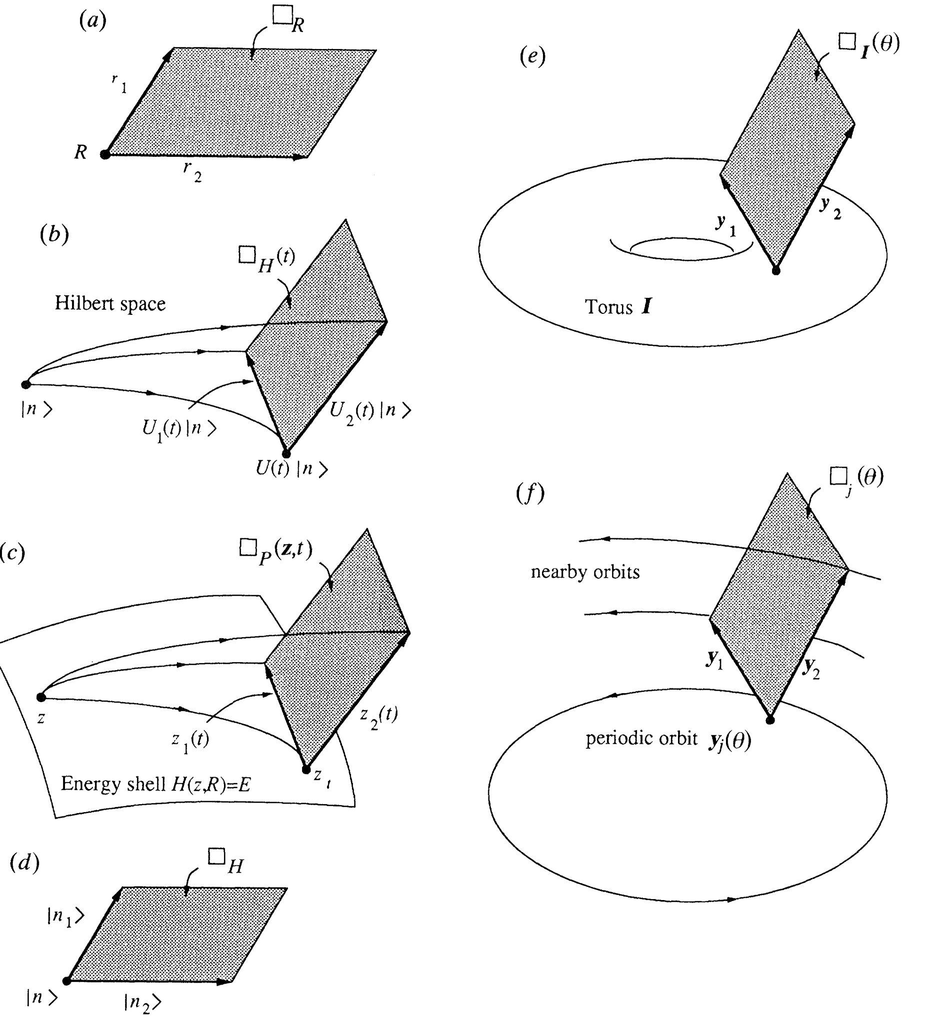

Figure 1. (a) area element $\square_R$ spanned by displacements r_1 and r_2 from R. (b)–(f) two-form fluxes through $\square_R$, as follows. (b) The time-dependent formula (6.2) relates $V_n \cdot \square_R$ to the time average of the symplectic area of $\square_H(t)$ in Hilbert space. (c) The time-dependent formula (6.8) relates $V^c(E) \cdot \square_R$ to the time and microcanonical averages of the symplectic area of $\square_P(z,t)$ in phase space. (d) The time-independent formula (1.2) relates $V_n \cdot \square_R$ to the symplectic area of $\square_H$ in Hilbert space. (e) The time-independent formula (G 1) relates $V^c_I \cdot \square_R$ to the symplectic area of $\square_P(\theta)$ in phase space. (f) The periodic orbit two-form (8.10).

(b) *Antiunitary symmetries*

An antiunitary symmetry $\hat{K}$, such as time-reversal, takes inner products to their complex conjugates and commutes with the hamiltonian;

$$\langle \hat{K}\cdot\psi \,|\, \hat{K}\cdot\phi\rangle = \langle\psi\,|\,\phi\rangle^*, \tag{2.11a}$$

$$\hat{H}\hat{K} = \hat{K}\hat{H}. \tag{2.11b}$$

If (2.11b) holds for all parameters, the two-form satisfies

$$V_n = -V_{\bar{n}}, \tag{2.12}$$

where $|\bar{n}\rangle = \hat{K}|n\rangle$. In particular, if $|n\rangle$ is invariant under $\hat{K}$, then V_n vanishes.

The symmetry property (2.12) is easily obtained from (1.2) and can be also made manifest in the new formula (2.10). We note that

$$\hat{K}(\mathrm{d}\hat{H})_t = (\mathrm{d}\hat{H})_{-t}\hat{K}, \tag{2.13}$$

because: (i) time-evolved operators $\hat{A}_t$ transform according to $\hat{K}\hat{A}_t = \bar{\hat{A}}_{-t}\hat{K}$, where $\bar{\hat{A}} = \hat{K}\hat{A}\hat{K}^{-1}$, and (ii) from (2.11$b$) $\mathrm{d}\bar{\hat{H}} = \mathrm{d}\hat{H}$. Turning to the expectation value in (2.10), computed for $|\bar{n}\rangle$ rather than $|n\rangle$,

$$\begin{aligned}\langle \bar{n}|[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]|\bar{n}\rangle &= \langle \hat{K}\cdot n|\,[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]\,\hat{K}\cdot n\rangle \\ &= \langle \hat{K}\cdot n|\,\hat{K}[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]\cdot n\rangle = \langle n|[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]|n\rangle^*,\end{aligned} \tag{2.14}$$

where in the third equality we have used (2.13), and in the last equality the antiunitary property (2.11a). Since the expectation value of the commutator in the last term is pure imaginary, it follows that

$$\begin{aligned}\langle \bar{n}|[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]|\bar{n}\rangle &= \langle n|[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]\cdot n\rangle^* \\ &= -\langle n|[(\mathrm{d}\hat{H})_t + (\mathrm{d}\hat{H})_{-t}, \wedge\, \mathrm{d}\hat{H}]\cdot n\rangle,\end{aligned} \tag{2.15}$$

and (2.12) follows immediately.

3. Classical limit

(a) *Wigner–Weyl formalism*

The classical limit of (2.9) is carried out within the Wigner–Weyl formalism, the defining relation of which is the following correspondence between operators $\hat{A}$ and phase space functions $A(z)$,

$$A(z) = \int \mathrm{d}^N \boldsymbol{s}\, \langle \boldsymbol{q} + \tfrac{1}{2}\boldsymbol{s}|\hat{A}|\boldsymbol{q} - \tfrac{1}{2}\boldsymbol{s}\rangle\, \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{s}/\hbar}, \tag{3.1}$$

where $z = (\boldsymbol{q}, \boldsymbol{p})$. $A(z)$ is called the Weyl symbol, or simply the symbol of $\hat{A}$; sometimes we write $(\hat{A})_W(z)$ for $A(z)$. There is nothing intrinsically semiclassical or approximate about the Wigner–Weyl correspondence; it is simply another formalism for exact quantum mechanics. However, it lends itself to semiclassical approximations in which the canonical structure of classical mechanics is manifest. For discussions and reviews, see Groenewold (1946), Moyal (1949), Baker (1958).

V_n is expressed in (2.9) as the time integral of an expectation value. In the Wigner–Weyl formalism, expectation values of operators correspond to phase space averages of symbols. In particular,

$$\langle n|[(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}]|n\rangle = \int \mathrm{d}^{2N} z\, W_n(z)\,([(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}])_W(z). \tag{3.2}$$

$W_n(z)$ is the symbol of the projection $|n\rangle\langle n|$, and is also called the Wigner function.

For chaotic systems, the simplest and crudest semiclassical approximation is to replace $W_n(z)$ by the microcanonical density, namely

$$W_n(z) \to \delta(E - H(z))/\Omega'(E) \tag{3.3}$$

Here $H(z)$, an abbreviation for $H(z, R)$, is the classical hamiltonian, i.e. the symbol of $\hat{H}$. The normalization factor

$$\Omega'(E) = \int \mathrm{d}^{2N} z\, \delta(E - H(z))$$

is the volume of the energy shell, whose energy E is quantized in this lowest approximation according to the rule

$$\Omega(E_n) = nh^N, \tag{3.4}$$

which associates a quantum state to each phase space cell of volume h^N.

$$\Omega(E) = \int \mathrm{d}^{2N}z\,\Theta(E-H(z))$$

is the phase space volume with energy less than E. Refinements to (3.3), involving classical periodic orbits, are discussed in §8.

Next we consider $([(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}])_W$. To lowest order in $\hbar$, the symbol of the commutator of two operators is given by $\mathrm{i}\hbar$ times the Poisson bracket of their symbols. Thus

$$([(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}])_W \rightarrow \mathrm{i}\hbar\{((\mathrm{d}\hat{H})_t)_W, \wedge\, \mathrm{d}H\}. \tag{3.5}$$

Like its commutator analogue, the Poisson bracket of one-forms is symmetric rather than antisymmetric in its arguments. (Explicitly, the flux of $\{\mathrm{d}A, \wedge\, \mathrm{d}B\}$ through $\square_R$ is given by $\{A_1, B_2\}+\{A_2, B_1\}$, where $A_i \overset{\text{def}}{=} \mathrm{d}A\cdot r_i$, $B_i \overset{\text{def}}{=} \mathrm{d}B\cdot r_i$.) The symbol of a time-evolved operator is given, to lowest order in $\hbar$, by its classically time-evolved symbol. If we define the time-evolved function $A_t(z) \overset{\text{def}}{=} A(z_t)$, where z_t is the trajectory from z at time t, then

$$((\mathrm{d}\hat{H})_t)_W \rightarrow (\mathrm{d}H)_t. \tag{3.6}$$

(An explication of notation might be helpful at this point: $(\mathrm{d}H)_t$, evaluated at z and R, is just $H(z_t, R+\mathrm{d}R)-H(z_t, R)$ 'to first order in $\mathrm{d}R$'.) Then from (3.5) and (3.6),

$$([(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}\hat{H}])_W \rightarrow \mathrm{i}\hbar\{(\mathrm{d}\hat{H})_t, \wedge\, \mathrm{d}H\}. \tag{3.7}$$

Let us mention that both (3.5) and (3.6) give the lowest-order terms in formal power series expansion in $\hbar$. The next terms are of order $\hbar^2$ higher than the leading one (see Voros 1976), so that the next term in (3.7) is of order $\hbar^3$.

Substituting (3.3) and (3.7) into (3.2) and (2.9) we obtain the classical limit of the two-form,

$$V_n \rightarrow V^{\mathrm{c}}(E) = -\frac{1}{2}\int_0^\infty \mathrm{d}t\, t\langle\{(\mathrm{d}H)_t, \wedge\, \mathrm{d}H\}\rangle_E. \tag{3.8}$$

(In general $\langle f\rangle_E$ denotes the microcanonical average

$$\int \mathrm{d}^{2N}z\,\delta(E-H)f/\Omega'(E).$$

When there is no risk of confusion we simply write $\langle f\rangle$, leaving the energy dependence implicit.) For given n, E is quantized according to the approximation (3.4).

(b) *Convergent formula*

For chaotic systems, it is not clear that the expression in (3.8) is convergent. The reason is that the Poisson bracket $\{(\mathrm{d}H)_t, \wedge\, \mathrm{d}H\}(z)$ grows exponentially in time. To see this, note that in general

$$\{A_t, B\}(z) = \boldsymbol{A}'(z_t)\cdot \boldsymbol{S}(z,t)\boldsymbol{J}\cdot \boldsymbol{B}'(z), \tag{3.9}$$

where $\boldsymbol{A}'(z)$ and $\boldsymbol{B}'(z)$ are phase space gradients, $\boldsymbol{J}$ is the Poisson tensor

$$\boldsymbol{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{3.10}$$

and

$$S_{ij}(z,t) = \partial Z_i(z,t)/\partial z_j \tag{3.11}$$

is the linearized flow, where $\boldsymbol{Z}(z,t) \overset{\text{def}}{=} z_t$ is the flow. The exponential growth of $\boldsymbol{S}(z,t)$ (which would imply the same of (3.9)) is the very definition of chaos.

To make sense of the classical limit of the two-form we require a manifestly convergent formula. This can be obtained by means of an identity which eliminates the z derivatives in (3.8),

$$\langle \{(\mathrm{d}A)_t, \wedge \mathrm{d}B\} \rangle_E = (1/\Omega')\,(\Omega' \langle (\mathrm{d}\dot{A})_t \wedge \mathrm{d}B \rangle_E)'. \tag{3.12}$$

The derivation is given in Appendix A. The prime ($'$) denotes the derivative with respect to energy, and the dot ($\cdot$) the derivative with respect to time. While (3.9) implies that $\{A_t, B\}$ (z) is exponentially divergent in t, (3.12) implies that it is oscillatory in z, and that the exponential oscillations cancel in the main when averaged over the energy shell. Substituting (3.12) into (3.8),

$$V^{\mathrm{c}}(E) = -\frac{1}{2\Omega'}\left(\Omega' \int_0^\infty \mathrm{d}t\, t \langle (\mathrm{d}\dot{H})_t \wedge \mathrm{d}H \rangle_E \right)'. \tag{3.13}$$

($(\mathrm{d}\dot{H})_t$ denotes the derivative of $(\mathrm{d}H)_t$ with respect to t.) We integrate by parts,

$$\int_0^\infty \mathrm{d}t\, t (\mathrm{d}\dot{H})_t = \lim_{\epsilon \to 0} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\epsilon t} t (\mathrm{d}\dot{H})_t = -\int_0^\infty \mathrm{d}t (\mathrm{d}H)_t \tag{3.14}$$

(the reinstated convergence factor of (2.2) justifies the neglect of the boundary term), and obtain

$$V^{\mathrm{c}}(E) = \frac{1}{2\Omega'}\left(\Omega' \int_0^\infty \mathrm{d}t \,\langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle_E \right)'. \tag{3.15}$$

This is our principal formula for the classical two-form. Like the quantum formula (2.9) it can be made more symmetrical with respect to time. Since microcanonical averages are time invariant, we get that $\langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle = \langle \mathrm{d}H \wedge (\mathrm{d}H)_{-t} \rangle = -\langle (\mathrm{d}H \rangle_{-t} \wedge \mathrm{d}H \rangle$. Therefore

$$V^{\mathrm{c}}(E) = \frac{1}{4\Omega'}\left(\Omega' \int_0^\infty \mathrm{d}t \,\langle ((\mathrm{d}H)_t - (\mathrm{d}H)_{-t}) \wedge \mathrm{d}H \rangle_E \right)'. \tag{3.16}$$

From (3.15), the convergence of $V^{\mathrm{c}}(E)$ depends on the behaviour of the correlation function $\langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle$. If the dynamics is *mixing* (Arnold & Avez 1989), then

$$\lim_{t \to \infty} \langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle = \langle \mathrm{d}H \rangle \wedge \langle \mathrm{d}H \rangle = 0. \tag{3.17}$$

In fact, we shall assume the rate of mixing (i.e. the rate at which $\langle A_t B \rangle \to \langle A \rangle \langle B \rangle$) is sufficiently rapid so that

$$\int_0^\infty \mathrm{d}t \,\langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle$$

converges. This is certainly true for hyperbolic (or Axiom A) systems, for which the mixing rate is exponential (see Ruelle 1986), but clearly holds for power law mixing rates $t^{-\nu}$ with $\nu > 1$. (As discussed in §4*c*, (3.15) also holds for integrable systems, which are not mixing at all, essentially because the correlation functions are quasi-periodic.)

Because the dynamics is ergodic,

$$\langle (\mathrm{d}H)_t \wedge \mathrm{d}H \rangle_E = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}\tau \, \mathrm{d}H(z_{t+\tau}) \wedge \mathrm{d}H(z_\tau) \tag{3.18}$$

for almost all initial conditions z. Therefore, the phase space integrals of (3.15) may be replaced by time integrals along a single trajectory, and the energy derivative obtained by varying the energy of the initial condition. Use of (3.18) would considerably facilitate numerical computations, as $V^{\mathrm{c}}(E)$ could be computed from just a pair of trajectories with slightly separated energies E and $E+\epsilon$.

Finally, let us mention an equivalent form of (3.15) of some theoretical interest. Considering the quantum two-form for the moment, we note that because it depends only on the eigenstates of $\hat{H}$ (and not on the energy levels), it is unchanged if $\hat{H}$ is replaced by a (possibly parameter-dependent) function of itself. The same is true of the classical two-form; it is easy to verify that V^{c} remains unchanged if $H(z, R)$ is replaced by

$$G(z,R) \overset{\mathrm{def}}{=} g(H(z,R),R), \tag{3.19}$$

where $g = g(E,R)$ is a function of energy and parameters. (The effect on the dynamics of this substitution is simply to rescale the time.) A natural representative for the family of 'hamiltonians' defined by (3.19) is the volume function

$$\Omega_P(z,R) \overset{\mathrm{def}}{=} \Omega(H(z,R),R)$$

(whose quantum analogue is the counting operator $\hat{\Omega} = \Sigma_n n \,|\, n\rangle \langle n|$), in terms of which

$$V^{\mathrm{c}}(\omega) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\omega} \int_0^\infty \mathrm{d}\sigma \, \langle (\mathrm{d}\Omega_P)_\sigma \wedge \mathrm{d}\Omega_P \rangle_\omega. \tag{3.20}$$

Here the expectation value $\langle \cdot \rangle_\omega$ is taken over that energy shell which contains phase volume ω, and $(\mathrm{d}\Omega_P)_\sigma$ denotes $\mathrm{d}\Omega_P$ evolved under the dynamics of Ω_P for a fictitious time σ. For one-dimensional systems, (3.20) is closely related to equation (9) of Hannay (1985).

4. Symmetries

(*a*) *Anticanonical symmetries*

The classical analogue of an antiunitary symmetry $\hat{K}$ (cf. (2.11)) is an anticanonical symmetry K (Robnik & Berry 1986), a phase space transformation which reverses the sign of Poisson brackets and commutes with the hamiltonian;

$$\{A \circ K, B \circ K\} = -\{A, B\} \circ K, \tag{4.1a}$$

$$H \circ K = H. \tag{4.1b}$$

(Here $\circ$ denotes composition, so that $(H \circ K)(z) = H(K(z))$.) Time reversal, in the form $K(\boldsymbol{q}, \boldsymbol{p}) = (\boldsymbol{q}, -\boldsymbol{p})$, is the prototypical example.

Suppose a system possesses an anticanonical symmetry K. In general, the energy shell $\{z \mid H(z) = E\}$ will be composed of distinct connected components mapped into each other by K. Let Γ_E and $\bar{\Gamma}_E$ be two such components, related by $\bar{\Gamma}_E = K(\Gamma_E)$ (it could be that $\Gamma_E = \bar{\Gamma}_E$, i.e. that Γ_E is invariant under K). Let $V^c(E)$ and $\bar{V}^c(E)$ be the associated two-forms obtained by restricting the microcanonical average in (3.16) to Γ_E and $\bar{\Gamma}_E$ respectively. Then, in analogy with (2.12), the classical two-form obeys

$$\bar{V}^c(E) = -V^c(E). \tag{4.2}$$

In particular, if $\Gamma_E = \bar{\Gamma}_E$, then $V^c(E)$ vanishes.

The proof of (4.2) is quite similar to that of (2.12). Calculating $\bar{V}^c(E)$ from (3.16) and integrating over $K(z)$ rather than z (a volume-preserving change of variable),

$$\begin{aligned}\bar{V}^c(E) &= \frac{1}{4\Omega'}\int_0^\infty \mathrm{d}t \int \mathrm{d}^{2N} z\, \delta'_{\bar{\Gamma}}(E-H)\,((\mathrm{d}H)_t - (\mathrm{d}H)_{-t}) \wedge \mathrm{d}H \\ &= \frac{1}{4\Omega'}\int_0^\infty \mathrm{d}t \int \mathrm{d}^{2N} z\, \delta'_{\bar{\Gamma}}(E-H\circ K)\,((\mathrm{d}H)_t\circ K - (\mathrm{d}H)_{-t}\circ K) \wedge (\mathrm{d}H\circ K). \end{aligned} \tag{4.3}$$

Here $\delta'_{\bar{\Gamma}}(E-H)$ denotes the restriction of $\delta'(E-H)$ to $\bar{\Gamma}_E$, and $\Omega'(E) = \bar{\Omega}'(E)$ is the volume of Γ_E or $\bar{\Gamma}_E$. Since anticanonical symmetries reverse the sense of time (easily shown), $\boldsymbol{Z}(t)\circ K = K\circ \boldsymbol{Z}(-t)$, or more explicitly $\boldsymbol{Z}(K(z), t) = K(\boldsymbol{Z}(z, -t))$. Therefore $(\mathrm{d}H)_t\circ K \overset{\text{def}}{=} \mathrm{d}H\circ \boldsymbol{Z}(t)\circ K = \mathrm{d}H\circ K\circ \boldsymbol{Z}(-t)$. But $\mathrm{d}H\circ K = \mathrm{d}H$ (K is a symmetry), so that

$$(\mathrm{d}H)_t\circ K = \mathrm{d}H\circ \boldsymbol{Z}(-t) = (\mathrm{d}H)_{-t}, \quad (\mathrm{d}H)_{-t}\circ K = (\mathrm{d}H)_t. \tag{4.4}$$

Substituting the preceding into (4.3),

$$\bar{V}^c(E) = -\frac{1}{4\Omega'}\int_0^\infty \mathrm{d}t \int \mathrm{d}^{2N} z\, \delta'_{\bar{\Gamma}}(E-H\circ K)\,((\mathrm{d}H)_t - (\mathrm{d}H)_{-t}) \wedge \mathrm{d}H. \tag{4.5}$$

Since $\delta'_{\bar{\Gamma}}(E-H\circ K) = \delta'_{\Gamma}(E-H)$, the right-hand side is just $-V^c(E)$, and the symmetry property (4.2) follows directly.

(*b*) *Additional constants of the motion*

Before considering integrable systems we first consider the more general case in which there are k commuting constants of the motion, with $1 \leqslant k \leqslant N$. Ergodic systems correspond to $k = 1$, integrable systems to $k = N$. Let $\boldsymbol{F} = (F_1, \ldots, F_k)$ denote the constants of motion.

Assuming the dynamics is ergodic on the invariant manifold $\{z \mid \boldsymbol{F}(z) = \boldsymbol{f}\}$, there is a straightforward generalization of the classical two-form. Equation (3.8) is still valid if the microcanonical density is reinterpreted to be $\delta^k(\boldsymbol{f}-\boldsymbol{F})/D(\boldsymbol{f})$, where

$$D(\boldsymbol{f}) = \int \mathrm{d}^{2N} z\, \delta^k(\boldsymbol{f}-\boldsymbol{F})$$

is the volume of the invariant manifold. Thus

$$V^c(\boldsymbol{f}) = -\frac{1}{2}\int_0^\infty \mathrm{d}t\, t \langle\{(\mathrm{d}H)_t, \wedge\, \mathrm{d}H\}\rangle_{\boldsymbol{f}}. \tag{4.6}$$

From a straightforward generalization of (3.12) (derived in Appendix A),

$$\langle\{(\mathrm{d}H)_t, \wedge\, \mathrm{d}H\}\rangle_{\boldsymbol{f}} = (1/D)\,\nabla_{\boldsymbol{f}}\cdot(D\langle\{(\mathrm{d}H)_t, \boldsymbol{F}\}\wedge \mathrm{d}H\rangle_{\boldsymbol{f}}). \tag{4.7}$$

But $\{(\mathrm{d}H)_t, \boldsymbol{F}\} = \{\mathrm{d}H, \boldsymbol{F}_{-t}\}_t$, since Poisson brackets are preserved by the dynamics, and $\{\mathrm{d}H, \boldsymbol{F}_{-t}\}_t = \{\mathrm{d}H, \boldsymbol{F}\}_t$, since $\boldsymbol{F}$ is a constant of the motion. However, $\{\mathrm{d}H, \boldsymbol{F}\} = \mathrm{d}\{H, \boldsymbol{F}\} - \{H, \mathrm{d}\boldsymbol{F}\}$, and $\mathrm{d}\{H, \boldsymbol{F}\} = 0$, again because $\boldsymbol{F}$ is a constant of the motion. Therefore

$$\{(\mathrm{d}H)_t, \boldsymbol{F}\} = -\{H, \mathrm{d}\boldsymbol{F}\}_t = (\mathrm{d}\dot{\boldsymbol{F}})_t. \tag{4.8}$$

Substituting (4.8) and (4.7) into (4.6) and integrating by parts over t, we obtain

$$V^{\mathrm{c}}(\boldsymbol{f}) = \frac{1}{2D}\nabla_f \cdot \left(D\int_0^\infty \mathrm{d}t\, \langle (\mathrm{d}\boldsymbol{F})_t \wedge \mathrm{d}H\rangle_f\right), \tag{4.9}$$

the required generalization of (3.15).

(c) *Integrable systems*

Take the constants of motion $\boldsymbol{F}$ to be the actions $\boldsymbol{I}$. Then $D(\boldsymbol{I}) = (2\pi)^N$ (obtained from integration over the angles $\boldsymbol{\theta}$), and

$$V^{\mathrm{c}}(\boldsymbol{I}) = \frac{1}{2}\int_0^\infty \mathrm{d}t\, \nabla_I \cdot \langle (\mathrm{d}\boldsymbol{I})_t \wedge \mathrm{d}H\rangle_I. \tag{4.10}$$

We obtain a more explicit formula by expanding $\mathrm{d}H$ in a Fourier series,

$$\mathrm{d}H(\boldsymbol{\theta}, \boldsymbol{I}) = \sum_{\boldsymbol{m}} h_{\boldsymbol{m}}(\boldsymbol{I}) \exp(\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{\theta}), \tag{4.11}$$

in which the coefficients $h_{\boldsymbol{m}}$ are one-forms. (Note that $\mathrm{d}H$ is the derivative of $H(\boldsymbol{z}, R)$ with $\boldsymbol{z}$, rather than $(\boldsymbol{\theta}, \boldsymbol{I})$, held fixed.) The Fourier coefficients $\boldsymbol{i}_{\boldsymbol{m}}$ of $\mathrm{d}\boldsymbol{I}$ may be expressed in terms of the $h_{\boldsymbol{m}}$s. Expanding the relation $\{\mathrm{d}\boldsymbol{I}, H\} = \{\mathrm{d}H, \boldsymbol{I}\}$ (the derivative of $\{\boldsymbol{I}, H\} = 0$) in a Fourier series, we obtain $\mathrm{i}(\boldsymbol{m}\cdot\boldsymbol{\omega})\,\boldsymbol{i}_{\boldsymbol{m}} = \mathrm{i}\boldsymbol{m}h_{\boldsymbol{m}}$, where $\boldsymbol{\omega} = \nabla_I H$ are the frequencies. Therefore

$$\boldsymbol{i}_{\boldsymbol{m}} = h_{\boldsymbol{m}}\boldsymbol{m}/(\boldsymbol{m}\cdot\boldsymbol{\omega}). \tag{4.12}$$

The dynamics is simply $\boldsymbol{\theta}_t = \boldsymbol{\theta} + \boldsymbol{\omega}t$. Substituting the Fourier series for $(\mathrm{d}\boldsymbol{I})_t$ and $\mathrm{d}H$ into (4.9), we readily carry out the torus average $\langle\cdot\rangle_I$ and time integral (the latter after reinstating the convergence factor of (2.2)) and obtain

$$V^{\mathrm{c}}(\boldsymbol{I}) = \tfrac{1}{2}\mathrm{i}\sum_{\boldsymbol{m}\neq 0} (\boldsymbol{m}\cdot\nabla_I)\frac{h_{\boldsymbol{m}} \wedge h_{-\boldsymbol{m}}}{(\boldsymbol{m}\cdot\boldsymbol{\omega})^2}. \tag{4.13}$$

As $h_{-\boldsymbol{m}} = h_{\boldsymbol{m}}^*$, $V^{\mathrm{c}}(\boldsymbol{I})$ is real. In Appendix B we show that (4.13) is equivalent to the Hannay two-form.

5. Examples

(a) *Uniform magnetic field*

In appropriate units the hamiltonian of a three-dimensional charged particle in a uniform magnetic field $\boldsymbol{B}$ is given by

$$H = \tfrac{1}{2}(\boldsymbol{p} - \boldsymbol{A})^2 + V(\boldsymbol{r}), \quad \boldsymbol{A} = \tfrac{1}{2}\boldsymbol{B}\times\boldsymbol{r}. \tag{5.1}$$

We take the parameters of H to be the components of the magnetic field and use vector notation for parameter space, writing $\nabla_{\boldsymbol{B}}$ instead of d. Straightforward calculation gives

$$\nabla_{\boldsymbol{B}} H = -\tfrac{1}{2}\boldsymbol{l}, \tag{5.2}$$

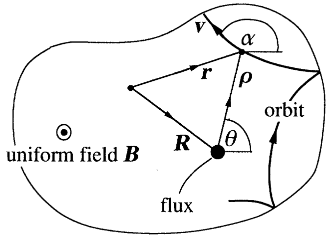

Figure 2. Aharonov–Bohm billiard. The particle at $\boldsymbol{r}$ moves with velocity $\boldsymbol{v} = (v, \alpha)$ in uniform background field B, and a flux line is located at $\boldsymbol{R}$. $\boldsymbol{\rho} = \boldsymbol{r} - \boldsymbol{R} = (\rho, \theta)$.

where $\boldsymbol{l} = \boldsymbol{r} \times \boldsymbol{v}$ is the mechanical angular momentum and $\boldsymbol{v} = \boldsymbol{p} - \boldsymbol{A}$ is the velocity $\dot{\boldsymbol{r}}$. The two-form $\boldsymbol{V}^{\mathrm{c}}(E, \boldsymbol{B})$ is a vector field in $\boldsymbol{B}$-space and is given by

$$\boldsymbol{V}^{\mathrm{c}}(E, \boldsymbol{B}) = \frac{1}{4\Omega'}\left(\Omega' \int_0^\infty \mathrm{d}t \, \langle (\boldsymbol{l}_t - \boldsymbol{l}_{-t}) \times \boldsymbol{l} \rangle_{E, \boldsymbol{B}}\right)'. \tag{5.3}$$

At $\boldsymbol{B} = 0$ the hamiltonian is invariant under the time reversal transformation $(\boldsymbol{r}, \boldsymbol{v}) \rightarrow (\boldsymbol{r}, -\boldsymbol{v})$. Under this transformation $\boldsymbol{l} \rightarrow -\boldsymbol{l}$ and $\boldsymbol{l}_t \rightarrow -\boldsymbol{l}_{-t}$. Since microcanonical averages are invariant under time reversal,

$$\langle (\boldsymbol{l}_t - \boldsymbol{l}_{-t}) \times \boldsymbol{l} \rangle = -\langle (\boldsymbol{l}_t - \boldsymbol{l}_{-t}) \times \boldsymbol{l} \rangle, \tag{5.4}$$

which in turn implies that $V^{\mathrm{c}}(E, \boldsymbol{B})$ vanishes when $\boldsymbol{B} = 0$. Note that this conclusion is *not* a consequence of (4.2). Equation (4.2) is derived for an anticanonical symmetry which holds for all parameters, whereas the hamiltonian (5.1) is time-reversal invariant only for $\boldsymbol{B} = 0$.

$V^{\mathrm{c}}(E, \boldsymbol{B})$ is not invariant under parameter-dependent gauge transformations of the vector potential $\boldsymbol{A}$, in spite of its expression in terms of the mechanical angular momentum. Under the gauge transformation $\boldsymbol{A}(\boldsymbol{r}) \rightarrow \boldsymbol{A}(\boldsymbol{r}) + \nabla_{\boldsymbol{r}} \psi(\boldsymbol{r}, \boldsymbol{B})$,

$$\nabla_{\boldsymbol{B}} H \rightarrow \nabla_{\boldsymbol{B}} H - \nabla_{\boldsymbol{B}}(\boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} \psi), \tag{5.5}$$

and $\boldsymbol{V}^{\mathrm{c}}(E, \boldsymbol{B})$ transforms accordingly. The analogous behaviour of the quantum two-form is discussed in Mondragon & Berry (1988). (There it is noted that, although the geometrical and dynamical phases are not separately gauge invariant, their sum is.)

(*b*) *Aharonov–Bohm billiard in uniform magnetic field.*

A particle is confined to a two-dimensional billiard threaded by an infinitely thin unit solenoid (e.g. the flux line of a magnetic monopole) in a constant background magnetic field. In suitable units the hamiltonian is

$$\boldsymbol{H} = \tfrac{1}{2}(\boldsymbol{p} - \boldsymbol{A}_{\mathrm{s}} - \boldsymbol{A}_{\mathrm{b}})^2, \quad \boldsymbol{A}_{\mathrm{s}} = (\hat{\boldsymbol{z}} \times \boldsymbol{\rho})/\rho^2, \quad \boldsymbol{A}_{\mathrm{b}} = \tfrac{1}{2}B\hat{\boldsymbol{z}} \times \boldsymbol{r}, \tag{5.6}$$

where (see figure 2) $\boldsymbol{r} = (x, y)$ are the particle coordinates, $\boldsymbol{R} = (X, Y)$ are the solenoid coordinates, and $\boldsymbol{\rho} = \boldsymbol{r} - \boldsymbol{R}$. $\boldsymbol{A}_{\mathrm{s}}$ and $\boldsymbol{A}_{\mathrm{b}}$ are the vector potentials of the solenoid and the background field, respectively. One can verify that $\boldsymbol{B}_{\mathrm{s}} = 2\pi\delta^2(\boldsymbol{\rho})\,\hat{\boldsymbol{z}}$ and $\boldsymbol{B}_{\mathrm{b}} = B\hat{\boldsymbol{z}}$.

We take $\boldsymbol{R}$, the coordinates of the solenoid, as the parameters of the system. (We could if we wished include B, the background field strength, and introduce another parameter for the solenoid strength.) We use vector notation for parameter space, writing $\nabla_{\boldsymbol{R}}$ instead of d. Omitting straightforward calculations, we get that

$$\nabla_{\boldsymbol{R}} H = \hat{\boldsymbol{z}} \times (\boldsymbol{v}_{\perp} - \boldsymbol{v}_{\parallel})/\rho^2 \tag{5.7a}$$

$$= (-v/\rho^2)\,(\sin(\alpha - 2\theta), \cos(\alpha - 2\theta)), \tag{5.7b}$$

where $\boldsymbol{v} = \boldsymbol{p} - \boldsymbol{A}_s - \boldsymbol{A}_b$ is the velocity $\dot{\boldsymbol{r}}$. Equation (5.5a) is expressed in terms of the components of $\boldsymbol{v}$ parallel and perpendicular to $\hat{\boldsymbol{\rho}}$, namely $\boldsymbol{v}_\parallel = (\hat{\boldsymbol{\rho}}\cdot\boldsymbol{v})\,\hat{\boldsymbol{\rho}}$ and $\boldsymbol{v}_\perp = \boldsymbol{v} - \boldsymbol{v}_\parallel$. Equation (5.5$b$) is expressed in terms of the polar coordinates of $\boldsymbol{v}$ and $\boldsymbol{\rho}$, namely $\boldsymbol{\rho} = \rho\,(\cos\theta, \sin\theta)$ and $\boldsymbol{v} = v\,(\cos\alpha, \sin\alpha)$.

For this system Ω' is a constant equal to $2\pi A$, where A is the area of the billiard, and $v = |\boldsymbol{v}|$ is a constant of the motion. The two-form is a scalar field in $\boldsymbol{R}$-space given by

$$V^{\mathrm{c}}(E,R) = \left(\int_0^\infty \mathrm{d}t \left\langle \frac{(\boldsymbol{v}_\perp)_t - (\boldsymbol{v}_\parallel)_t}{\rho_t^2} \times \frac{\boldsymbol{v}_\perp - \boldsymbol{v}_\parallel}{\rho^2} \right\rangle\right)' \tag{5.8a}$$

$$= \left(-v^2 \int_0^\infty \mathrm{d}t \left\langle \frac{\sin\left(2(\theta_t - \theta) - (\alpha_t - \alpha)\right)}{\rho_t^2\,\rho^2} \right\rangle\right)'. \tag{5.8b}$$

Let us point out some features of (5.8). For trajectories which either start (resp. end) at the solenoid, ρ (resp. ρ_t) vanishes, and the integrand is singular. However, the contribution of these singularities to $V^{\mathrm{c}}(E,\boldsymbol{R})$ is finite. (See Appendix C.) Next, in the absence of a background field (i.e. $B = 0$), the dynamics is time-reversal invariant, and with an argument similar to the one in §5a, one can show that $V^{\mathrm{c}}(E,\boldsymbol{R})$ vanishes identically. Thus, even though the solenoid breaks the time-reversal invariance of the hamiltonian, the background field is needed to produce a non-zero two-form. Finally, one can show that $V^{\mathrm{c}}(E,\boldsymbol{R})$ vanishes if the solenoid lies outside the billiard. (This is intuitively clear but is not obvious from (5.8). It does follow immediately from the alternative formula (6.8) derived in the next section.) Thus $\boldsymbol{R}$-space is effectively the billiard itself.

The Aharonov–Bohm billiard in a uniform background field is perhaps the simplest example of a chaotic system for which the classical two-form is non-trivial. It is two-dimensional, the minimum required for chaos. The dynamics may be computed without having to solve differential equations (the trajectories are circular arcs specularly reflected at the billiard boundary.) Finally, the dynamics is independent of the parameters $\boldsymbol{R}$ (as $\boldsymbol{B}_s$ vanishes everywhere but at a point, only a zero measure set of trajectories is affected by it.) In light of the discussion following (3.18), a numerical calculation would require only a pair of trajectories, with slightly separated energies, to determine $V^{\mathrm{c}}(E,\boldsymbol{R})$ for all $\boldsymbol{R}$. A variant of this example (not quite as simple) is a billiard in crossed uniform electric and magnetic fields. The magnetic field is normal to the billiard, the electric field tangent to it, and the two field strengths and the direction of the electric field are natural parameters.

6. Alternative form

We obtain a useful alternative expression for the classical two-form, (6.8) below. Instead of deriving it directly from (3.15), we begin with an alternative expression for the quantum two-form (6.2) below) which is of independent interest.

(a) *Quantum formula*

The alternative quantum formula follows from an identity,

$$-\tfrac{1}{2}\mathrm{i}\hbar\langle \mathrm{d}U(t)\cdot n| \wedge |\,\mathrm{d}U(t)\cdot n\rangle = V_n + \tfrac{1}{2}\mathrm{i}\hbar \sum_{j\neq n} \langle \mathrm{d}n\,|j\rangle \wedge \langle j\,|\,\mathrm{d}n\rangle \cos\omega_{nj}t, \tag{6.1}$$

derived in Appendix D. $\mathrm{d}U(t)$ is the derivative of the propagator. Upon averaging over time the oscillatory terms vanish, and we obtain

$$V_n = -\tfrac{1}{2}\mathrm{i}\hbar\,\overline{\langle \mathrm{d}U(t)\cdot n\,| \wedge |\,\mathrm{d}U(t)\cdot n\rangle}. \tag{6.2}$$

(Here and hereafter, $\bar{f}$ denotes the time average

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\, f(t).)$$

With a similar calculation one can also show that

$$V_n = -\mathrm{i}\hbar\overline{\langle \mathrm{d}U(t)\cdot n|}\wedge\overline{|\mathrm{d}U(t)\cdot n\rangle}. \tag{6.2$'$}$$

In (6.2′) the time averages over the bra and ket are performed separately, or incoherently, whereas in (6.2) they are performed simultaneously, or coherently; the factor of $\frac{1}{2}$ accounts for this difference. One can develop the formalism starting from either the coherent or the incoherent expression; for brevity we present the coherent version only.

Equation (6.2) has an interesting geometrical interpretation. Suppose we want the flux of V_n through $\square_R$ (see figure 1*a*). We apply $U(t,R)$, $U(t,R+r_1)$ and $U(t,R+r_2)$ to $|n,R\rangle$. The states obtained describe an area element $\square_H(t)$ in Hilbert space (see figure 1*b*), spanned by displacements $U_1(t)|n\rangle$ and $U_2(t)|n\rangle$ from $U(t)|n\rangle$ (here $U_i(t) \overset{\mathrm{def}}{=} \mathrm{d}U(t)\cdot r_i$). By virtue of the canonical structure of quantum mechanics, $\square_R(t)$ has a (naturally defined) symplectic area $-2\hbar\,\mathrm{Im}\,\langle U_1(t)\cdot n\,|\,U_2(t)\cdot n\rangle$ (see Appendix E). According to (6.2), the time average of the symplectic area of $\square_H(t)$ is just (minus twice) the required flux. (Note there is a factor of two which arises from the definition of the wedge product.)

The equivalence of (6.2) and (2.9) can be established by expressing $\mathrm{d}U(t)$ in terms of $(\mathrm{d}\hat{H})_t$. These are related by the formula for the derivative of an exponential (see Bellman 1960),

$$\mathrm{d}U(t) = -\frac{\mathrm{i}}{\hbar}U(t)\int_0^t \mathrm{d}\tau(\mathrm{d}\hat{H})_\tau. \tag{6.3}$$

Substituting into (6.2),

$$V_n = -\frac{\mathrm{i}}{4\hbar}\overline{\int_0^t \mathrm{d}\tau\int_0^t \mathrm{d}\tau'\langle n\,|\,[(\mathrm{d}\hat{H})_\tau, \wedge\,(\mathrm{d}\hat{H})_{\tau'}]\,|\,n\rangle}, \tag{6.4}$$

in which, because the τ and τ' integrals appear symmetrically, we have replaced $(\mathrm{d}\hat{H})_\tau\wedge(\mathrm{d}\hat{H})_{\tau'}$ by its symmetrized part, $\frac{1}{2}[(\mathrm{d}\hat{H})_\tau, \wedge\,(\mathrm{d}\hat{H})_{\tau'}]$ (cf. (2.6)). Since expectation values of eigenstates are time invariant,

$$\langle n\,|\,[(\mathrm{d}\hat{H})_\tau, \wedge\,(\mathrm{d}\hat{H})_{\tau'}]\,|\,n\rangle = \langle n\,|\,[(\mathrm{d}\hat{H})_{\tau-\tau'}, \wedge\,\mathrm{d}\hat{H}]\,|\,n\rangle.$$

Making this substitution in (6.4) enables the τ' integral to be performed, and (2.9) follows from a few more manipulations.

(*b*) *Classical formula*

The corresponding classical alternative is obtained directly from (6.4). Taking its classical limit as in §3, we get

$$V_n \to V^{\mathrm{c}}(E) = \frac{1}{4}\overline{\int_0^t \mathrm{d}\tau\int_0^t \mathrm{d}\tau'\langle\{(\mathrm{d}H)_\tau, \wedge\,(\mathrm{d}H)_{\tau'}\}\rangle_E}. \tag{6.5}$$

In Appendix F we show that

$$\int_0^t \mathrm{d}\tau\int_0^t \mathrm{d}\tau'\{(\mathrm{d}H)_\tau, \wedge\,(\mathrm{d}H)_{\tau'}\} = -[\mathrm{d}\boldsymbol{Z}(t), \wedge\,\mathrm{d}\boldsymbol{Z}(t)]. \tag{6.6}$$

where $\mathrm{d}\boldsymbol{Z}(t)$ is the derivative of the flow with respect to parameters, in which the dependence on initial conditions z has been left implicit. The square brackets denote the symplectic inner product (Arnold 1978), defined as follows: Given vectors $\boldsymbol{u} = (\boldsymbol{q},\boldsymbol{p})$ and $\boldsymbol{v} = (\boldsymbol{q}',\boldsymbol{p}')$ in phase space,

$$[\boldsymbol{u},\boldsymbol{v}] \stackrel{\text{def}}{=} \boldsymbol{u}\cdot\boldsymbol{J}^{-1}\cdot\boldsymbol{v} = \boldsymbol{p}\cdot\boldsymbol{q}' - \boldsymbol{q}\cdot\boldsymbol{p}', \tag{6.7}$$

where $\boldsymbol{J}$ is given by (3.10). (The symplectic inner product $[\boldsymbol{u},\boldsymbol{v}]$ should not be confused with the commutator $[\hat{A},\hat{B}]$; in the latter the quantum operators are distinguished by carats.) Substituting (6.6) into (6.5) we obtain

$$V^{\mathrm{c}}(E) = -\tfrac{1}{4}\langle\overline{[\mathrm{d}\boldsymbol{Z}(t),\ \wedge\,\mathrm{d}\boldsymbol{Z}(t)]}\rangle_E = -\tfrac{1}{2}\langle\overline{[\mathrm{d}\boldsymbol{P}(t),\ \wedge\,\mathrm{d}\boldsymbol{Q}(t)]}\rangle_E, \tag{6.8}$$

where in the last expression we have taken $\mathrm{d}\boldsymbol{Z}(t) = (\mathrm{d}\boldsymbol{Q}(t), \mathrm{d}\boldsymbol{P}(t))$. This is the alternative formula for the classical two-form.

Equation (6.8) is a precise version of a formula (eq. (4.18)) derived in Berry (1990) (there the time dependence was integrated over, but the interpretation of the differentials $\mathrm{d}\boldsymbol{Q}$ and $\mathrm{d}\boldsymbol{P}$ was left ambiguous). Equation (6.8) might appear to be the simplest expression for the classical two-form, but its simplicity is deceptive (cf. the discussion in Berry (1990)). As with (3.8), the fact that (6.8) converges is not obvious, because if the dynamics is chaotic, both $\mathrm{d}\boldsymbol{Z}(z,t)$ and $[\mathrm{d}\boldsymbol{Z}(z,t),\ \wedge\,\mathrm{d}\boldsymbol{Z}(z,t)]$ grow exponentially in time for fixed z. (We shall not give the somewhat involved general argument here – none of our results depend on it – but the particular case of periodic orbits is treated in appendix K.) However, since the microcanonical average $\langle[\mathrm{d}\boldsymbol{Z}(t),\ \wedge\,\mathrm{d}\boldsymbol{Z}(t)]\rangle$ does not in fact diverge, it follows that $[\mathrm{d}\boldsymbol{Z}(z,t),\ \wedge\,\mathrm{d}\boldsymbol{Z}(z,t)]$ oscillates with z, and that the exponentially large oscillations must cancel in the main when averaged over the energy shell.

Like (6.2), (6.8) has a geometrical interpretation. Suppose we want the flux of $V^{\mathrm{c}}(E)$ through $\square_R$. To a point z on the energy shell we apply the hamiltonians $H(R)$, $H(R+r_1)$ $H(R+r_2)$ for a time t. The resulting trajectories describe an area element $\square_P(z,t)$ in phase space drawn in figure 1c, spanned by displacements $\boldsymbol{Z}_1(z,t)$ and $\boldsymbol{Z}_2(z,t)$ from z_t, where $\boldsymbol{Z}_i(z,t) \stackrel{\text{def}}{=} \mathrm{d}\boldsymbol{Z}(z,t)\cdot r_i$. The symplectic area of $\square_P(z,t)$ is $[\boldsymbol{Z}_1(z,t), \boldsymbol{Z}_2(z,t)]$, and according to (6.8), its microcanonical and time average is just (minus twice) the required flux. In light of figure 1b and c, the correspondence between quantum and classical two-forms, (6.2) and (6.8), is immediate.

(c) *An equivalent form*

Differentiating Hamilton's equations $\dot{\boldsymbol{Z}}(t) = \boldsymbol{J}\cdot(\boldsymbol{H}')_t$ with respect to parameters, we find that $\mathrm{d}\boldsymbol{Z}(t)$ satisfies the linear inhomogeneous equation

$$\mathrm{d}\dot{\boldsymbol{Z}}(t) = \boldsymbol{J}(\boldsymbol{H}'')_t\cdot\mathrm{d}\boldsymbol{Z}(t) + \boldsymbol{J}\cdot(\mathrm{d}\boldsymbol{H}')_t, \tag{6.9}$$

with initial conditions $\mathrm{d}\boldsymbol{Z}(z,0) = 0$. (Here $(\boldsymbol{H}'')_{ij} = \partial^2 H/\partial z_i\,\partial z_j$.) It is often useful to express $\mathrm{d}\boldsymbol{Z}(t)$ in terms of other solutions $\mathrm{d}\boldsymbol{Y}(t)$ of (6.9), to be specified later, which will of course satisfy different initial conditions. (Here we make a slight abuse of notation, as we will not assume that $\mathrm{d}\boldsymbol{Y}(t)$ is an exact differential.) In general, any two solutions of (6.9) differ by a solution of the homogeneous equation $\mathrm{d}\dot{\boldsymbol{X}}(t) = \boldsymbol{J}(\boldsymbol{H}'')_t\cdot\mathrm{d}\boldsymbol{X}(t)$, and solutions of the homogeneous equation are of the form $\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{S}(t)\cdot\mathrm{d}\boldsymbol{X}(0)$. (Here $\boldsymbol{S}(t)$ is an abbreviation for $\boldsymbol{S}(z,t)$, the linearized flow of (3.11).) Therefore

$$\mathrm{d}\boldsymbol{Z}(t) = \mathrm{d}\boldsymbol{Y}(t) - \boldsymbol{S}(t)\cdot\mathrm{d}\boldsymbol{Y}(0). \tag{6.10}$$

Substituting (6.10) into (6.8) we obtain

$$V^{c}(E) = -\tfrac{1}{4}\overline{\langle[\mathrm{d}\boldsymbol{Y}(t),\wedge\mathrm{d}\boldsymbol{Y}(t)]\rangle}+\tfrac{1}{2}\overline{\langle[\mathrm{d}\boldsymbol{Y}(t),\wedge\boldsymbol{S}(t)\cdot\mathrm{d}\boldsymbol{Y}(0)]\rangle}-\tfrac{1}{4}\overline{\langle[\mathrm{d}\boldsymbol{Y}(0),\wedge\mathrm{d}\boldsymbol{Y}(0)]\rangle}, \tag{6.11}$$

an equivalent expression for the classical two-form. In the last term we have used

$$[\boldsymbol{S}(t)\cdot\mathrm{d}\boldsymbol{Y}(0),\wedge\boldsymbol{S}(t)\cdot\mathrm{d}\boldsymbol{Y}(0)] = [\mathrm{d}\boldsymbol{Y}(0),\wedge\mathrm{d}\boldsymbol{Y}(0)], \tag{6.12}$$

the canonical invariance of the symplectic inner product. Equation (6.11) is particularly useful in deriving the two-form for integrable systems (Appendix G) and periodic orbits (§§8 and 9).

7. Is the classical two-form closed?

The question as to whether $V^{c}(E)$ is closed is of central importance, but it is not easily answered. Here we present a formal derivation of closedness,

$$\mathrm{d}V^{c}(E) = 0. \tag{7.1}$$

First, let us point out that it is not correct to argue, on the basis of the correspondence principle, that because the quantum two-form is closed, so must be its classical limit. The reason is that V_n is not closed, as $\mathrm{d}V_n$ is singular at eigenvalue degeneracies. (Indeed this property was one of the motivations underlying the discovery of the geometric phase (see Shapere & Wilczek 1989, p. 26).) Thus $\mathrm{d}V_{\mathrm{c}}(E) \neq 0$ would have implications for the distribution of degeneracies in the classical limit, as will be explained in §9. On the other hand, $\mathrm{d}V_c(E) = 0$ would imply that (at least locally) $V^{c}(E)$ is the derivative of a one-form, whose integral around a closed loop in parameter space one might expect to describe a classical anholonomy for adiabatically cycled chaotic systems, analogous to the Hannay angles for integrable systems.

From the formulas derived so far it is not even clear that the three-form $\mathrm{d}V^{c}(E)$ converges. For example, the derivative of (3.15) introduces the two-form $\mathrm{d}((\mathrm{d}H)_t)$. While $\mathrm{d}(\mathrm{d}H)$ vanishes, $\mathrm{d}((\mathrm{d}H)_t)$ does not, due to the parameter dependence of the dynamics. In fact, for fixed z, $\mathrm{d}((\mathrm{d}H)_t)(z)$ grows exponentially in time, since

$$\mathrm{d}((\mathrm{d}H)_t)(z) = \mathrm{d}\boldsymbol{H}'(z_t)\wedge\cdot\mathrm{d}\boldsymbol{Z}(z,t) \tag{7.2}$$

and $\mathrm{d}\boldsymbol{Z}(z,t)$ grows exponentially.

The alternative form (6.8) turns out to be the most convenient for calculating $\mathrm{d}V^{c}(E)$. To proceed, we first note that upon differentiating an ensemble average such as $\langle\phi\rangle_E$ (here ϕ is any differential form), account must be taken of both the explicit parameter dependence of ϕ and the implicit parameter dependence of the ensemble. Also, the derivative of the ensemble is to be taken at fixed volume rather than fixed energy (cf. of the Weyl rule (3.4)). As shown in Appendix H,

$$\mathrm{d}\langle\phi\rangle_E = \langle\mathrm{d}\phi\rangle_E+(1/\Omega')\,(\Omega'\langle(\mathrm{d}E-\mathrm{d}H)\wedge\phi\rangle_E)', \quad \text{where} \quad \mathrm{d}E = \langle\mathrm{d}H\rangle_E. \tag{7.3}$$

Thus differentiation of (6.8) gives

$$\mathrm{d}V^{c}(E) = -(1/4\Omega')\,(\Omega'\overline{\langle(\mathrm{d}E-\mathrm{d}H)\wedge[\mathrm{d}\boldsymbol{Z}(t),\wedge\boldsymbol{Z}(t)]\rangle_E})' \tag{7.4}$$

(we have used the closedness of $[\mathrm{d}\boldsymbol{Z}(t),\wedge\mathrm{d}\boldsymbol{Z}(t)]$). In what follows we show that

$$\tfrac{1}{4}\overline{\langle\mathrm{d}H\wedge[\mathrm{d}\boldsymbol{Z}(t),\wedge\mathrm{d}\boldsymbol{Z}(t)]\rangle} = \tfrac{1}{4}\mathrm{d}E\wedge\overline{\langle[\mathrm{d}\boldsymbol{Z}(t),\wedge\mathrm{d}\boldsymbol{Z}(t)]\rangle_E}, \tag{7.5}$$

which together with (7.4) implies that $V^{c}(E)$ is closed. To streamline the presentation we have left some details to Appendix I.

In Appendix I we show that

$$\tfrac{1}{4}\overline{\langle \mathrm{d}H \wedge [\mathrm{d}\boldsymbol{Z}(t),\, \wedge\, \mathrm{d}\boldsymbol{Z}(t)]\rangle} = \lim_{s\to 0} G(s,s), \tag{7.6}$$

where

$$\left.\begin{aligned} G(s,s') &= -\int_0^\infty \mathrm{d}\tau \frac{\mathrm{e}^{-s\tau}}{s} s' \int_0^\infty \mathrm{d}\tau' \, \mathrm{e}^{-s'\tau'} F(\tau,\tau'), \\ F(\tau,\tau') &= \tfrac{1}{2}\langle (\mathrm{d}H)_{-\tau'} \wedge \{(\mathrm{d}H)_\tau,\, \wedge\, \mathrm{d}H\}\rangle. \end{aligned}\right\} \tag{7.7}$$

The principal steps leading to (7.6) involve replacing $[\mathrm{d}\boldsymbol{Z}(t),\, \wedge\, \mathrm{d}\boldsymbol{Z}(t)]$ by its expression in (6.6) and writing its time average as the residue of its Laplace transform at the origin (as in Appendix J). Instead of taking both arguments of $G(s,s')$ to zero simultaneously, let us take the limit $s'\to 0$ first. From Appendix J

$$\lim_{s'\to 0} s' \int_0^\infty \mathrm{d}\tau' \, \mathrm{e}^{-s'\tau'} F(\tau,\tau') = \lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{d}\tau' F(\tau,\tau'), \tag{7.8}$$

because the right-hand side is the τ'-average of $F(\tau,\tau')$ and the left-hand side is the residue of its τ'-Laplace transform at the origin. But from (7.7) the τ'-average of $F(\tau, \tau')$ is $\tfrac{1}{2}\mathrm{d}E \wedge \langle\{(\mathrm{d}H)_\tau,\, \wedge\, \mathrm{d}H\}\rangle$, as implied by the *weak mixing property* $\overline{\langle A_{\tau'} B\rangle} = \langle A\rangle\,\langle B\rangle$ (Arnold & Avez 1989) (weak mixing is implied by mixing, which we have already assumed the dynamics to be). Therefore

$$\lim_{s'\to 0} G(s,s') = -\mathrm{d}E \wedge \frac{1}{2}\int_0^\infty \mathrm{d}\tau \frac{\mathrm{e}^{-s\tau}}{s} \langle\{(\mathrm{d}H)_\tau,\, \wedge\, \mathrm{d}H\}\rangle. \tag{7.9}$$

The remaining limit $s\to 0$ is straightforward. As shown in Appendix I,

$$\lim_{s\to 0}\frac{1}{2}\int_0^\infty \mathrm{d}\tau \frac{\mathrm{e}^{-s\tau}}{s} \langle\{(\mathrm{d}H)_\tau,\, \wedge\, \mathrm{d}H\}\rangle_E = V^{\mathrm{c}}(E). \tag{7.10}$$

Thus $\lim_{s\to 0}(\lim_{s'\to 0} G(s,s')) = -\mathrm{d}E \wedge V^{\mathrm{c}}(E)$, which in turn is equal to

$$\tfrac{1}{4}\mathrm{d}E \wedge \overline{\langle[\mathrm{d}\boldsymbol{Z}(t),\, \wedge\, \mathrm{d}\boldsymbol{Z}(t)]\rangle_E}.$$

Together with (7.6) and (7.4), this implies the closedness of the classical two-form.

The preceding derivation is purely formal in that we have not established the convergence of the expressions involved nor justified the interchange of limits. These difficulties might yield to a more technically rigorous treatment but might also conceal some interesting behaviour. One possibility is that $V^{\mathrm{c}}(E)$ is in a sense exact but not closed; it might be the derivative of a one-form (in which case its integral over a closed surface would vanish), but it might not be differentiable itself.

8. The spectral two-form

Just as the Weyl density of states $\bar{\mathrm{d}}(E) = \Omega'/h^N$ describes smooth variations in the exact density of states $\mathrm{d}(E) = \Sigma_n \delta(E - E_n)$, so too $V^{\mathrm{c}}(E)$ describes smooth variations in V_n on a classical energy scale. Similarly, just as quantum fluctuations in the density of states are described by classical periodic orbits, so too are fluctuations in the two-form. The starting point for these considerations is not the two-form itself but rather the *spectral two-form*

$$D(E) = \sum_n \delta(E - E_n)\, V_n. \tag{8.1}$$

We can write the previously derived quantum formula (6.2) as

$$V_n = -\tfrac{1}{2}\mathrm{i}\hbar\,\overline{\mathrm{Tr}\,[P_n\,\mathrm{d}U^{\dagger}(t)\wedge\mathrm{d}U(t)]}, \tag{6.2$''$}$$

where $P_n = |n\rangle\langle n|$; this is a time-dependent version of the manifestly gauge-invariant formula $V_n = -\mathrm{i}\hbar\,\mathrm{Tr}\,[P_n\,\mathrm{d}P_n\wedge\mathrm{d}P_n]$ (see Avron *et al.* 1987, 1989) in which the two-form is expressed in terms of spectral projections. Thus we may express the spectral two-form in a form more suitable for semiclassical approximation,

$$D(E) = -\tfrac{1}{2}\mathrm{i}\hbar\,\overline{\mathrm{Tr}\,[\delta(E-\hat{H})\,\mathrm{d}U^{\dagger}(t)\wedge\mathrm{d}U(t)]}. \tag{8.2}$$

Here $\delta(E-\hat{H}) = \Sigma_n\,\delta(E-E_n)\,P_n$ is the *spectral operator*.

The classical limit of (8.2) is taken exactly as in §§3 and 6, with the result

$$D(E)\rightarrow D^{\mathrm{c}}(E) = -\frac{1}{4}\overline{\int \mathrm{d}^{2N}z\,W(z,E)\,[\mathrm{d}\boldsymbol{Z}(z,t),\wedge\,\mathrm{d}\boldsymbol{Z}(z,t)]}. \tag{8.3}$$

In place of the Wigner function $W_n(z)$ (taken to be the microcanonical density in §§3 and 6) there appears the *spectral Wigner function* (Berry 1989)

$$W(z,E) = (\delta(E-\hat{H}))_W(z), \tag{8.4}$$

the symbol of the spectral operator, whose semiclassical approximation is given by

$$W(z,E) = \frac{1}{h^N}\,\delta(E-H(z))\left(1+2h^{N-1}\sum_j A_j(E)\,\delta_j(z)\right). \tag{8.5}$$

The first term in (8.5) is just the microcanonical density weighted by the Weyl density of states. The additional terms, whose amplitudes are of order h^{N-1} less than the leading one, are the periodic orbit contributions. $\delta_j(z)$ is a normalized δ-function on the jth periodic orbit, and

$$A_j(E) = \frac{T_j}{\det|\boldsymbol{M}_j-\boldsymbol{I}|^{\frac{1}{2}}}\cos\,(S_j/\hbar-\tfrac{1}{2}\mu_j\,\pi) \tag{8.6}$$

are the oscillatory amplitudes of the Gutzwiller trace formula (Gutzwiller 1971, 1990). S_j is the action, T_j the period of a single repetition, $\boldsymbol{M}_j$ the linearized Poincaré map and μ_j the Maslov index of the jth orbit. (In fact, (8.5) is a limiting form of a more refined expression, in which the delta functions are replaced by smooth functions localized on the energy shell and the periodic orbits.)

Substituting (8.5) into (8.3), we obtain the classical limit of the spectral two-form,

$$D^{\mathrm{c}}(E) = \bar{D}^{\mathrm{c}}(E)+\sum_j D^{\mathrm{c}}_j(E). \tag{8.7}$$

The smooth contribution

$$\bar{D}^{\mathrm{c}}(E) = (\Omega'/h^N)\,V^{\mathrm{c}}(E) \tag{8.8}$$

is simply the classical two-form weighted by the Weyl density of states. Our interest here is in the periodic orbit contributions $(2/h)\,A_j(E)\,V^{\mathrm{sc}}_j(E)$, where

$$V^{\mathrm{sc}}_j(E) = -\tfrac{1}{4}\langle[\mathrm{d}\boldsymbol{Z}(t),\,\wedge\,\mathrm{d}\boldsymbol{Z}(t)]\rangle_{jE}. \tag{8.9}$$

(In general $\langle f\rangle_{jE}$ denotes the average of f round the jth orbit at energy E.)

There is a natural two-form associated with periodic orbits, analogous to the Hannay two-form for one-dimensional systems. Periodic orbits belong to continuous families $\boldsymbol{y}_j(\theta, S, R)$, labelled by action S (in preference to the energy) and parameters R. θ, the coordinate along the orbits, is the scaled time ('angle'), in terms of which $\boldsymbol{y}_j(\theta, S, R)$ is 2π-periodic. Then the periodic orbit two-form is given by

$$V_j^{\mathrm{c}}(S) = -\tfrac{1}{2}\langle[\mathrm{d}\boldsymbol{y}_j, \wedge \mathrm{d}\boldsymbol{y}_j)]\rangle_{jS}. \tag{8.10}$$

(Here $\langle\cdot\rangle_{jS}$ denotes the average around the jth orbit at action S.) As shown in Appendix K, $V_j^{\mathrm{c}}(S)$ is well-defined. Like (6.2) and (6.8), it has a geometrical interpretation. Suppose we want the flux of $V_j^{\mathrm{c}}(S)$ through $\square_R$. We draw vectors from $\boldsymbol{y}_j(\theta, S, R)$ to points on neighbouring orbits at the same action and scaled time, but with parameters $R+r_1$ and $R+r_2$. These vectors span an area element $\square_j(\theta)$ in phase space drawn in figure 1f. The symplectic area of $\square_j(\theta)$ averaged round the orbit is (minus) the required flux.

In Appendix K we show that the two-forms (8.9) and (8.10) are the same, i.e.

$$V_j^{\mathrm{c}}(S_j(E)) = V_j^{\mathrm{sc}}(E). \tag{8.11}$$

Thus the periodic orbit contribution to the spectral two-form is

$$D_j^{\mathrm{c}}(E) = (2/h)\, A_j(E)\, V_j^{\mathrm{c}}(S_j). \tag{8.12}$$

For unstable periodic orbits the derivation of (8.11) is not straightforward. As shown in Appendix K, $[\mathrm{d}\boldsymbol{Z}(z,t), \wedge \mathrm{d}\boldsymbol{Z}(z,t)]_{jE}$ diverges exponentially in time, and while the divergent behaviour disappears when z is averaged over the energy shell, it does *not* when z is averaged only over a periodic orbit. Thus $\langle[\mathrm{d}\boldsymbol{Z}(t), \wedge \mathrm{d}\boldsymbol{Z}(t)]\rangle_{jE}$ grows exponentially with t, and its time average must be defined by analytic continuation (as in Appendix J). The origin of the divergence is the singular nature of the periodic orbit delta function, itself an artefact of the semiclassical approximation (8.5). We would like a derivation of (8.12) free of all divergences (possibly based on the Airy-function smoothing of Berry (1989)), but have not yet found one.

9. Semiclassical density of degeneracies

In this section, we consider systems without time-reversal symmetry and for the sake of explicitness take parameter space to be three-dimensional.

The distribution of energy level degeneracies in parameter space is of considerable interest. While degeneracies are exceptional – according to a well-known theorem of Von Neumann & Wigner (1929), for systems without time reversal symmetry at least three parameters must be varied to find one – they provide a mechanism for dissipation in adiabatic processes. As a hamiltonian is varied in time, its path through parameter space passes near degeneracies; these near-approaches violate the conditions of the quantum adiabatic theorem and generate transitions of Landau–Zener type between states. This subject has received and continues to receive much attention, as described in Hill & Wheeler (1952) and Wilkinson (1990).

As discussed in the original work on the subject, the geometric phase is intimately connected to degeneracies (Berry 1984). It turns out that $\mathrm{d}V_n(\boldsymbol{R})$ (a scalar density in three-dimensional $\boldsymbol{R}$-space) has δ-function singularities at degeneracies (generically these occur at isolated points) and is zero elsewhere. Explicitly, letting $\boldsymbol{R}_{n,\alpha}$ denote the degeneracies between the states $|n\rangle$ and $|n+1\rangle$,

$$\mathrm{d}V_n(\boldsymbol{R}) = 2\pi \sum_\alpha (\sigma_{n,\alpha}\, \delta^3(\boldsymbol{R}-\boldsymbol{R}_{n,\alpha}) - \sigma_{n-1,\alpha}\, \delta^3(\boldsymbol{R}-\boldsymbol{R}_{n-1,\alpha}))\, \rho, \tag{9.1}$$

where $\rho = \mathrm{d}R_1 \wedge \mathrm{d}R_2 \wedge \mathrm{d}R_3$ is the coordinate volume form and the σs denote ± 1, as we discuss presently. Note that degeneracies with both the state above and below $|n\rangle$ contribute to $\mathrm{d}V_n$, and that the degeneracies between, say, $|n\rangle$ and $|n+1\rangle$ contribute to $\mathrm{d}V_n$ and $\mathrm{d}V_{n+1}$ with opposite signs.

The σs are defined as in Simon (1983). Assuming the eigenstates are continuous functions of parameters, let $|+\rangle \overset{\text{def}}{=} |n+1(\boldsymbol{R}_{n,\alpha})\rangle, |-\rangle \overset{\text{def}}{=} |n(\boldsymbol{R}_{n,\alpha})\rangle$ denote the pair of degenerate states at $\boldsymbol{R} = \boldsymbol{R}_{n,\alpha}$. We construct a two-dimensional hermitian matrix $H(\boldsymbol{R})$ with matrix elements $H_{\pm}(\boldsymbol{R}) \overset{\text{def}}{=} \langle +|\hat{H}(\boldsymbol{R})|-\rangle$, $H_{\mp}(\boldsymbol{R}) \overset{\text{def}}{=} \langle -|\hat{H}(\boldsymbol{R})|+\rangle$, etc. The expansion of H in terms of the Pauli matrices, $H = A\boldsymbol{I} + \boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}}$, determines a vector field $\boldsymbol{B}(\boldsymbol{R})$ on parameter space. Then $\sigma_{n,\alpha}$ is given by $-\operatorname{sgn}\det(\partial B_i/\partial R_j)|_{\boldsymbol{R}_{n,\alpha}}$; that is, $\sigma_{n,\alpha}$ is negative if at $\boldsymbol{R}_{n,a}$ the mapping from $\boldsymbol{R}$ to $\boldsymbol{B}$ is orientation preserving, and is positive if it is not.

The quantity we will consider is not $\mathrm{d}V_n$ itself but rather the sum

$$M_n = \sum_{m=1}^{n} \mathrm{d}V_m. \tag{9.2}$$

From (9.1) we get that

$$M_n = 2\pi \sum_{\alpha} \sigma_{n,\alpha}\, \delta^3(\boldsymbol{R}-\boldsymbol{R}_{n,\alpha})\,\rho, \tag{9.3}$$

as the alternating contributions from $m < n$ cancel each other. Thus M_n gives the algebraic or signed density of degeneracies between $|n\rangle$ and $|n+1\rangle$. M_n should be distinguished from the absolute density of degeneracies,

$$|M|_n \overset{\text{def}}{=} 2\pi \sum_{\alpha} \delta^3(\boldsymbol{R}-\boldsymbol{R}_{n,\alpha})\,\rho.$$

An interesting question (we will not pursue it here) is which of the two densities, M_n or $|M|_n$, determines the rate of Landau–Zener transitions; does each play a distinctive role in the description? Let us just mention that $|M|_n$ can also be expressed in terms of the two-form; explicitly

$$|M|_n(\boldsymbol{R}) = \lim_{\delta\to 0} \frac{1}{2\pi}\left(\int_{|\boldsymbol{R}-\boldsymbol{R}'|<\delta} \mathrm{d}^3\boldsymbol{R}'\, M_n(\boldsymbol{R}')\right) M_n(\boldsymbol{R}). \tag{9.4}$$

In terms of the spectral two-form (8.1),

$$M_n = \lim_{\epsilon\to 0^+} \mathrm{d}\int_{-\infty}^{E_n(\boldsymbol{R})+\epsilon} \mathrm{d}E\, D(E), \tag{9.5}$$

an expression whose classical limit $M^{\mathrm{c}}(E)$ is readily obtained from (8.7), (8.8) and (8.12). $M^{\mathrm{c}}(E)$ like $D^{\mathrm{c}}(E)$ contains smooth and oscillatory terms, but since $V^{\mathrm{c}}(E)$ is closed according to (7.1), it follows directly from (9.2) that the smooth contribution vanishes.

The periodic orbit contributions $M^{\mathrm{c}}_j(E)$ are given by

$$M^{\mathrm{c}}_j(E) = \frac{2}{\hbar}\mathrm{d}\int_{-\infty}^{E} \mathrm{d}\epsilon\, A_j(\epsilon)\, V^{\mathrm{c}}_j(S_j(\epsilon)), \tag{9.6}$$

where A_j is given by (8.6) and V_j^c by (8.10). Because the factor $\cos(S_j/\hbar - \frac{1}{2}\mu_j \pi)$ oscillates rapidly, to lowest order in $\hbar$ we may neglect the energy dependence of the other factors in the integrand. (In so doing we ignore singularities in $\det|M_j - I|^{-\frac{1}{2}}$ at bifurcations.) Then

$$M_j^c(E) = \frac{2}{\hbar}\mathrm{d}\left(\hbar\frac{\sin(S_j/\hbar - \frac{1}{2}\mu_j\pi)}{\det|M_j - I|^{\frac{1}{2}}}V_j^c(S_j)\right). \tag{9.7}$$

To lowest order in $\hbar$, d acts only on the oscillatory factor, and $\mathrm{d}\sin(S_j/\hbar - \frac{1}{2}\mu_j\pi) = \cos(S_j/\hbar - \frac{1}{2}\mu_j\pi)\,\mathrm{d}S_j/\hbar$. Also

$$\mathrm{d}S_j = T_j(\mathrm{d}E - \langle \mathrm{d}H\rangle_j), \tag{9.8}$$

as shown in Appendix K. Combining these results, we obtain

$$M_j^c(E) = (2/\hbar)A_j(E)(\mathrm{d}E - \langle \mathrm{d}H\rangle_j) \wedge V_j^c(S_j). \tag{9.9}$$

(Note that for long periodic orbits $\mathrm{d}E - \langle \mathrm{d}H\rangle_j$ approaches zero, as $\langle \mathrm{d}H\rangle_j \rightarrow \langle \mathrm{d}H\rangle_E = \mathrm{d}E$.) Thus the density of degeneracies, while neutral on a classical scale, is resolved semiclassically into oscillations described by classical periodic orbits.

10. Discussion

Our principal result (3.15) is an explicit and explicitly finite expression for the classical limit of the geometric phase two-form which is valid for chaotic systems. In the derivation we have assumed the dynamics is ergodic and mixing at a sufficiently rapid rate. We have given a formal derivation of the closedness of the classical two-form, obtained semiclassical corrections to it associated with periodic orbits, and derived a semiclassical expression for the algebraic density of degeneracies in parameter space. We have also discussed the case of additional constants of the motion and specific examples including the Aharonov–Bohm billiard in a uniform magnetic field.

From this investigation there emerge a number of questions to be pursued. One would like to test these formulas numerically, particularly the periodic orbit contributions. The Aharonov–Bohm billiard is one candidate system, although for the version we are considering the quantum calculations might not be simple. Maps (classical and quantum) present alternative and possibly simpler test cases; the necessary modifications to the formalism presented here should be straightforward. It would also be interesting to see if the periodic orbit two-form plays some role in purely classical mechanics, for instance in the study of bifurcations.

The most important question is whether the classical two-form itself has any intrinsic significance in classical mechanics. Does it describe an anholonomy in adiabatically cycled chaotic systems, as the Hannay two-form does for integrable systems? If so, it must be derivable purely within classical mechanics (as the Hannay two-form is). In this connection there remains the related question of the closedness of the two-form (another question amenable to numerical investigation.) The formal argument of §7 should be right in some sense, but precisely how requires further study, perhaps facilitated by consideration of the purely classical problem.

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Appendix A. Derivations of (3.12) and (4.7)

By definition

$$\langle\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\rangle_E = \frac{1}{\Omega'}\int \mathrm{d}^{2N}\boldsymbol{z}\,\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\,\delta(E-H\rangle. \tag{A 1}$$

Using the Leibniz rule for Poisson brackets, $\{F,G\}K = \{F,GK\}-\{F,K\}G$, the integrand $\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\,\delta(E-H)$ may be written as

$$\{(\mathrm{d}A)_t, \wedge\,\delta(E-H)\,\mathrm{d}B\}-\{(\mathrm{d}A)_t, \delta(E-H)\}\wedge \mathrm{d}B. \tag{A 2}$$

The first term vanishes when integrated over phase space because: (i) it is a Poisson bracket and therefore a pure divergence (explicitly, $\{F,G\} = \nabla_z\cdot(F\boldsymbol{J}\cdot\boldsymbol{G}')$, and (ii) its surface integral at infinity vanishes because $\delta(E-H(\boldsymbol{z}))$ does. As for the second term,

$$\{(\mathrm{d}A)_t, \delta(E-H)\} = -\{(\mathrm{d}A)_t, H\}\,\delta'(E-H) = -(\mathrm{d}\dot{A})_t\,\delta'(E-H), \tag{A 3}$$

where the prime denotes the derivative with respect to energy and the dot the derivative with respect to time. From (A 1)–(A 3) we obtain

$$\langle\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\rangle_E = \frac{1}{\Omega'}\int \mathrm{d}^{2N}\boldsymbol{z}\,\delta'(E-H)\,(\mathrm{d}\dot{A})_t \wedge \mathrm{d}B = \frac{1}{\Omega'}(\Omega'\langle(\mathrm{d}\dot{A})_t\wedge \mathrm{d}B\rangle_E)', \tag{A 4}$$

the required result (3.12).

A similar argument establishes (4.7). By definition

$$\langle\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\rangle_f = \frac{1}{D}\int \mathrm{d}^{2N}\boldsymbol{z}\,\delta^k(\boldsymbol{f}-\boldsymbol{F})\,\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}. \tag{A 5}$$

The integrand $\delta^k(\boldsymbol{f}-\boldsymbol{F})\,\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}$ may be expressed as

$$\{(\mathrm{d}A)_t, \wedge\,\delta^k(\boldsymbol{f}-\boldsymbol{F})\,\mathrm{d}B\}-\{(\mathrm{d}A)_t, \delta^k(\boldsymbol{f}-\boldsymbol{F})\}\wedge \mathrm{d}B. \tag{A 6}$$

The first term is a pure divergence which does not contribute to the phase space integral, and the second is

$$-\nabla_f\delta^k(\boldsymbol{f}-\boldsymbol{F})\cdot\{(\mathrm{d}A)_t, \boldsymbol{F}\}\wedge \mathrm{d}B. \tag{A 7}$$

Therefore
$$\langle\{(\mathrm{d}A)_t, \wedge \mathrm{d}B\}\rangle_f = (1/D)\,\nabla_f\cdot(D\langle\{(\mathrm{d}A)_t, \boldsymbol{F}\}\wedge \mathrm{d}B\rangle_f). \tag{A 8}$$

Appendix B. The integrable case: first derivation

We establish the equivalence of the classical two-form $V^{\mathrm{c}}(\boldsymbol{I})$ and the Hannay two-form

$$V^{\mathrm{H}}(\boldsymbol{I}) = -\langle \mathrm{d}\boldsymbol{p}\wedge \mathrm{d}\boldsymbol{q}\rangle_I \tag{B 1}$$

for integrable systems. In (B 1), $\boldsymbol{q}$ and $\boldsymbol{p}$ are functions of $\boldsymbol{\theta}$, $\boldsymbol{I}$ and R, and the average is taken over an invariant torus; for convenience a minus sign has been introduced into the usual definition. For the sake of simplicity, we restrict ourselves to one degree of freedom; the generalization to higher dimensions is straightforward.

Hamilton's equations and (4.11) give

$$\left.\begin{aligned} \mathrm{d}\dot{p} &= -\mathrm{d}\partial_q H = -\partial_q\,\mathrm{d}H = -\partial_q\sum_m h_m \exp(\mathrm{i}m\theta),\\ \mathrm{d}\dot{q} &= \partial_p\sum_m h_m^* \exp(-\mathrm{i}m\theta), \end{aligned}\right\} \tag{B 2}$$

where we have used the fact that phase space and parameter differentials commute. Inserting the time dependence $\theta_t = \theta + \omega t$ and integrating gives

$$\left.\begin{aligned} \mathrm{d}p &= \mathrm{i}\partial_q \sum_{m \neq 0} h_m \exp(\mathrm{i}m\theta)/m\omega + \partial_q F(I), \\ \mathrm{d}q &= \mathrm{i}\partial_p \sum_{m \neq 0} h_m^* \exp(-\mathrm{i}m\theta)/m\omega - \partial_p F(I), \end{aligned}\right\} \tag{B 3}$$

where F is a non-oscillatory 1-form describing the mean displacement of the torus labelled I.

These expressions for $\mathrm{d}q$ and $\mathrm{d}p$ must be substituted into (B 1) and integrated over θ. The terms involving F cancel because

$$\partial_q F \wedge \partial_p F = \tfrac{1}{2}\{F, \wedge F\} = \partial_\theta F \wedge \partial_I F = 0. \tag{B 4}$$

The other terms give

$$\begin{aligned} V^{\mathrm{H}}(I) = &-\sum_m \left[\partial_I\left(\frac{h_m}{\omega}\right) \wedge \frac{1}{m^2}\partial_I\left(\frac{h_m^*}{\omega}\right)\partial_q I\, \partial_p I + \frac{1}{\omega^2} h_m \wedge h_m^*\, \partial_q\theta\, \partial_p\theta\right] \\ &-\mathrm{i}\sum_m \frac{1}{m}\left[\left(\frac{h_m}{\omega}\right) \wedge \partial_I\left(\frac{h_m^*}{\omega}\right)\partial_q\theta\, \partial_p I - \partial_I\left(\frac{h_m}{\omega}\right) \wedge \left(\frac{h_m^*}{\omega}\right)\partial_p\theta\, \partial_q I\right]. \end{aligned} \tag{B 5}$$

Now $h_m \wedge h_m^*$ is odd in m, causing the terms in the first line to cancel. The remaining terms can be replaced by their average over m and $-m$ which gives

$$V^{\mathrm{H}}(I) = -\frac{\mathrm{i}}{2}\sum_m \partial_I(h_m \wedge h_m^*/\omega^2)\,(\partial_q\theta\, \partial_p I - \partial_p\theta\, \partial_q I)/m \tag{B 6}$$

which is the same as (4.13), because (θ, I) are canonical variables.

Appendix C. Convergence of billiard two-form

First we write (5.8*b*) in a more explicit form. The microcanonical average $\langle\cdot\rangle$ is given by

$$\frac{1}{\Omega'}\int_0^{2\pi} \mathrm{d}\alpha \int_A \mathrm{d}^2\boldsymbol{r}$$

(the $\boldsymbol{r}$ integral is taken over the billiard), and it is readily shown that $V^{\mathrm{c}}(E, \boldsymbol{R}) = -2(EI)'/\Omega'$, where

$$I = \int_0^\infty \mathrm{d}t \int_0^{2\pi} \mathrm{d}\alpha \int_A \mathrm{d}^2\boldsymbol{r}\, \frac{\sin(2(\theta_t - \theta) - (\alpha_t - \alpha))}{\rho_t^2 \rho^2}. \tag{C 1}$$

Equation (C 1) is an integral in four-dimensional $(\alpha, t, \boldsymbol{r})$ space, and the integrand exhibits four types of singularities: (*a*) $\rho = 0$, (*b*) $\rho_t = 0$, (*c*) $\rho = \rho_t = 0$, $t \neq 0$, (*d*) $\rho = 0, t = 0$. We consider these in turn.

(*a*) $\rho = 0$. The singularity is a two-dimensional surface in $(\alpha, t, \boldsymbol{r})$ space and corresponds to trajectories which begin at the solenoid. Regarding α and t as fixed, we consider the contribution $I_a(\alpha, t)$ of a two-dimensional pencil of trajectories beginning near $\rho = 0$ in direction α. Changing integration variables from $\boldsymbol{r}$ to (ρ, θ),

$$I_a(\alpha, t) = \int_0 \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta\, \frac{\sin(2(\theta_t - \theta) - (\alpha_t - \alpha))}{\rho_t^2 \rho}. \tag{C 2}$$

As our concern is the singularity at $\rho = 0$, the upper limit of the ρ-integral is left indefinite. Let ρ', θ' and α' denote the final coordinates of the central trajectory from $\rho = 0$. Since final conditions depend smoothly on initial conditions, $\rho_t = \rho' + O(\rho)$, and analogous relations hold for θ_t and α_t. Expanding the integrand about $\rho = 0$,

$$\frac{\sin(2(\theta_t - \theta) - (\alpha_t - \alpha))}{\rho_t^2 \rho} = \frac{\sin(\delta - 2\theta)}{\rho'^2 \rho} + \frac{O(\rho)}{\rho}, \tag{C 3}$$

where $\delta = 2\theta' - \alpha' + \alpha$. Only the first term is singular, and it vanishes upon integration over θ. Therefore (C 2) converges conditionally. The divergence itself is only logarithmic.

(*b*) $\rho_t = 0$. Again the singularity is two dimensional, and it corresponds to trajectories which end at the solenoid. The analysis proceeds exactly as in (*a*) and is therefore omitted.

(*c*) $\rho = \rho_t = 0, t \neq 0$. These occur at isolated points in $(\alpha, t, \boldsymbol{r})$ space, and correspond to trajectories which begin and end at the solenoid. In the neighbourhood of such a point it is convenient to change variables from α and t to $\rho' \stackrel{\text{def}}{=} \rho_t$ and $\theta' \stackrel{\text{def}}{=} \theta_t$. I_c, the contribution of the neighbourhood of the singularity, is given by

$$I_c = \int_0 \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta \int_0 \mathrm{d}\rho' \int_0^{2\pi} \mathrm{d}\theta' \frac{1}{J} \frac{\sin(2(\theta' - \theta) - (\alpha_t - \alpha))}{\rho' \rho}, \tag{C 4}$$

where J is the jacobian $|\partial \boldsymbol{r}_t / \partial(\alpha, t)|$. Expanding about $\rho = 0$ and $\rho' = 0$, we get that $\alpha_t - \alpha$ is of the form $(\text{const.} + f(\theta)\rho + g(\theta')\rho' + O(\rho^{1+m}\rho'^{1+n}))$, where $m, n \geqslant 0$. Assuming that J does not vanish at $\rho = \rho' = 0$, the singular terms in the integrand vanish upon integration over θ and θ', and the divergences in ρ and ρ' are logarithmic. (The case where J does vanish corresponds to a coincidence of closed orbits and caustics, and occurs only on a one-dimensional set in parameter space, and therefore not for generic $\boldsymbol{R}$. This set includes self-conjugate points along periodic orbits.)

(*d*) $\rho = 0$, $t = 0$. The singularity is one dimensional (it is parametrized by the initial direction α) and is the strongest of the four. As in (*c*) we change variables from α and t to $\rho' \stackrel{\text{def}}{=} \rho_t$ and $\theta' \stackrel{\text{def}}{=} \theta_t$. To first order in $L \stackrel{\text{def}}{=} |\boldsymbol{\rho}' - \boldsymbol{\rho}|$, i.e. short times,

$$t = \frac{L}{v}, \quad \alpha = \arctan\left(\frac{\rho' \sin\theta' - \rho \sin\theta}{\rho' \cos\theta' - \rho\cos\theta}\right), \quad J \stackrel{\text{def}}{=} \left|\frac{\partial(\alpha, t)}{\partial(\rho', \theta')}\right| = \frac{\rho'}{vL}. \tag{C 5}$$

Also, $\alpha_t - \alpha = \omega t = \omega L / v$, where ω is the Larmor frequency ($= B$ in our units.) Thus to first order in L,

$$I_d = \int_0 \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta \int_0 \mathrm{d}\rho' \int_0^{2\pi} \mathrm{d}\theta' \left[\frac{\sin 2(\theta' - \theta)}{v\rho\rho' L} - \frac{\omega \cos 2(\theta' - \theta)}{v^2 \rho\rho'}\right]. \tag{C6}$$

Both terms vanish on integrating over $\theta' - \theta$, the first because the θ and θ' dependence in L is through $\cos(\theta' - \theta)$. Thus I_d is conditionally convergent, although the leading-order divergence is stronger than logarithmic.

Appendix D. Derivation of (6.1)

Differentiating the spectral resolution of the propagator

$$U(t) = \sum_j P_j \exp(-\mathrm{i}\omega_j t) \tag{D 1}$$

with respect to parameters (here $P_j = |j\rangle\langle j|$ and $\omega_j = E_j/\hbar$), we get that

$$\langle \mathrm{d}U(t)\cdot n| \wedge |\mathrm{d}U(t)\cdot n\rangle = \sum_{jk} \langle n|(\mathrm{d}P_j + \mathrm{i}tP_j\,\mathrm{d}\omega_j) \wedge (\mathrm{d}P_k - \mathrm{i}tP_k\,\mathrm{d}\omega_k)|n\rangle\,\mathrm{e}^{\mathrm{i}\omega_{jk}t}, \tag{D 2}$$

where $\omega_{jk} = \omega_j - \omega_k$. The terms quadratic in t are of the form $\delta_{j,n}\,\delta_{k,n}(\mathrm{d}\omega_j \wedge \mathrm{d}\omega_k)$ and vanish by antisymmetry. The terms linear in t are of the form $\delta_{k,n}\langle n|\mathrm{d}P_j|n\rangle \wedge \mathrm{d}\omega_k$. These vanish because $\langle n|\mathrm{d}P_j|n\rangle = 0$. We are left with

$$\langle \mathrm{d}U(t)\cdot n| \wedge |\mathrm{d}U(t)\cdot n\rangle = \sum_{jk} \langle n|\mathrm{d}P_j \wedge \mathrm{d}P_k|n\rangle\,\mathrm{e}^{\mathrm{i}\omega_{jk}t}. \tag{D 3}$$

Next we substitute $|\mathrm{d}j\rangle\langle j| + |j\rangle\langle \mathrm{d}j|$ for $\mathrm{d}P_j$ and similarly for $\mathrm{d}P_k$ to obtain

$$\begin{aligned}\langle \mathrm{d}U(t)\cdot n| \wedge |\mathrm{d}U(t)\cdot n\rangle = \langle \mathrm{d}n| \wedge |\mathrm{d}n\rangle + \sum_j \langle n|\mathrm{d}j\rangle \wedge \langle \mathrm{d}j|n\rangle \\ + \sum_j(\langle n|\mathrm{d}j\rangle \wedge \langle j|\mathrm{d}n\rangle\,\mathrm{e}^{\mathrm{i}\omega_{jn}t} + \langle \mathrm{d}n|j\rangle \wedge \langle \mathrm{d}j|n\rangle\,\mathrm{e}^{\mathrm{i}\omega_{nj}t}).\end{aligned} \tag{D 4}$$

Differentiating $\langle n|j\rangle = \delta_{nj}$, we get that $\langle n|\mathrm{d}j\rangle = -\langle \mathrm{d}n|j\rangle$. This implies that (i) the second sum may be written as $\Sigma_j \langle \mathrm{d}n|j\rangle \wedge \langle j|\mathrm{d}n\rangle$ and the sum performed to give $\langle \mathrm{d}n| \wedge |\mathrm{d}n\rangle$, and (ii) the prefactors of the two exponentials in the third sum are the same, and the $j = n$ term vanishes. Thus we obtain

$$\langle \mathrm{d}U(t)\cdot n| \wedge |\mathrm{d}U(t)\cdot n\rangle = 2\langle \mathrm{d}n| \wedge |\mathrm{d}n\rangle - 2\sum_{j\neq n} \langle \mathrm{d}\,n|j\rangle \wedge \langle j|\mathrm{d}n\rangle \cos\omega_{jn}t, \tag{D 5}$$

which when multiplied by $-\frac{1}{2}\mathrm{i}\hbar$ gives (6.1).

Appendix E. Symplectic form on Hilbert space

It is well known that the equations of quantum mechanics can be cast in hamiltonian form (see, for example, Abraham & Marsden 1978). Our purpose here is to do so in a manner motivated by the correspondence principle; we make the convention that the hamiltonian functional $\mathscr{H}(\psi)$ (which plays the role of H in Hamilton's equations) should be given by the energy expectation value $\langle\psi|\hat{H}|\psi\rangle$ (usually it is taken to be half of this). As we now show, this convention implies the following definition of the symplectic form:

$$[\phi, \chi] \stackrel{\mathrm{def}}{=} -2\hbar\,\mathrm{Im}\,\langle\phi|\chi\rangle. \tag{E 1}$$

Our main interest is to explain the origin of the numerical factor $-2\hbar$, so we do not take pains to introduce a precise notation. Formally Hamilton's equations are $\dot{\psi} = \boldsymbol{J}\cdot\mathscr{H}'(\psi)$. Therefore $\boldsymbol{J}^{-1}\cdot\dot{\psi} = \mathscr{H}'(\psi)$, so that for arbitrary ϕ,

$$[\phi, \dot{\psi}] \stackrel{\mathrm{def}}{=} \langle\phi|\boldsymbol{J}^{-1}\cdot\dot{\psi}\rangle = \mathscr{H}'(\psi)\cdot\phi.$$

But $$\mathscr{H}'(\psi)\cdot\phi \stackrel{\mathrm{def}}{=} (\mathrm{d}/\mathrm{d}\epsilon)_0\,\mathscr{H}(\psi + \epsilon\phi) = 2\,\mathrm{Re}\,\langle\phi|\hat{H}\cdot\psi\rangle,$$

and from Schrödinger's equation, $\hat{H}\cdot\psi = \mathrm{i}\hbar\dot{\psi}$. Therefore

$$[\phi, \dot{\psi}] = 2\,\mathrm{Re}\,\langle\phi|\mathrm{i}\hbar\dot{\psi}\rangle = -2\hbar\,\mathrm{Im}\,\langle\phi|\dot{\psi}\rangle.$$

As $\dot{\psi}$ is arbitrary, (E 1) follows.

Appendix F. Derivation of (6.6)

Consider the quantity $[\boldsymbol{S}^{-1}(\tau)\cdot \mathrm{d}\boldsymbol{Z}(\tau), \wedge \boldsymbol{S}^{-1}(\tau')\cdot \mathrm{d}\boldsymbol{Z}(\tau')]$ and its derivative with respect to τ and τ'. (Here $\boldsymbol{Z}(\tau)$ and $\boldsymbol{S}(\tau)$ are abbreviations for the flow $\boldsymbol{Z}(\boldsymbol{z},\tau)$ and the linearized flow $S(\boldsymbol{z},\tau)$ of (3.11); the $\boldsymbol{z}$ dependence is left implicit.) From (6.9) and from $\dot{\boldsymbol{S}}^{-1}(\tau) = -\boldsymbol{S}^{-1}(\tau)\boldsymbol{J}(H'')_\tau$ we get that

$$\frac{\partial}{\partial \tau}(\boldsymbol{S}^{-1}(\tau)\cdot \mathrm{d}\boldsymbol{Z}(\tau)) = \boldsymbol{S}^{-1}(\tau)\boldsymbol{J}\cdot(\mathrm{d}\boldsymbol{H}')_\tau = \boldsymbol{J}\cdot\nabla_z((\mathrm{d}H)_\tau), \tag{F 1}$$

as the terms in H'' cancel. In the last equality we have used $\boldsymbol{S}^{-1} = -\boldsymbol{J}\boldsymbol{S}^{\mathrm{T}}\boldsymbol{J}$. (We remark in passing that (F 1) is the classical analogue of the t-derivative of (6.3).) Therefore

$$\frac{\partial^2}{\partial\tau\,\partial\tau'}[\boldsymbol{S}^{-1}(\tau)\cdot \mathrm{d}\boldsymbol{Z}(\tau), \wedge \boldsymbol{S}^{-1}(\tau')\cdot \mathrm{d}\boldsymbol{Z}(\tau')] = [\boldsymbol{J}\cdot\nabla_z((\mathrm{d}H)_\tau), \wedge \boldsymbol{J}\cdot\nabla_z((\mathrm{d}H)'_\tau)]$$

$$= -\nabla_z((\mathrm{d}H)_\tau)\cdot\boldsymbol{J}\cdot\nabla_z((\mathrm{d}H)_{\tau'}), \tag{F 2}$$

by using (6.7) and $\boldsymbol{J} = -\boldsymbol{J}^{\mathrm{T}}$. But the last expression is just $-\{(\mathrm{d}H)_\tau, \wedge(\mathrm{d}H)_{\tau'}\}$. Therefore

$$\{(\mathrm{d}H)_\tau, \wedge(\mathrm{d}H)_{\tau'}\} = -\frac{\partial^2}{\partial\tau\,\partial\tau'}[\boldsymbol{S}^{-1}(\tau)\cdot \mathrm{d}\boldsymbol{Z}(\tau), \wedge \boldsymbol{S}^{-1}(\tau')\cdot \mathrm{d}\boldsymbol{Z}(\tau')]. \tag{F 3}$$

Integrating τ and τ' from 0 to t, and noting that $\mathrm{d}\boldsymbol{Z}(0) = 0$ and

$$[\boldsymbol{S}^{-1}(t)\cdot \mathrm{d}\boldsymbol{Z}(t), \wedge \boldsymbol{S}^{-1}(t)\cdot \mathrm{d}\boldsymbol{Z}(t)] = [\mathrm{d}\boldsymbol{Z}(t), \wedge \mathrm{d}\boldsymbol{Z}(t)] \tag{F 4}$$

(the invariance of the symplectic inner product under canonical transformations) we obtain (6.6).

Appendix G. The integrable case: second derivation

We give an alternative derivation of the equivalence of the classical two-form $V^{\mathrm{c}}(\boldsymbol{I})$ and the Hannay two-form $V^{\mathrm{H}}(\boldsymbol{I})$ based on the formalism of §6, in terms of which (B 1) may be rewritten as

$$V^{\mathrm{H}}(\boldsymbol{I}) = -\tfrac{1}{2}\langle[\mathrm{d}\boldsymbol{y}, \mathrm{d}\boldsymbol{y}]\rangle_I. \tag{G 1}$$

Here $\boldsymbol{y}(\boldsymbol{\theta},\boldsymbol{I},R) = (\boldsymbol{q}(\boldsymbol{\theta},\boldsymbol{I},R), \boldsymbol{p}(\boldsymbol{\theta},\boldsymbol{I},R))$. As in Appendix B, we restrict ourselves to one degree of freedom, but the generalization to higher dimensions is straightforward.

Let $\boldsymbol{v} = \partial\boldsymbol{y}/\partial\theta$. Then $\frac{1}{2}\langle[\boldsymbol{y},\boldsymbol{v}]\rangle_I = \langle p\partial_\theta q\rangle_I = I$. Differentiating with respect to R, $\langle[\mathrm{d}\boldsymbol{y},\boldsymbol{v}]\rangle_I + \langle[\boldsymbol{y},\mathrm{d}\boldsymbol{v}]\rangle_I = 0$. But $\langle[\boldsymbol{y},\mathrm{d}\boldsymbol{v}]\rangle_I = \langle[\mathrm{d}\boldsymbol{y},\boldsymbol{v}]\rangle_I$ (this follows from integration by parts over θ and interchanging the arguments of the symplectic inner product), so that

$$\langle[\mathrm{d}\boldsymbol{y},\boldsymbol{v}]\rangle_I = 0. \tag{G 2}$$

Let $\boldsymbol{Y}(\theta,t) \overset{\mathrm{def}}{=} \boldsymbol{y}(\theta+\omega t)$ (the I and R dependence is left implicit). Equivalently $\boldsymbol{Y}(\theta,t) \overset{\mathrm{def}}{=} \boldsymbol{y}_t(\theta)$ (since in general $f_t(\theta) = f(\theta+\omega t)$), or more simply $\boldsymbol{Y}(t) \overset{\mathrm{def}}{=} \boldsymbol{y}_t$. Since $\boldsymbol{Y}(t)$ satisfies Hamilton's equations, its derivative with respect to parameters,

$$\mathrm{d}\boldsymbol{Y}(t) = \mathrm{d}(\boldsymbol{y}_t) = (\mathrm{d}\boldsymbol{y})_t + \mathrm{d}\omega\, t\boldsymbol{v}_t, \tag{G 3}$$

is a solution of (6.9). Substituting (G 3) into (6.11) we get that

$$V^{\mathrm{c}} = -\tfrac{1}{4}\overline{\langle[(\mathrm{d}\boldsymbol{y})_t, \wedge (\mathrm{d}\boldsymbol{y})_t]\rangle_I} + \tfrac{1}{2}\overline{\langle[\mathrm{d}\boldsymbol{Y}(t), \wedge \boldsymbol{S}(\boldsymbol{y},t)\cdot\mathrm{d}\boldsymbol{y}]\rangle_I} - \tfrac{1}{4}\langle[\mathrm{d}\boldsymbol{y}, \wedge \mathrm{d}\boldsymbol{y}]\rangle_I, \tag{G 4}$$

as terms of the form $\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_I$ vanish in light of (G 2). The first and third terms in (G 4) are both equal to $\frac{1}{2}V^{\mathrm{H}}(I)$. It remains to show that the second term vanishes.

Letting $\boldsymbol{w} \stackrel{\mathrm{def}}{=} \partial \boldsymbol{y}/\partial I$, and resolving $\mathrm{d}\boldsymbol{y}$ into its $\boldsymbol{v}$ and $\boldsymbol{w}$ components,

$$\mathrm{d}\boldsymbol{y} = \alpha^v \boldsymbol{v} + \alpha^w \boldsymbol{w}. \tag{G 5}$$

It is straightforward to verify that $\boldsymbol{S}(\boldsymbol{y},t)\cdot\boldsymbol{v} = \boldsymbol{v}_t$ (or more explicitly, $\boldsymbol{S}(\boldsymbol{y}(\theta),t)\cdot\boldsymbol{v}(\theta) = \boldsymbol{v}(\theta+\omega t)$) and $\boldsymbol{S}(\boldsymbol{y},t)\cdot\boldsymbol{w} = \boldsymbol{w}_t + (\partial\omega/\partial I)\, t\boldsymbol{v}_t$. Therefore

$$\boldsymbol{S}(\boldsymbol{y},t)\cdot\mathrm{d}\boldsymbol{y} = (\alpha^v + (\partial\omega/\partial I)\, t\alpha^w)\, \boldsymbol{v}_t + \alpha^w \boldsymbol{w}_t. \tag{G 6}$$

Also, since $\omega\boldsymbol{v} = \boldsymbol{J}\cdot\boldsymbol{H}'(\boldsymbol{y})$, it follows that

$$[\boldsymbol{w}, \boldsymbol{v}] = (1/\omega)\, \boldsymbol{w}\cdot\boldsymbol{H}' = (1/\omega)\, \partial H/\partial I = 1. \tag{G 7}$$

By using (G 3) and (G 5)–(G 7), the second term in (G 4) may be written as half the time average of

$$\langle(\alpha^w)_t \wedge \alpha^v\rangle_I + (\partial\omega/\partial I)\, t\, \langle(\alpha^w)_t \wedge \alpha^w\rangle_I - \langle(\alpha^v)_t \wedge \alpha^w\rangle_I - \mathrm{d}\omega \wedge \langle\alpha^w\rangle_I\, t. \tag{G 8}$$

From (G 2), (G 5) and (G 7) it follows that

$$\langle\alpha^w\rangle_I = \overline{(\alpha^w)_t} = 0. \tag{G 9}$$

One can show that (G 9) implies the vanishing of the time average of (G 8), which in turn implies that $V^{\mathrm{c}}(I) = V^{\mathrm{H}}(I)$. (Note that $\overline{t(\alpha^w)_t}$ vanishes in the generalized sense of Appendix J.) A similar though more involved argument appears in Appendix K for the periodic orbit two-form.

Let us point out that (G 1) has a geometrical interpretation similar to those described in §6. Suppose we want the flux of $V^{\mathrm{H}}(\boldsymbol{I})$ through $\square_R$. From a point $\boldsymbol{y}$ on an invariant torus we draw vectors $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ to points on neighbouring tori with the same actions and angles but with parameters $R+r_1$ and $R+r_2$. $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ span an area element $\square_I(\boldsymbol{\theta})$ in phase space, as drawn in figure 1*e*. According to (G 1), the required flux is (minus) the symplectic area of $\square_I(\boldsymbol{\theta})$ averaged over the torus. There is a similar construction for the fundamental formula (1.2) for the quantum two-form V_n. From $|n(R)\rangle$ we draw vectors $|n_1\rangle$ and $|n_2\rangle$ in Hilbert space to $|n(R+r_1)\rangle$ and $|n(R+r_2)\rangle$. $|n_1\rangle$ and $|n_2\rangle$ span an area element $\square_H$ in Hilbert space, as in figure 1*d*. According to (1.2), the flux of V_n through $\square_R$ is just (minus) the symplectic area of $\square_H$ (as defined in Appendix E). In this light, the correspondence of the quantum and classical two-forms, (1.2) and (G 1), is immediate.

Appendix H. Derivative at constant volume

The microcanonical average, regarded as a function of phase volume ω rather than energy E, is given by

$$\langle\phi\rangle_\omega = \int \mathrm{d}^{2N}\boldsymbol{z}\, \delta(\omega - \Omega_P)\, \phi, \tag{H 1}$$

where $\Omega_P(\boldsymbol{z}) \stackrel{\mathrm{def}}{=} \Omega(H(\boldsymbol{z}))$ is the volume of phase space with energy less than $H(\boldsymbol{z})$. (More explicitly, $\Omega_P(\boldsymbol{z},R) \stackrel{\mathrm{def}}{=} \Omega(H(\boldsymbol{z},R),R)$.) Equation (H 1) is correctly normalized since

$$\delta(\Omega(E) - \Omega_P(\boldsymbol{z})) = \delta(E - H(\boldsymbol{z}))/\Omega'(E).$$

Differentiating (H 1) with respect to parameters at fixed ω, we get

$$\mathrm{d}\langle\phi\rangle_\omega = \langle\mathrm{d}\phi\rangle_\omega - \int \mathrm{d}^{2N}z\,\delta'(\omega-\Omega_P)\,\mathrm{d}\Omega_P \wedge \phi = \langle\mathrm{d}\phi\rangle_\omega - \frac{\mathrm{d}}{\mathrm{d}\omega}\langle\mathrm{d}\Omega_P \wedge \phi\rangle_\omega. \quad \text{(H 2)}$$

But $\mathrm{d}\Omega_P = \mathrm{d}\Omega + \Omega'\mathrm{d}H$, and

$$\mathrm{d}\Omega = -\int \mathrm{d}^{2N}z\,\delta(E-H)\,\mathrm{d}H = -\Omega'\langle\mathrm{d}H\rangle.$$

Therefore

$$\mathrm{d}\Omega_P = -\Omega'(\mathrm{d}E-\mathrm{d}H), \quad \text{(H 3)}$$

where $\mathrm{d}E \overset{\mathrm{def}}{=} \langle\mathrm{d}H\rangle$. We substitute (H 3) into (H 2), and express the result in terms of E rather than ω, via $\omega = \Omega(E)$. Noting that $\mathrm{d}/\mathrm{d}\omega = (\Omega')^{-1}\,\mathrm{d}/\mathrm{d}E$,

$$\mathrm{d}\langle\phi\rangle = \langle\mathrm{d}\phi\rangle + (1/\Omega')\,(\Omega'\langle(\mathrm{d}E-\mathrm{d}H)\wedge\phi\rangle)'. \quad \text{(H 4)}$$

Appendix I. Derivations of (7.6) and (7.10)

First we derive (7.6). Starting with the expression $\frac{1}{4}\overline{\langle \mathrm{d}H \wedge [\mathrm{d}\boldsymbol{Z}(t), \wedge\, \mathrm{d}\boldsymbol{Z}(t)]\rangle}$ on the left side of (7.6), we express the time average as the residue of the Laplace transform at the origin (as in Appendix J), and replace $[\mathrm{d}\boldsymbol{Z}(t), \wedge\, \mathrm{d}\boldsymbol{Z}(t)]$ by its expression in (6.6). The result is

$$-\tfrac{1}{2}\lim_{s\to 0} s \int_0^\infty \mathrm{d}t\,\mathrm{e}^{-st}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'\,\langle \mathrm{d}H \wedge \{(\mathrm{d}H)_\tau, \wedge\,(\mathrm{d}H)_{\tau'}\}\rangle. \quad \text{(I 1)}$$

In writing (I 1) we have used the symmetry of the τ and τ' integrals to restrict the domain of integration to $\tau > \tau'$; this restriction is compensated by an additional factor of 2. Reversing the order of the integrations allows the t integral to be performed, with the result

$$-\tfrac{1}{2}\lim_{s\to 0} s \int_0^\infty \mathrm{d}\tau' \int_{\tau'}^\infty \mathrm{d}\tau\,\mathrm{e}^{-s\tau}\,\langle \mathrm{d}H \wedge \{(\mathrm{d}H)_\tau, \wedge\,(\mathrm{d}H)_{\tau'}\}\rangle. \quad \text{(I 2)}$$

Since microcanonical averages are time invariant, $\langle \mathrm{d}H \wedge \{(\mathrm{d}H)_\tau, \wedge\,(\mathrm{d}H)_{\tau'}\}\rangle$ may be replaced by $\langle \mathrm{d}H_{-\tau'} \wedge \{(\mathrm{d}H)_{\tau-\tau'}, \wedge\,\mathrm{d}H\}\rangle$. After changing variables from τ to $\tau-\tau'$, (I 2) becomes

$$-\lim_{s\to 0} \int_0^\infty \mathrm{d}\tau'\,\mathrm{e}^{-s\tau'} \int_0^\infty \mathrm{d}\tau\,\mathrm{e}^{-s\tau}\,\langle (\mathrm{d}H)_{-\tau'} \wedge \{(\mathrm{d}H)_\tau, \wedge\,\mathrm{d}H\}\rangle. \quad \text{(I 3)}$$

This expression may be written as $\lim_{s\to 0} G(s,s)$, where

$$\left.\begin{aligned} G(s,s') &= -\int_0^\infty \mathrm{d}\tau\,\frac{\mathrm{e}^{-s\tau}}{s}\,s' \int_0^\infty \mathrm{d}\tau'\,\mathrm{e}^{-s'\tau'}\,F(\tau,\tau'),\\ F(\tau,\tau') &= \langle (\mathrm{d}H)_{-\tau'} \wedge \{(\mathrm{d}H)_\tau, \wedge\,\mathrm{d}H\}\rangle, \end{aligned}\right\} \quad \text{(I 4)}$$

as asserted in (7.6) and (7.7). In passing from (I 3) to (I 4) we have in effect multiplied and divided by s.

Next we derive (7.10). Consider

$$\lim_{s\to 0}\frac{1}{2}\int_0^\infty \mathrm{d}\tau\,\frac{\mathrm{e}^{-s\tau}}{s}\,\langle\{(\mathrm{d}H)_\tau, \wedge\,\mathrm{d}H\}\rangle. \quad \text{(I 5)}$$

From (3.12), $\langle\{(\mathrm{d}H)_\tau, \wedge \mathrm{d}H\}\rangle = (\Omega'\langle(\mathrm{d}\dot{H})_\tau \wedge \mathrm{d}H\rangle)'/\Omega'$. Making this substitution in (I 5) and integrating by parts over τ, we obtain

$$\lim_{s\to 0}\frac{1}{2\Omega'}\int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-s\tau}(\Omega'\langle(\mathrm{d}H)_\tau \wedge \mathrm{d}H\rangle)' = \frac{1}{2\Omega'}\int_0^\infty \mathrm{d}\tau(\Omega'\langle(\mathrm{d}H)_\tau \wedge \mathrm{d}H\rangle)'. \tag{I 6}$$

But from (3.15), this last expression is just $V^{\mathrm{c}}(E)$, as asserted in (7.10).

Appendix J. Time average as residue of Laplace transform

Assuming that $\bar{f}$ exists, we show that

$$\lim_{s\to 0} sF(s) = \bar{f}, \tag{J 1}$$

where F is the Laplace transform of f. The result is true for constant functions (easily verified). Then taking $\tilde{f} = f - \bar{f}$ to be the oscillatory part of f, it suffices to show that

$$\lim_{s\to 0} s\tilde{F}(s) = 0, \tag{J 2}$$

where $\tilde{F}$ is the Laplace transform of $\tilde{f}$. Integrating the left-hand side of (J 2) by parts, we get

$$\lim_{s\to 0} s\tilde{F}(s) = \lim_{s\to 0} s^2\int_0^\infty \mathrm{d}t\, \tilde{g}(t)\, \mathrm{e}^{-st}, \tag{J 3}$$

where $\tilde{g}(t) = \int_0^t \mathrm{d}\tau \tilde{f}(\tau)$. Since the time average of $\tilde{f}$ vanishes, $|\tilde{g}(t)|/t \to 0$ as $t \to \infty$. Thus for any $\epsilon > 0$ we can take T sufficiently large so that $|\tilde{g}(t)| < \epsilon t$ for $t > T$. Then dividing the integral in (J 3) between $[0, T]$ and $[T, \infty]$,

$$\lim_{s\to 0}|s\tilde{F}(s)| < \lim_{s\to 0} s^2\int_0^T \mathrm{d}t\,|\tilde{g}(t)|\,\mathrm{e}^{-st} + \lim_{s\to 0} s^2\int_T^\infty \mathrm{d}t\,\epsilon t\,\mathrm{e}^{-st}. \tag{J 4}$$

Taking the $s \to 0$ limit on the right-hand side, we get $\lim_{s\to 0}|s\tilde{F}(s)| < \epsilon$. Since ϵ is arbitrary, (J 2) follows. If F has a meromorphic extension to a neighbourhood of the origin, (J 1) is equivalent to

$$\bar{f} = \mathrm{Res}_0 F(s), \tag{J 5}$$

where $\mathrm{Res}_0 F(s)$ denotes the residue of F at the origin. If $\bar{f}$ does not exist, we may regard (J 5) as its definition. In this way we can say that t^n $(n > 0)$ and $\mathrm{e}^{\lambda t}$ have time averages equal to zero.

Appendix K. The periodic orbit two-form

$\boldsymbol{y}_j(\theta, S, R)$ denotes a family of periodic orbits parametrized by an angle θ (proportional to the time), action S and parameters R. For convenience we drop the subscript j from $\boldsymbol{y}_j$. Usually the R dependence is left implicit, and sometimes the S and θ dependence is left implicit as well. T_j is the period and $\omega_j = 2\pi/T_j$ is the frequency of the orbit; $\boldsymbol{v} \stackrel{\mathrm{def}}{=} \partial\boldsymbol{y}/\partial\theta$ is proportional to the velocity.

The periodic orbit two-form is given by

$$V_j^{\mathrm{c}}(S) = -\langle[\mathrm{d}\boldsymbol{y}, \wedge \mathrm{d}\boldsymbol{y}]\rangle_{jS}. \tag{K 1}$$

$\langle\cdot\rangle_{jS}$ denotes the orbit average $(2\pi)^{-1}\int_0^{2\pi}\mathrm{d}\theta$. While we will not use this result, let us point out that $V_j^c(S)$ is closed, simply because $\mathrm{d}\boldsymbol{y}(\theta, S)$ is closed. Note that in §8, the periodic orbit two-form is a function of energy rather than action, as S is set equal to $S_j(E)$. In general $\mathrm{d}(V_j^c(S_j(E)) \neq 0$.

The θ-origin along each periodic orbit is arbitrary and may be shifted by the transformation

$$\boldsymbol{y}(\theta, S, R) \rightarrow \boldsymbol{y}(\theta + F(S, R), S, R). \tag{K 2}$$

However $V_j^c(S)$ remains invariant under this transformation, as we now show. Under (K 2), $\mathrm{d}\boldsymbol{y}(\theta) \rightarrow \mathrm{d}\boldsymbol{y}(\theta+F) + \mathrm{d}F\boldsymbol{v}(\theta+F)$, and the two-form (K 1) acquires an additional term $-2\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS} \wedge \mathrm{d}F$. We have that $\frac{1}{2}\langle[\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS} = \langle \boldsymbol{p}\cdot\partial_\theta \boldsymbol{q}\rangle_{jS} = S/2\pi$. Differentiating, $\mathrm{d}\langle[\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS} = \langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS} + \langle[\boldsymbol{y}, \mathrm{d}\boldsymbol{v}]\rangle_{jS} = 0$. But $\langle[\boldsymbol{y}, \mathrm{d}\boldsymbol{v}]\rangle_{jS} = \langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS}$ (this follows from integration by parts over θ and reversing the arguments of the symplectic inner product). Therefore

$$\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS} = 0, \tag{K 3}$$

which in turn implies the invariance of the two-form.

Next we derive (9.8). The energy of an orbit $E_j(S, R) = H(\boldsymbol{y}(\theta, S, R), R)$ is independent of θ. Therefore its variation with R and S,

$$\delta E_j = (\mathrm{d}H + \boldsymbol{H}'(\boldsymbol{y})\cdot\mathrm{d}\boldsymbol{y})\cdot\delta R + (1/2\pi)\,(\boldsymbol{H}'(\boldsymbol{y})\cdot\boldsymbol{w})\,\delta S, \tag{K 4}$$

where $\boldsymbol{w} \overset{\mathrm{def}}{=} 2\pi\,\partial\boldsymbol{y}/\partial S$, is also θ-independent. Averaging (K 4) around the orbit, and using the fact that $\boldsymbol{J}\cdot\partial\boldsymbol{H}'(\boldsymbol{y}) = \omega_j\boldsymbol{v}$, we obtain

$$\delta E_j = (\langle \mathrm{d}H\rangle_{jS} + \omega_j\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS})\cdot\delta R + (\omega_j/2\pi)\langle[\boldsymbol{w}, \boldsymbol{v}]\rangle_{jS}\,\delta S. \tag{K 5}$$

From (K 3) $\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jS}$ vanishes. Also $[\boldsymbol{w}, \boldsymbol{v}] = (2\pi/\omega_j)\,\boldsymbol{H}'(\boldsymbol{y})\cdot\partial\boldsymbol{y}/\partial S = T_j\,\partial E_j/\partial S = 1$. Therefore (K 5) becomes $\delta E_j = \langle \mathrm{d}H\rangle_{jS}\cdot\delta R + \delta S/T_j$, or, if S is regarded as a function of E and R,

$$\mathrm{d}S_j = T_j(\mathrm{d}E - \langle \mathrm{d}H\rangle_{jS}), \tag{9.8}$$

the required result (9.8).

The last result to be derived is (8.11). The starting point is the alternative formula (6.11) for $V_j^{\mathrm{sc}}(E)$, which remains valid if the microcanonical average is replaced by an orbit average. Let $\boldsymbol{Y}(\theta, t) \overset{\mathrm{def}}{=} \boldsymbol{y}(\theta + \omega_j t)$ (the S and R dependence is left implicit.) Equivalently $\boldsymbol{Y}(\theta, t) \overset{\mathrm{def}}{=} \boldsymbol{y}_t(\theta)$ (since in general $f_t(\theta) = f(\theta + \omega_j t)$), or more simply $\boldsymbol{Y}(t) \overset{\mathrm{def}}{=} \boldsymbol{y}_t$. Since $\boldsymbol{Y}(t)$ satisfies Hamilton's equations, its derivative with respect to parameters,

$$\mathrm{d}\boldsymbol{Y}(t) = \mathrm{d}(\boldsymbol{y}_t) = (\mathrm{d}\boldsymbol{y})_t + \mathrm{d}\omega_j t\boldsymbol{v}_t \tag{K 6}$$

is a solution of (6.9). From (K 6), (6.11) and (8.9) we obtain

$$V_j^{\mathrm{sc}}(E) = -\tfrac{1}{4}\overline{\langle[(\mathrm{d}\boldsymbol{y})_t, \wedge (\mathrm{d}\boldsymbol{y})_t]\rangle_{jE}} + \tfrac{1}{2}\overline{\langle[\mathrm{d}\boldsymbol{Y}(t), \wedge \boldsymbol{S}(\boldsymbol{y}, t)\cdot\mathrm{d}\boldsymbol{y}]\rangle_{jE}} - \tfrac{1}{4}\overline{\langle[\mathrm{d}\boldsymbol{y}, \wedge \mathrm{d}\boldsymbol{y}]\rangle_{jE}}, \tag{K 7}$$

where the average $\langle\,\cdot\,\rangle_{jE}$ is taken over the orbit with energy E, and terms of the form $\langle[\mathrm{d}\boldsymbol{y}, \boldsymbol{v}]\rangle_{jE}$ vanish in light of (K 3). Both the first and third terms of (K 7) are equal to $\frac{1}{2}V_j^c(S_j(E))$. It remains to show that the second term vanishes.

Expressing its time average as the residue of the Laplace transform at the origin (as in Appendix J), we may write the second term of (K 7) as $\mathrm{Res}_0 F(s)$, where $F(s)$ is the Laplace transform of

$$f(t) = \langle[\mathrm{d}\boldsymbol{Y}(t), \boldsymbol{S}(\boldsymbol{y}, t)\cdot\mathrm{d}\boldsymbol{Y}(0)]\rangle_{jE}. \tag{K 8}$$

For the explicit evaluation of $f(t)$ we introduce a Floquet basis along the orbit, in terms of which the action of the linearized flow $\boldsymbol{S}(\boldsymbol{y},t)$ is simply expressed. The Floquet basis consists of $\boldsymbol{v}=\partial\boldsymbol{y}/\partial\theta$ tangent to the orbit, $\boldsymbol{w}=2\pi\,\partial\boldsymbol{y}/\partial S$ transverse to the energy shell on which the orbit lies, and $\boldsymbol{\xi}^{k+}$, $\boldsymbol{\xi}^{k-}$, $k=1,\dots,N-1$, which span the orbit's stable and unstable manifolds respectively; $\boldsymbol{v}$, $\boldsymbol{w}$ and $\boldsymbol{\xi}^{k\pm}$ are functions of θ, S, R. Then one can show that

$$\begin{gathered}\boldsymbol{S}(\boldsymbol{y},t)\cdot\boldsymbol{v}=\boldsymbol{v}_t,\quad \boldsymbol{S}(\boldsymbol{y},t)\cdot\boldsymbol{w}=\boldsymbol{w}_t+(\partial\omega_j/\partial S)\,t\boldsymbol{v}_t,\\ \boldsymbol{S}(\boldsymbol{y},t)\cdot\boldsymbol{\xi}^{k\pm}=\mathrm{e}^{\mp\lambda_k t}(\boldsymbol{\xi}^{k\pm})_t.\end{gathered}\tag{K 9}$$

(The first equation is written more explicitly as $\boldsymbol{S}(\boldsymbol{y}(\theta),t)\cdot\boldsymbol{v}(\theta)=\boldsymbol{v}(\theta+\omega_j t)$, and similarly for the others.) Both λ_k and $\boldsymbol{\xi}^{k\pm}$ may be complex, but we assume that

$$\lambda_k\neq \mathrm{i}n\omega_j,\tag{K 10}$$

i.e. that the stability exponents are either elliptic or hyperbolic.

The Floquet basis can be chosen to be symplectic, so that

$$[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l+}]=0,\quad[\boldsymbol{\xi}^{k-},\boldsymbol{\xi}^{l-}]=0,\quad[\boldsymbol{v},\boldsymbol{\xi}^{k\pm}]=0,\quad[\boldsymbol{w},\boldsymbol{\xi}^{k\pm}]=0,\tag{K 11a}$$

$$[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l-}]=\delta_{kl},\quad[\boldsymbol{w},\boldsymbol{v}]=1.\tag{K 11b}$$

Among these relations, the homogeneous equations (K 11a) are a direct consequence of (K 9). For example,

$$[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l+}]=[\boldsymbol{S}(\boldsymbol{y},T_j)\cdot\boldsymbol{\xi}^{k+},\boldsymbol{S}(\boldsymbol{y},T_j)\cdot\boldsymbol{\xi}^{l+}]=\exp\left(-(\lambda_k+\lambda_l)\,T_j\right)[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l+}];$$

(the first equality follows from the invariance of the symplectic inner product and the second from (K 9)). Therefore

$$(\exp\left(-(\lambda_k+\lambda_l)\,T_j\right)-1)\,[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l+}]=0.$$

Since $\exp\left(-(\lambda_k+\lambda_l)\,T_j\right)\neq 1$ (cf. (K 10)), this implies that $[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{l+}]=0$. Of the inhomogeneous equations (K 11b), $[\boldsymbol{\xi}^{k+},\boldsymbol{\xi}^{k-}]=1$ is simply a normalization convention, whereas $[\boldsymbol{w},\boldsymbol{v}]=1$ was shown in the discussion following (K 5).

Expanding $\mathrm{d}\boldsymbol{y}$ in the Floquet basis,

$$\left.\begin{gathered}\mathrm{d}\boldsymbol{y}=\alpha^v\boldsymbol{v}+\alpha^w\boldsymbol{w}+\sum_{k=1}^{N-1}(\alpha^{k+}\boldsymbol{\xi}^{k+}+\alpha^{k-}\boldsymbol{\xi}^{k-}),\\ \alpha^v=[\boldsymbol{w},\mathrm{d}\boldsymbol{y}],\quad\alpha^w=-[\boldsymbol{v},\mathrm{d}\boldsymbol{y}],\quad\alpha^{k\pm}=\mp[\boldsymbol{\xi}^{k\mp},\mathrm{d}\boldsymbol{y}];\end{gathered}\right\}\tag{K 12}$$

the expressions for the coefficients α (which are functions of θ, S, R) follow from (K 11). Substituting (K 9), (K 11) and (K 12) into (K 8) one can show that

$$f(t)=\phi^{wv}(t)+\phi^{wv}(-t)+(\partial\omega_j/\partial S)\,\phi^{ww}(t)\,t+\langle\alpha^w\rangle_{jE}\wedge\mathrm{d}\omega_j\,t+\sum_{k=1}^{N-1}(\phi^k(t)\,\mathrm{e}^{\lambda_k t}+\phi^k(-t)\,\mathrm{e}^{-\lambda_k t}),\tag{K 13}$$

where

$$\phi^{wv}(t)=\langle(\alpha^w)_t\wedge\alpha^v\rangle_{jE},\quad\phi^{ww}(t)=\langle(\alpha^w)_t\wedge\alpha^w\rangle_{jE},\quad\phi^k(t)=\langle(\alpha^{k+})_t\wedge\alpha^{k-}\rangle_{jE}.\tag{K 14}$$

From (K 3) and (K 12) it follows that

$$\langle\alpha^w\rangle_{jE}=\overline{(\alpha^w)_t}=0.\tag{K 15}$$

Equation (K 15) in turn implies that the Laplace transform of the first three terms in (K 13) have no poles at the origin. As for the remaining terms, since $\phi^k(t)$ is T_j-periodic, the Laplace transform of $\phi^k(\pm t)\exp(\pm\lambda_k t)$ can have poles only at $\pm\lambda_k + in\omega_j$; from (K 10) none of these lie at the origin. Thus $\mathrm{Res}_0 F(s) = 0$, and the second term in (K 7) vanishes, as claimed. This implies in turn than $V_j^{\mathrm{sc}}(E) = V_j^{\mathrm{c}}(S_j(E))$, the required result (8.11).

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