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COURSE ON GEOMETRIC PHASES

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"Chaos and the Geometric Phase"

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These are preliminary lecture notes, intended only for distribution to participants.

Chaos and the Geometric Phase.

In these lectures we'll explore the classical ($\hbar=0$) and semiclassical limits ($\hbar \to 0$) of the geometric phase for systems whose classical dynamics is chaotic. What do we mean by chaotic? We'll start by assuming the dynamics is <u>ergodic</u>, and will make additional assumptions later.

Integrable - N constants of motion

$H(z)$, N freedom Hamiltonian. $z=(q,p)$; $q,p \in \mathbb{R}^N$

$\{H, I_i\} = \{I_i, I_j\} = 0$, $1 \le i,j \le N$. COM's / Symmetries.

Motion on N-dim tori

Ergodic - 1 constant of motion

$\{H, F\} = 0 \Rightarrow F = f(H)$. H is only COM.

Motion on 2N-1 dim energy shell $\{z \mid H(z)=E\}$.

Time Average = Microcanonical Average

$$\bar{F} = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, F(z_t), \qquad z \longrightarrow z_t$$

$$\langle F \rangle_E = \frac{1}{\Omega'(E)} \int d^{2N}z\, \delta(E-H(z))\, F(z),$$

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

$\Omega'(E) = d\Omega/dE = \int d^{2N}z\, \delta(E-H)$, volume of energy s

For almost all initial conditions,

$$\overline{F} = \langle F \rangle .$$

1. $\hbar$-scaling

How does γ scale with $\hbar$? This will be a preliminary and rather heuristic discussion, part of whose purpose is to introduce concepts, notation that we'll use later. We'll give two arguments which will give conflicting results. The conflict calls into question the existence of the classical limit itself! We'll indicate the resolution here, though part of the discussion will be deferred till later.

Classical limit

$$\hbar \to 0, \; n \to \infty \quad \text{so that } E_n \approx \text{constant, macroscopic}$$

Classical observables are $\hbar$-independent

A. After adiabatic cycle,

$$|n\rangle \to \exp -\frac{i}{\hbar}\left[\int_0^T dt \, E_n(R_t) - \hbar \gamma_n \right].$$

Expect: $E_n = O(1) \Rightarrow \hbar\gamma_n \lesssim O(1)$, since geometric phase should not overwhelm dynamical phase in classical limit.

In what follows, absorb $\hbar$ into γ_n:

$$\gamma_n^0 \to \gamma_n = \hbar \gamma_n^0 , \quad V_n^0 \to V_n = \hbar V_n^0 .$$

Expect f_n, V_n to be $O(1)$ in classical limit.

B. Estimate

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

(Note factor of $\hbar$, and $-i$, which is equivalent to Im).

Require formula for energy levels, matrix elements.

Energy levels.

$$\mathcal{N}(E) = \#\ \text{levels} < E$$

$$= \frac{\Omega(E)}{(2\pi\hbar)^N} + O(\hbar^{-N+1}), \quad \text{Weyl rule}$$

$$\Omega(E_n) = n(2\pi\hbar)^N, \quad \text{implicit quantization.}$$

[[• Rigorous basis - Weyl calculus.

$$A(z) = \int d^N x \, \langle q + \tfrac{1}{2} x | \hat{A} | q - \tfrac{1}{2} x \rangle \, e^{-\frac{ip.x}{\hbar}}$$

$$\hat{A} = \hat{q} \longrightarrow A = q,$$

$$\hat{P}_n = |n\rangle\langle n| \longrightarrow \rho_n(z), \quad \text{Wigner function}$$

$$[\hat{A}, \hat{B}] \longrightarrow \{A, B\} + O(\hbar^2)$$

$$\mathrm{Tr}\, A^{+} B = \frac{1}{(2\pi\hbar)^N} \int d^{2N} z \, A^{*}(z) B(z)$$

Omitted in lecture

$$\langle n|\hat{A}|n\rangle = \mathrm{Tr}\ \hat{P}_n^{+}\hat{A} = \frac{1}{(2\pi\hbar)^N}\int d^{2N}z\ \rho_n(z)\,A(z).$$

Weyl rule follows from $\hbar$-expansion of $e^{-\beta\hat{H}}$ and its Laplace transform $\frac{1}{E-\hat{H}}$ via Weyl calculus.]

Matrix elements

- Diagonal matrix elements

$$\langle n|\hat{A}|n\rangle = \frac{1}{(2\pi\hbar)^N}\int d^{2N}z\ \rho_n(z)\,A(z) \approx O(1).$$

What is ρ_n? (classical phase distribution corresponding to expectation value wrt $|n\rangle$)

$$\langle n|\hat{A}_t|n\rangle = \langle n|\hat{A}_t|n\rangle\ ,\quad \hat{A}_t = U^+(t)\,\hat{A}\,U(t)\ ,\quad U(t) = e^{-\frac{i}{\hbar}\hat{H}t}.$$

time invariance of expectation values

$$\rightsquigarrow \int d^{2N}z\ \rho_n(z)\,A(z_t) = \int d^{2N}z\ \rho_n(z)\,A(z_t) = \int d^{2N}z\ \rho_n(z_{-t})\,A(z$$

Liouville theorem

$\Rightarrow$ $\rho_n(z_t) = \rho_n(z)$, ie ρ is invariant under dynamics

Ergodicity $\Rightarrow$ $\rho_n = \rho_n(H(z))$

Eigenstate $\Rightarrow$ $\rho_n = c\,\delta(E_n - H(z))$

Normalization $\Rightarrow$ $\rho_n = \delta(E_n - H(z))\,/\,\Omega'(E_n).$

$\langle n|\hat{A}|n\rangle \rightsquigarrow \langle A\rangle_{E_n}$, microcanonical average.

- Off diagonal Matrix elements

Proceed from diagonal result...

Variance:

$$\langle n|\hat{A}^2|n\rangle - \langle n|\hat{A}|n\rangle^2 \rightsquigarrow \langle A^2\rangle_{E_n} - \langle A\rangle_{E_n}^2 = O(1)$$

Insert resolution of identity on lhs:

$$\langle n|\hat{A}^2|n\rangle - \langle n|\hat{A}|n\rangle^2 = \sum_{m\neq n} |\hat{A}_{mn}|^2$$

For purposes of estimation, truncate sum:

$$|\hat{A}_{mn}|^2 = \left.\begin{array}{l} 0, \ |E_m - E_n| > \Delta \\ a^2, \ |E_m - E_n| < \Delta \end{array}\right\} .$$

Δ is small classical energy interval. a^2 = const.

So

$$\sum_{m\neq n} |\hat{A}_{mn}|^2 \sim \Bigg(\underbrace{\frac{\Omega'(E_n)\Delta}{(2\pi\hbar)^N}}_{\text{(\# of states in range } E_n \pm \Delta)}\Bigg) a^2 = O(1)$$

$$|\langle m|\hat{A}|n\rangle|^2 \gtrsim O(\hbar^N).$$

The off-diagonal elements can be larger, of course. For integrable systems, for example, certain matrix elements satisfying selection rules are $O(1)$, ie much larger than $O(\hbar^N)$, whereas the vast majority are exponentially small $\sim e^{-1/\hbar}$, ie much smaller than $O(\hbar^N)$. For chaotic systems, however, matrix elements are roughly the same size, and most are therefore of $O(\hbar^N)$. A narrow band about the diagonal (energy width $\Delta \sim \hbar$) is of $O(\hbar^{N-1})$, but this does not contradict sum rule. It is this "equipartition" which makes random matrix theory applicable.

- Estimate of two-form

We are now in a position to estimate two-form

$$V_n = -i\hbar \sum_{m\neq n} \frac{\langle n|\nabla\hat{H}|m\rangle \wedge \langle m|\nabla\hat{H}|n\rangle}{(E_m - E_n)^2} \qquad \hat{H}(R),\ |n(R)\rangle$$

$$\langle n|\nabla H|m\rangle \sim O(\hbar^{N/2})$$

$$(E_m - E_n)^2 \sim (n-m)^2\, O(\hbar^{2N})$$

$$V_n \sim \hbar \sum_{m\neq n} \frac{O(\hbar^N)}{O(\hbar^{2N})} \frac{1}{(n-m)^2}$$

$$\sim \hbar^{-(N-1)}.$$

It would appear that two-form diverges in classical limit for $N > 1$. Integrable systems are exceptional, because when $E_n - E_m$ is minimal, ie $|m-n|$ small, $\langle n|\nabla h|m\rangle$ is typically exponentially small.

So does the semiclassical limit exist?

It does, provided we consider an averaged two-form

$$\sim \frac{1}{2N} \sum_{n=n_*-N}^{n_*+N} V_n .$$

Divergent behaviours cancel, and what remains is $O(1)$. We'll return to this point. Next, we'll see to get

Classical Limit

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

Identity:

$$\frac{1}{(E_m - E_n)^2} = -\frac{1}{\hbar^2} \int_0^\infty dt \; t e^{\frac{-i}{\hbar}(E_m - E_n)t}$$

Take first factor from above.

$$\frac{\langle n | \nabla\hat{H} | m \rangle}{(E_m - E_n)^2} = -\frac{1}{\hbar^2} \int_0^\infty dt \; t \, \langle n | e^{itE_n/\hbar} \; \nabla\hat{H} \; e^{-itE_m/\hbar} | m \rangle$$

$$= \langle n | U^\dagger(t) \nabla\hat{H} \, U(t) | m \rangle , \quad U(t) = e^{-it\hat{H}/\hbar}.$$

$$= \langle n | (\nabla\hat{H})_t | m \rangle, \text{ Heisenberg picture}$$

Then

$$V_n = \frac{i}{\hbar} \int_0^\infty dt \; t \sum_{m \neq n} \langle n | (\nabla\hat{H})_t | m \rangle \wedge \langle m | \nabla\hat{H} | n \rangle$$

(m=n term vanishes

$$= \frac{i}{\hbar} \int_0^\infty dt \; t \; \langle n | (\nabla\hat{H})_t \wedge \nabla\hat{H} | n \rangle .$$

$$= \frac{1}{2} \langle n | (\nabla\hat{H})_t \wedge \nabla\hat{H} - \nabla\hat{H} \wedge (\nabla\hat{H})_t | n \rangle \quad \text{(symmetrizin}$$

$$= \frac{1}{2} \langle n | [(\nabla\hat{H})_t , \wedge \nabla\hat{H}] | n \rangle .$$

Notation. $[\hat{\underline{A}}, \wedge \hat{\underline{B}}]_z = [\hat{A}_x, \hat{B}_y] - [\hat{A}_y, \hat{B}_x]$.

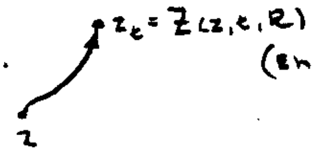
$$V_n = \frac{i}{2\hbar} \int_0^\infty dt \, t \, \langle n | \, [(\nabla \hat{H})_t , \wedge \nabla \hat{H}] \, | n \rangle$$

classical limit:

$$\langle n | \cdot | n \rangle \longrightarrow \langle \cdot \rangle_{E_n} .$$

$$[\hat{A}, \hat{B}] \longrightarrow i\hbar \, \{ A, B \} \qquad \text{(Dirac)}$$

$$\hat{A}_t \longrightarrow A_t , \; A_t(z) = A(z_t) .$$



(Ehrenfest)

Thus,

$$V_n \to -\frac{1}{2} \int_0^\infty dt \, t \, \langle \{ (\nabla H)_t , \wedge \nabla H \} \rangle_{E_n} , \text{ independent of } \hbar !$$

Convergence of t-integral is not evident. ∴ Poisson bracket is badly behaved, because system is chaotic.

$$\{ A, B \} = \partial_z A . J . \partial_z B , \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} .$$

$$\{ A_t, B \} = (\partial_z A)_t . \frac{\partial z_t}{\partial z} . J . \partial_z B , \text{ chain rule.}$$

$$\frac{\partial z_t}{\partial z} \sim e^{\lambda t} , \; \lambda = \text{Liapunov exponent.}$$

However, microcanonical average is well-behaved by virtue of the following identity:

$$\langle \{ A_t, B \} \rangle_E = \frac{1}{\Omega'(E)} \partial_E \left(\Omega' \langle \dot{A}_t B \rangle_E \right) , \quad \dot{A}_t = \frac{d A_t}{dt} .$$

Sketch of derivation:

Consider $\int d^{2N}z \;\; \{A_t, B\}\, \delta(E-H)$

$$\{A_t, B\}\,\delta = \{A_t, B\delta\} - \{A_t, \delta(E-H)\}\, B \; , \text{ Leibnitz.}$$

$$\{A_t, \delta(E-H)\} = \{A_t, H\}(-\delta'(E-H)) \, , \text{ chain rule}$$

$$= -\dot{A}_t \;\delta'(E-H) .$$

$$\{A_t, B\delta\} = -\partial_z \cdot (B\delta\, J \cdot \partial_z A) \, , \text{ pure divergence vanishes on volume integration}$$

Exponential growth isolated in pure divergence term.

Thus,

$$\langle \{(\nabla H)_t, \wedge \nabla H\} \rangle = \frac{1}{\Omega'} \partial_E \left(\Omega' \langle (\dot{\nabla H})_t \wedge \nabla H \rangle \right),$$

$$\int_0^\infty dt\; t\; (\dot{\nabla H})_t = - \int_0^\infty dt\, (\nabla H)_t \; , \text{ formally by parts.}$$

Then

$$\boxed{V_n(R) \longrightarrow V^c(E;R) = \frac{1}{2\Omega'} \partial_E \left(\Omega' \int_0^\infty dt \;\; \langle (\nabla H)_t \wedge \nabla H \rangle_E \right)}$$

Convergence:

Mixing implies

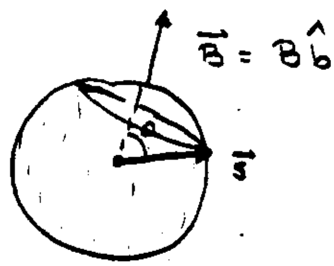
$$\langle A_t B \rangle \xrightarrow[t \to \infty]{} \langle A \rangle \langle B \rangle \, , \text{ correlations decay.}$$

Thus, assuming mixing,

$$\langle (\nabla H)_t \wedge \nabla H \rangle \longrightarrow \langle (\nabla H) \rangle \wedge \langle \nabla H \rangle = 0.$$

Assume correlations decay sufficiently fast for t-integra to converge, eg $\sim e^{-\alpha t}$, $\sim 1/t^{1+\beta}$.

<u>Example</u>: Spin in $\vec{B}$-field



$$H = \vec{B}.\vec{s} = Bs\cos\theta,$$

$s\cos\theta = E/B$

$$dq\,dp = s\sin\theta\,d\theta\,d\phi$$

$$\Omega(E) = s \cdot 2\pi(1-\cos\theta) = 2\pi s(1 - E/Bs).$$

$$\Omega'(E) = -2\pi s/Bs = -2\pi/B, \text{ const.}$$

Thus

$$V^c(E) = -\frac{1}{2}\partial_E \int_0^\infty dt \langle (\nabla H)_t \wedge \nabla H \rangle_E.$$

$$\nabla_B H = \vec{s} = s_{\parallel}\hat{b} + \vec{s}_{\perp}, \quad s_{\parallel} = s\cos\theta = E/B$$

$$\vec{s}_t = s_{\parallel}\hat{b} + \cos Bt\,\vec{s}_{\perp} + \sin Bt\,\hat{b} \wedge \vec{s}_{\perp},$$

$$\langle \vec{s}_{\parallel}\vec{s}_{\perp} \rangle = 0.$$

$$\langle \vec{s}_t \wedge \vec{s} \rangle = \sin Bt \langle (\hat{b} \wedge \vec{s}_{\perp}) \wedge \vec{s}_{\perp} \rangle = -\langle \vec{s}_{\perp} \cdot \vec{s}_{\perp} \rangle \sin Bt\,\hat{b}$$
$$= -s^2 \sin^2\theta \sin Bt\,\hat{b}.$$

$$\langle \bar{s}_t \wedge \bar{s} \rangle = -(s^2 - E^2/B^2) \sin Bt \, \hat{b}.$$

$$\checkmark \int_0^\infty dt \sin Bt = \mathrm{Im} \int_0^\infty dt \, e^{iBt - \epsilon t} = \mathrm{Im} \frac{-1}{iB} = \frac{1}{B}.$$

So,

$$\checkmark \; V^c = \frac{-1}{2} \partial_E \int_0^\infty dt \langle s_t \wedge s \rangle$$

$$= \frac{1}{2} \partial_E \left(E^2/B^2 - s^2\right) \frac{1}{B} \hat{b} = \frac{\overset{\overset{Bs_{\parallel}}{\shortparallel}}{E}}{B^3} \hat{b}$$

$$\checkmark \; = \frac{s_{\parallel}}{B^2} \hat{b}, \text{ solid angle result.}$$

Comments.

1) System is integrable, not chaotic. Correlation function is periodic, not decaying to constant. t-integral converges provided it is suitably interpreted. Formula applies to integrable case.

2) Manifest gauge invariance. No reference to action/angle variables, an in particular to choice of angle origin,

$$\theta \rightarrow \theta + \chi(R),$$

Price paid for gauge independence is extra time integral in addition to ensemble average.

Some Properties

1. Time Reversal.

Simplest case:

If $H(q,p,R) = H(q,-p,R)$, then $V^c(E,R) = 0$.

(Needn't always vanish, as with QM systems with T-symmetry but where states themselves are not T-symmetric.)

2. Rescaling.

$$H(z,R) \longrightarrow G(z,R) = g(H(z,R),R); \ V^c \text{ unchanged.}$$

(As in QM, where rescaling changes energies but not eigenstates, and so not the two-form. A geometrical property.

Geometrical Interpretation

We'll give geometrical interpretations for classical and quantum two-forms, starting with familiar interpretations for the familiar cases.

QM. $V_n = -i\hbar \langle \nabla n | \wedge \nabla n \rangle$

R-space

(oriented area element) R

Hilbert space

$|n(R)\rangle$

$$V_n \cdot \square = -\mathcal{A}(\square) \quad (= -2\hbar \, \mathrm{Im}\langle \delta_1 n | \delta_2 n \rangle)$$

CM, integrable. $V^c = \langle \nabla p \wedge \nabla q \rangle_I$, $z = z(\theta, I, R)$

Phase space

R

$$V^n \cdot \square = - \langle a(\square_\theta) \rangle_I , \quad a(\square_\theta) = \delta p_1 . \delta q_2 - \delta q_2 . \delta p_1 .$$

In this context, quantum and classical stand in natural analogy.

Time dependent versions

QM. $V_n = -\frac{i\hbar}{2} \overline{\langle n | \nabla U^+(t) \wedge \nabla U(t) | n \rangle}$, $\overline{} = \lim_{T\to\infty} \int_0^T dt$, time average

(This is another formula for phase. Derivation is discussed below.)

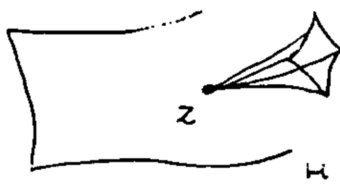
R

$|n(R)\rangle$ $\square_t = U(t, \square)|n\rangle$

$$V_n \cdot \square = -\frac{1}{2} \overline{a(\square_t)} .$$

CM. Chaotic. $V^c = -\frac{1}{2} \overline{\langle \nabla p_t \wedge \nabla q_t \rangle_E}$.

R



z $\square_t(z)$

H = E

$$V^c \cdot \square = -\frac{1}{2} \overline{\left\langle a(\square_t(z)) \right\rangle}_E .$$

Quantum and classical formulas stand in natural analogy. Note that $\square_t(z)$ diverges exponentially in time. However, z-average of area does not.

Formulas for derivation:

$$QM: \quad \nabla(\hat{F}_t) = (\nabla\hat{F})_t - \frac{i}{\hbar}\int_0^t d\tau \; [(\nabla\hat{F})_t, (\nabla\hat{H})_\tau].$$

$$CM: \quad \nabla(F_t) = (\nabla F)_t + \int_0^t d\tau \; \{(\nabla F)_t, (\nabla H)_\tau\}.$$

These are both exact.

Clash of Limits.

A subtlety in derivation of V^c has been overlooked. V^c was obtained by replacing quantum correlation fn. by classical one. Let's consider simpler ~~example~~:

$$Q(t) = \langle n | \tfrac{1}{2}(\hat{A}_t\hat{A} + \hat{A}\hat{A}_t) | n \rangle - \langle n | \hat{A} | n \rangle^2 .$$

Moments:

$$Q_r = \int_{-\infty}^{\infty} dt \; t^r \; Q(t) \, e^{-\epsilon|t|}, \quad \epsilon \to 0^+.$$

$$Q(t) = Q(-t) \text{ (easily checked)} \Rightarrow \boxed{Q_{2r+1} = 0}$$

Even moments:

$$Q_{2r} = 2\int_0^\infty dt\, t^{2r}\, Q(t)\, e^{-\epsilon t}, \quad \epsilon \to 0.$$

$$Q(t) = \sum_{m \neq n} |\hat{A}_{mn}|^2 \underbrace{\cos \omega_{mn} t}_{= \,\mathrm{Re}\, e^{i\omega_{mn} t}}, \quad \omega_{mn} = \frac{E_m - E_n}{\hbar}$$

Consider $\displaystyle\int_0^\infty dt\, t^{2r}\, e^{i\omega_{mn}t - \epsilon t} \xrightarrow[\epsilon \to 0]{} \frac{(-1)^{r+1}(2r)!}{\omega^{2r+1}}\, i$

$$\mathrm{Re} \text{ " } \quad \text{ " } = 0.$$

$\Rightarrow$ $\boxed{Q_{2r} = 0}$. All moments vanish.

Classical limit.

$$C(t) = \langle A_t A \rangle_E - \langle A \rangle_E^2 .$$

$$C_r = \int_{-\infty}^{\infty} dt\, t^r C(t), \quad (\text{OK if } C(t) \sim e^{-|t|}).$$

$$C(t) \text{ even} \Rightarrow \boxed{C_{2r+1} = 0}$$

For strongly chaotic systems, can show

$$A \neq 0 \Rightarrow \boxed{C_{2r} \neq 0}, \text{ some } r.$$

(Argument: Anosov $\Rightarrow$ $\hat{C}(\omega)$ analytic in strip about $\mathrm{Im}\,\omega = 0$.
$\forall r,\ C_r = 0 \Rightarrow \hat{C}^{(r)}(0) = 0,\ \forall r \Rightarrow \hat{C}(\omega) \equiv 0 \Rightarrow C(t) \equiv 0$.

Not a violation of correspondence principle because two limits are involved. Result depends on order.

$t \to \infty \; (\epsilon \to 0)$, then $\hbar \to 0 \;\Rightarrow\; Q_r = 0$

$\hbar \to 0$, then $t \to \infty \;\Rightarrow\; C_r \neq 0$.

(Explanation: Classical correlation functions have continuous spectrum, quantum cf's have discrete spectrum. $Q_r = 0$ is property of discrete spectrum. Long times are need to resolve discreteness,

$$T \sim O(1/\hbar^{N-1}).$$

For two form, can show:

$$\text{ave}\,[V_n]_n \approx \frac{1}{2N}\sum_{j=n-N}^{n+N} V_j \xrightarrow[\hbar\to 0]{} V^c(E). \quad \text{No clash.}$$

Average is needed, of course. Not true for scalar potential:

$$\text{ave}\,[\phi_n]_n \underset{\hbar \to 0}{\not\longrightarrow} \phi^c.$$

So clashes occur. Most interesting is associated with appearance of friction, in next lecture.

Quantum Corrections

Want semiclassical corrections to V^c. Use as model the Gutzwiller trace formula for density of states, $N = 2$ for simplicity.

$$\mathcal{N}(E) = \sum_n \Theta(E - E_n) \approx \Omega(E)/(2\pi\hbar)^2$$

$$\mathcal{N}'(E) = \sum_n \delta(E - E_n) \approx \frac{\Omega'}{(2\pi\hbar)^2} + \cdots + \frac{1}{\pi\hbar}\sum_{\text{po's}} K_j(E)$$

$$K_j(E) = \frac{T\cos(S(E)/\hbar - \mu\pi/2)}{r\,|\det(M-I)^{1/2}|}.$$

Quantum Corrections - Spectral Two-Form

Want $\hbar$-corrections to classical limit. Review situation for density of states. $N=2$, for simplicity.

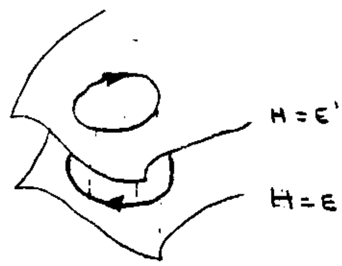
$$\mathcal{N}(E) = \sum_n \Theta(E-E_n) \approx \Omega(E)/(2\pi\hbar)^2$$

$$\mathcal{N}'(E) = \sum_n \delta(E-E_n) \approx \Omega'(E)/(2\pi\hbar)^2 + O\left(\frac{1}{\hbar}\right) + \cdots$$

$$+ \frac{1}{\pi\hbar} \sum_{\substack{\text{periodic}\\ \text{orbits}}} K_j(E)$$

$z_T = z$. Parameterized by E, R.

Isolated on energy shell.



$S(E) = \oint p \cdot dq$, $T = S'$.

$M(E)$, monodromy matrix

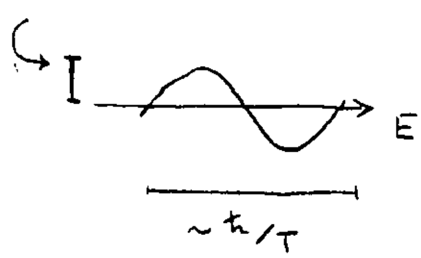
$Mu = u'$

u = transverse displacement, on shell

evals: $e^{\pm\lambda T}$

$e^{-r\lambda T/2}$

$$K_{jr}(E) = \frac{\cos\left(r S_j/\hbar - \mu_j \pi/2\right)}{\det|M_j^r - I|}$$



As function of Energy?

r = repetitions

μ = Maslov index

Comments:

1) Truncated sum (up to fixed period) describes modulations in low resolution density

2) ∞-sum does not converge (or if it does, only conditionally) as # of orbits proliferates with period at an exponential rate faster than decrease in amplitude

3) Recently, tremendous progress has been made in recasting formula so as to obtain energy levels from periodic orbits. See Berry + Keating (1992), for examp

Spectral Two-Form.

We consider not V_n itself but

$$D(E) = \sum_n \delta(E - E_n) V_n \text{ , " two-form density per unit energy "}$$

$$\approx \frac{\Omega'(E)}{(2\pi\hbar)^2} V^c(E) + \frac{1}{\pi\hbar} \sum_j K_j(E) V_j^c(E)$$

Orbit two-form.

First, reparameterize. $z(t, E, R) \longrightarrow z(\theta, S, R)$, $\theta = \frac{2\pi t}{T}$

Then $V_j^c(E,R) = \langle \nabla p \wedge \nabla q \rangle_{orbit} (S(E,R), R)$

Just like torus two-form for family of 1D tori.

Comments.

Derivation produces divergent terms. $\{A_t, B\}$

$$\langle \{A_t, B\} \rangle_E \xrightarrow[t \to \infty]{} \text{finite}$$

$$\langle \{A_t, B\} \rangle_{orbit} \xrightarrow[t \to \infty]{} \infty .$$

Infinities can be removed by analytic prescription. Result is satisfying, but means is not. Interesting to explore in examples, eg maps.

Closedness of Classical Two-Form

$$\nabla \cdot V^c = ?$$

Closedness (zero divergence) not automatically inherited from quantum mechanics.

$$\nabla \cdot V_n = 2\pi \sum_\alpha \sigma_\alpha \, \delta^3(R - R_\alpha),$$

R_α denotes degeneracy; $E_n(R_\alpha) = E_{n+1}(R_\alpha)$.

Comments.

- Degeneracies have codimension 3 for systems w/o time reversal invariance. (Von Neumann-Wigner). Degeneracies are point monopoles in $\vec{R}$-space
- $\sigma_\alpha = \pm 1$, given by signature of determinant of mapping from $\vec{R}$ to parameters $\vec{b}$ of 2-state Hamiltonian, $\vec{b}(\vec{R}) \cdot \vec{\sigma}$.

$$\nabla \cdot V^c \approx \operatorname{ave}\Big(\sum_{n\alpha} 2\pi \sigma_n \, \delta(R - R_\alpha)\Big]_n,$$

smooth density of monopoles.

Interesting to know: Asymptotic behavior of topological quantity

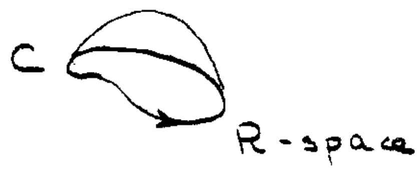
- Formal arguments for $\nabla \cdot V^c = 0$, but these are not satisfactory. Involve some interchange of limits which cannot be justified.

- Do not have good formula for evaluating $\nabla \cdot V^c$. Simply taking divergence inevitably leads to integrals of divergent quantities like $\{A_e, B\}$. Integrals may converge, but this isn't clear. And numerical calculation using these formulas is not possible, because of divergent quantities

One-form

$$V^c = \nabla \wedge A^c \quad \text{requires} \quad \nabla \cdot V^c = 0.$$

Therefore, so does existence of chaos analogue of Hannay angle.



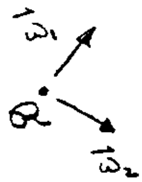
Putative: $\theta_c = \oint A^c \cdot dR$.

$\theta_c = \int_S V^c \cdot dS$ depends not just on C, but on bounding surface S, if V^c is not closed.

Special Case

Parameters describe orientation in space ($N=3$)

$$H(\vec{q},\vec{p},\mathcal{R}) = H_0(\mathcal{R}^{-1}\cdot\vec{r},\mathcal{R}^{-1}\cdot\vec{p}), \quad \mathcal{R}\in SO(3).$$



$$V^c(E,\mathcal{R})\cdot\square = \langle\vec{L}\rangle_{E,\mathcal{R}}\cdot(\vec\omega_1\wedge\vec\omega_2)$$

(Follows from formula - time integral of correlation function becomes trivial)

For QM case,

$$V_n(\mathcal{R})\cdot\square = \langle n|\vec{L}|n\rangle\cdot(\vec\omega_1\wedge\vec\omega_2)$$

Simplifications:

- PO corrections straightforward
- $\nabla\cdot V^c = 0$. $\quad A^c = \langle\vec{L}\rangle_{E,\mathcal{R}}$ (in suitable frame).
  Note: No degeneracies!
- Possible chaos Hannay angle
- Generalization: Canonical/Unitary families.
  $$H(z,R) = H_0(\phi^{-1}(z,R))$$
  $$\hat{H}(R) = U(R)\,\hat{H}_0\,U^{+}(R).$$

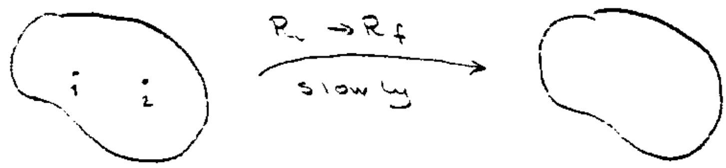
Why special? No intrinsic dependence of dynamics on parameters.

Forces of Reaction

Does V^c appear in the dynamics of classical chaotic systems? Look in context of adiabatic processes...

Classical adiabatic theorem, Ergodic case.

$S_i = \{H(z, R_i) = E_i\}$



S_f

What can be said about final surface S_f?

Liouville: $\mathrm{Vol}(S_f) = \mathrm{Vol}(S_i)$ (exact)

Ergodicity, Adiabatics: $\Delta E_1 \approx \Delta E_2$

$\Rightarrow$ S_f is energy surface wrt $H(z, R_f)$,

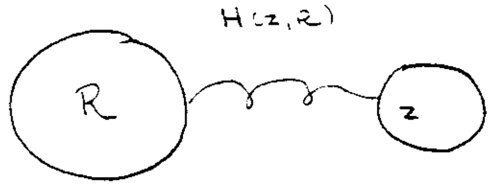
$$\Omega(E_f, R_f) = \Omega(E_i, R_i).$$

(Consistent with quantum adiabatic theorem via Weyl rule, $\Omega \propto n$).

Then
$$\boxed{\begin{aligned} E &= E(R, \Omega) \\ \nabla E &= \langle \nabla H \rangle_{E(R,\Omega)}. \end{aligned}}$$
along adiabats,

"Classical Helleman-Feynman theorem"

Coupled Systems



Regard parameters as slow dynamical variables.

Fast z's : adiabatic, anholonomy

Slow R's : perturbation theory, geometric reaction forces

· Program: Born-Oppenheimer, Mead-Truhlar for fast system which is classical + chaotic. First, a slight variation on the treatment of the quantum case, useful for comparison...

Half-classical Case

fast quantum: $\hat{\rho}(t)$, density operator

slow classical: $R_t, \dot{R}_t$, coordinates + velocities

$$\mathcal{E} = \frac{1}{2}\dot{R}^2 + \mathrm{Tr}[\hat{\rho}\hat{H}(R)], \text{ total energy}$$

Proceed directly to equations of motion:

$$i\hbar\dot{\hat{\rho}} = \frac{1}{\epsilon}[\hat{H},\hat{\rho}], \text{ Schrödinger.}$$

$$\ddot{R} = F = -\mathrm{Tr}[\hat{\rho}\,\nabla\hat{H}], \text{ Newton.}$$

Slow time ~ $O(1)$, Fast time ~ $O(\epsilon)$, $\epsilon \sim \sqrt{m/M} \ll 1$.

Adiabatic ansatz.

$$\hat{\rho}(t) = \sum_{n=0}^{\infty} \epsilon^n \hat{\rho}_n(t),$$

$$F(R,t) = \sum_n \epsilon^n F_n(R,t), \quad F_n = -\mathrm{Tr}[\hat{\rho}_n \nabla \hat{H}].$$

Require: F_0, F_1.

Recursion relation:

$$i\hbar \dot{\hat{\rho}}_n = [\hat{H}, \hat{\rho}_{n-1}], \text{ or}$$

$$\boxed{[\hat{H}, \hat{\rho}_n] = i\hbar \dot{\hat{\rho}}_{n-1}}.$$

<u>n = 0</u>

$$[\hat{H}, \hat{\rho}_0] = 0 \Rightarrow \boxed{\hat{\rho}_0(t) = |n(R_t)\rangle\langle n(R_t)|}$$ (assume $\hat{\rho}$ is pure state

$$F_0 = -\mathrm{Tr}\left[|n\rangle\langle n| \nabla H\right] = -\langle n|\nabla H|n\rangle = -\nabla E_n(R),$$ Helleman-Feynman

$$\boxed{F_0 = -\nabla E_n(R)},$$ Born-Oppenheimer

<u>n = 1</u>

$[\hat{H}, \hat{\rho}_1] = i\hbar \dot{\hat{\rho}}_0$. Compute $\langle k| \;\; |l\rangle$, off-diagonals:

$$\langle k|\hat{\rho}_1|l\rangle = i\hbar \frac{\langle k|\dot{\hat{\rho}}_0|l\rangle}{E_k - E_l}.$$

$\dot{\hat{\rho}}_0$ obtained from above. Diagonal elements vanish for pure state.
Obtain:

$$\boxed{F_1 = \dot{R} \wedge B_n}, \quad B_n = i\hbar \langle \nabla n| \wedge |\nabla n\rangle = -V_n.$$

geometric magnetism.

Comment: Using Newtonian rather than Hamiltonian formulation, vector potential does not appear.

Full Classical Case

fast: $\rho(z,t)$, Liouville density
slow: $R_t, \dot{R}_t$ (as before)

$$\mathcal{E} = \frac{1}{2}\dot{R}^2 + \int dz\, \rho\, H(z,R) \text{ , total energy.}$$

Equations of motion:

$$\partial_t \rho = \frac{1}{\epsilon}\{H,\rho\} \text{, Liouville}$$

$$\ddot{R} = F = -\int dz\, \rho\, \nabla H \text{, Newton}$$

Adiabatic Ansatz:

$$\rho = \sum_n \epsilon^n \rho_n \,,\quad F = \sum \epsilon^n F_n \,,\quad F_n = -\int dz\, \rho_n \nabla H .$$

Require: F_0, F_1

Recurrence relation:

$$\partial_t \rho_n = \{H, \rho_{n+1}\} \text{, or}$$

$$\boxed{\{H,\rho_n\} = \partial_t \rho_{n-1} .}$$

n = 0

$$\{H, \rho_0\} = 0 \Rightarrow \rho_0 = \text{fn of } H \text{ (ergodicity)}$$

Take: $\rho_0(z,t) = \dfrac{\delta(E_t - H(z, R_t))}{\Omega'(E_t, R_t)}$, normalized microcanonical.

(More general sol'n's obtained by superposition.) E_t is as yet undetermined, but turns out (see below) that

$$E_t = E(R_t, \Omega), \text{ adiabatic energy.}$$

$$F_0 = -\int dz\, \rho_0 \nabla H = -\langle \nabla H \rangle_{E(R,\Omega)} = -\nabla E, \text{ Hellman-Feynma[n]}$$

$$\boxed{F_0 = -\nabla E(R)}, \text{ classical Born-Oppenheimer.}$$

n = 1

$$\{H, \rho_1\} = \partial_t \rho_0, \text{ i.e. } \{H, f\} = g.$$

Can't take matrix elements, as in quantum case!

Necessary condition:

$$\langle \{H, f\} \rangle_E = 0, \ \forall E \text{ (constancy of microcanonical average)}$$

$$\Rightarrow \boxed{\langle g \rangle_E = 0}.$$

Letting $g = \partial_t \rho_0$, we obtain the condition

$$\dot{E}_t = \dot{R}_t \cdot \langle \nabla H \rangle_{E_t}, \text{ (short calculation)}$$

i.e. $\boxed{E_t = E(R_t, \Omega)}$, Ω const

Thus microcanonical energy obeys adiabatic thm., as claimed.

Note that

$$\{H, f(z_\tau)\} = -\frac{d}{d\tau} f(z_\tau),$$

so that

$$\{H, f\} = g \quad \Rightarrow \quad \frac{d}{d\tau} f(z_\tau) = -g(z_\tau),$$

ie (t-deriv. of f along orbits) = g.

Formal sol'n:

$$f(z) = -\int_{-\infty}^{0} d\tau\, g(z_\tau), \text{ integral over infinite past of } z.$$

Integral does not converge, but makes sense as distribution:

$$\langle A f \rangle_\varepsilon = -\int_{-\infty}^{0} d\tau\, \langle A g_\tau \rangle_\varepsilon, \quad \langle A g_\tau \rangle \xrightarrow[\tau\to\infty]{} \langle A \rangle \langle g \rangle = 0,$$

by necessary condition. Integral converges if correlations decay fast enough. Effectively, f is integral of random function with zero mean (ie g_τ).

Returning to problem at hand, general sol'n is

$$\rho_1(z,t) = -\int_{-\infty}^{0} d\tau\, \partial_t \rho_0(z_\tau, R_\tau) + f_1(H)$$

sol'n of homogeneous eqn, $\{H, f_1\} = 0$

from which we obtain

$$F_1 = -\int dz\, \rho_1 \nabla H.$$

We shall not discuss the homogeneous term f_1 in detail. The force it produces is, unlike the ones below, <u>independent</u> of velocity. As shown by Jarzynski, f_1 can be determined by imposing the necessary condition on the second ($n=2$) equation in the hierarchy $\{H, \rho_n\} = \partial_t \rho_{n+1}$. The resulting force is conservative, in that it can be expressed as the gradient of a potential, but the potential depends not only on R_t, but also on its history (i.e. the trajectory to R_t). Thus it is a "memory" effect

Result:

$$\boxed{\begin{aligned} F_1(R, \dot{R}) &= -K \cdot \dot{R} = -K_a \cdot \dot{R} - K_s \cdot \dot{R}, \\ K_{ij}(R) &= \frac{1}{\Omega'} \partial_E \left[\Omega' \int_0^\infty d\tau \, C_{ij}(\tau) \right], \\ C_{ij}(\tau) &= \Big\langle (\nabla_i H - \nabla_i E)_\tau (\nabla_j H - \nabla_j E) \Big\rangle_{E(R)} , \end{aligned}}$$

C is force-force correlation tensor.

Discussion

1. $K_a \cdot \dot{R}$, Geometric Magnetism

$K_a \cdot \dot{R} = B \wedge \dot{R}$, $B = -V^c$, classical limit of two-form.

So V^c acts as magnetic force on parameters, as in QM.

2. $K_s \cdot \dot{R}$, Deterministic Friction

Deterministic, because it follows from eqns. of motion, Dissipative, because

$K_s > 0$ (positive definite)

i) microcanonical ensemble 

is replaced by


,

$\bar{\rho}' < 0.$

ii) even in microcanonical case, if certain reasonable scaling assumptions are satisfied

(Note: Overall sign (negative) followed from using causal sol'n to $\{H, \rho_1\} = \partial_t \rho_0$, i.e. integral over past rather than future.)

3. Linear response theory. $F_1 = K \cdot \dot{R}$

$$\left.\begin{array}{l} T\text{-symmetry} \Rightarrow K \text{ symmetric} \\ \text{no } T\text{-symmetry} \Rightarrow K_a^* = -K_a \end{array}\right\} \text{Onsager relations}$$

Geomagnetism is antisymmetric partner of dissipation, as with Hall conductance.

F_1 produced by fluctuations, i.e. departures from adiabaticity  .

Such considerations lead to version of fluctuation-dissipation thm.

4. Absence of Quantum Friction

Friction did not appear in quantum analysis. This is another example of quantum/classical clash of the kind discussed in II. Quantum correlation fn. has discrete spectrum.

5. Friction and Chaos

If fast system is integrable, friction vanishes, again because correlation fn. is quasiperiodic.

6. Finite # of particles

$\rho \to \delta(z - z_t)$, then $F_0 = -\nabla E(R) \to -\nabla H(z_t, R) = -\nabla E + \widetilde{\nabla H}(z_t, R)$

Fluctuations at 0^{th}-order overwhelm reaction forces at 1^{st} order

Suppose: $\rho \to \sum_1^N \delta(z - z_{i\,t})$.

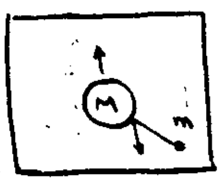
Require:

$$\frac{1}{\epsilon^2} \gg N \gg \frac{1}{\epsilon^{1/2}}.$$

N large enough so as to smooth out fluctuations,
small enough so that $\sqrt{Nm/M}$ remains small.

7. Canonical Families

$H(z,R) = H_0(\Phi^{-1}(z,R)) \Rightarrow$ No friction.



hard walls ⇒ friction

periodic boundary conditions ⇒ no friction

Open question:

Is it possible to obtain slow equations to arbitrary order in ϵ (as divergent series)?

To what extent can a system be separated from its environment?

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LETTER TO THE EDITOR

Discordance between quantum and classical correlation moments for chaotic systems

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Abstract. For systems whose classical orbits are chaotic, a set of quantum expectation values Q_r is constructed which vanish for all $\hbar$, unlike their classical counterparts C_r which are finite. This behaviour is not paradoxical because Q_r and C_r are moments of time correlation functions, which are dominated by the long-time limit where quantum and classical evolutions disagree.

According to the correspondence principle, quantum observables (expectations of Hermitian operators) should tend to their classical counterparts in the semiclassical limit, i.e. as Planck's constant $\hbar \to 0$. However, the semiclassical limit is highly singular (Berry 1991), and is vulnerable to disruption by any other limit with which it does not commute. An example is the long-time limit $t \to \infty$. In the combined semiclassical long-time limit, the correspondence principle need not apply, and very complicated behaviour can occur (see e.g. Berry 1988).

Here we give an example where the quantum–classical clash is extreme: the quantum observable is zero independently of $\hbar$, while if the orbits are chaotic its classical limit does not vanish. A related result was given by Kosloff and Rice (1980), who argued that the quantum mechanical value of a suitably defined Kolmogorov entropy vanishes, whereas the classical value does not. Another example has been presented by Ford *et al* (1991); they showed that the algorithmic complexity of computations for the quantum Arnold cat map always vanishes, while the classical complexity, reflecting the chaotic evolution, does not (of course, complexity is not the expectation of a Hermitian operator and so is not a quantum observable in any obvious way). In both the above examples, as with ours, the apparent breakdown of correspondence originates in the fact that the development of chaos involves the long-time limit. The example we give here has the virtue that the transcription from quantum to classical is particularly straightforward.

Let $\hat{A}$ and $\hat{B}$ be Hermitian operators that depend on the fundamental coordinate and momentum operators $\hat{q}$, $\hat{p}$ for a bound system whose evolution is governed by a time-independent Hamiltonian $\hat{H}$. Then we can define the quantum correlation function

$$Q(t) \equiv \tfrac{1}{2}\langle n|(\hat{A}_t\hat{B} - \hat{A}\hat{B}_t + \hat{B}\hat{A}_t - \hat{B}_t\hat{A})|n\rangle. \tag{1}$$

This involves the nth eigenstate $|n\rangle$ of $\hat{H}$, and the Heisenberg (time-evolved) operators

$$\hat{A}_t \equiv \exp\{i\hat{H}t/\hbar\}\hat{A}\exp\{-i\hat{H}t/\hbar\} \tag{2}$$

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and similarly for $\hat{B}_t$. $Q(t)$ is real because the operator in parentheses in (1) is Hermitian. The correlation moments, with which we will be concerned, are

$$Q_r \equiv \int_{-\infty}^{\infty} \mathrm{d}t\, t^r Q(t). \tag{3}$$

Elementary arguments (involving independence of expectation value to a shift in the time at which Heisenberg operators are evaluated) show that $Q(t)$ is an odd function, so that all the even moments are zero. Now we show that the Q_r also vanish when r is odd. After introducing the resolution of the identity to separate the operators in (1), and the frequencies

$$\omega_{nm} \equiv \frac{E_n - E_m}{\hbar} \tag{4}$$

where E_n are the energy levels (discrete eigenvalues of $\hat{H}$), an elementary calculation gives

$$Q(t) = -2\sum_m \sin\{\omega_{nm}t\}\ \mathrm{Im}\{\langle n|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle\}. \tag{5}$$

Thus $Q(t)$ is an almost-periodic function. That its moments vanish can be seen by expressing them as derivatives of the Fourier transform of $Q(t)$ at the origin, and observing that (5) has no Fourier component at $\omega = 0$. Alternatively, we can use

$$\int_0^{\infty} \mathrm{d}t\, t^r \sin\{\omega t\} = 0 \qquad \omega > 0,\ r \text{ odd} \tag{6}$$

whose truth can be established by a variety of arguments, for example expressing the integral as a derivative of a delta-function of ω, or introducing a convergence factor $\exp\{-\varepsilon t\}$ and taking the limit $\varepsilon \to 0$.

Let the classical counterpart of the quantum system have N (≥ 2) freedoms, and let

$$z \equiv (q, p) = (q_1, \ldots, q_N, p_1, \ldots, p_N) \tag{7}$$

denote position in the $2N$-dimensional phase space. Then corresponding to the quantum operators $\hat{A}$ and $\hat{B}$ are classical functions $A(z)$ and $B(z)$. The corresponding classical Hamiltonian $H(z)$ generates from the initial point z the orbit $Z_t(z)$ in time t, and the classical counterpart of the time-evolved operator (2) is

$$A_t(z) \equiv A(Z_t(z)). \tag{8}$$

To define the classical counterpart of the correlation function (1) we need to know what corresponds to the quantum expectation value in the state $|n\rangle$. This is a phase-space average over whatever classical invariant manifold corresponds to $|n\rangle$. By assumption, the classical systems we are considering are chaotic, so almost all orbits are ergodic on their energy surfaces. Thus the appropriate average is microcanonical, and the classical correlation function is

$$\begin{aligned} C(t) &= \langle A_t B - B_t A\rangle_E \\ &\equiv \frac{\int \mathrm{d}^{2N}z\, \delta\{E - H(z)\}(A_t(z)B(z) - B_t(z)A(z))}{\int \mathrm{d}^{2N}z\, \delta\{E - H(z)\}}. \end{aligned} \tag{9}$$

Of course this function is independent of $\hbar$. (There are also semiclassical 'scar' contributions to $Q(t)$ from each of the classical periodic orbits, but these are of order

$\hbar^{N-1}\exp\{i/\hbar\}$ (Berry 1991) and vanish in the classical limit, as the oscillations become infinitely fast and faint.) The classical correlation moments are

$$C_r \equiv \int_{-\infty}^{\infty} \mathrm{d}t\, t^r C(t). \tag{10}$$

Again, elementary arguments (involving conservation of H and the fact that time evolution is a canonical transformation) show that $C(t)$ is an odd function, so that all the even moments vanish. But the odd moments need not vanish. To see why, we observe that the mixing property associated with chaos means that

$$C(t) \xrightarrow[t\to\infty]{} \langle A\rangle_E\langle B\rangle_E - \langle B\rangle_E\langle A\rangle_E = 0 \tag{11}$$

so that $C(t)$ rises from zero at $t=0$ and then decays to zero at infinity. Provided the decay is sufficiently fast, $C(t)$ has a continuous spectrum, and so is not an almost-periodic function. Therefore it can possess some non-zero moments, and typically will do so.

We can prove this for hyperbolic systems, for which it is known (Pollicott 1985, Ruelle 1986) that $\bar{C}(\omega)$, the Fourier transform of $C(t)$, is meromorphic in a strip including the real axis. But if all the moments of $C(t)$ are to vanish, then all derivatives of $\bar{C}(\omega)$ must vanish at $\omega=0$; by analytic continuation this implies that $\bar{C}(\omega)$, and hence $C(t)$, vanish identically. Thus any non-zero $C(t)$ must have non-zero moments.

We are unable to generalize this argument to arbitrary classical chaotic systems, because not enough is known about the analytic structure of their correlations. Therefore we cannot exclude cases such as

$$\bar{C}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, C(t)\exp\{\mathrm{i}\omega t\} = \mathrm{i}\omega\exp\left\{-\frac{1}{4|\omega|} - A|\omega|\right\} \tag{12}$$

where, because of the essential singularity, all derivatives at $\omega=0$, and therefore all moments of $C(t)$, are zero. Moreover, $C(t)$, in addition to having a continuous spectrum, decays exponentially. This can be seen by Fourier inversion, which gives

$$C(t) = -\frac{1}{2\pi}\,\mathrm{Im}\,\frac{1}{\xi^2}K_2\{\xi\} \qquad \xi = \sqrt{t-\mathrm{i}A}\,\exp\{\mathrm{i}\pi/4\} = \sqrt{A+\mathrm{i}t} \tag{13}$$

where K denotes the modified Bessel function (Abramowitz and Stegun 1964), whose limiting forms are

$$C(t) \approx \begin{cases} \dfrac{t}{4\pi A^{5/2}}[4\sqrt{A}\,K_0\{\sqrt{A}\} + (8+A)K_1\{\sqrt{A}\}] & |t| \ll A \\[2ex] \dfrac{\mathrm{sgn}(t)}{|t|^{5/4}2\sqrt{2\pi}}\exp\{-\sqrt{\tfrac{1}{2}|t|}\}\cos\{\sqrt{\tfrac{1}{2}|t|}+\tfrac{1}{8}\pi\} & |t| \gg A. \end{cases} \tag{14}$$

We consider such cases as special, and unlikely to occur in any real classical system.

If the classical motion is integrable, the above arguments do not apply. For then the motion *is* almost periodic (indeed multiply periodic, since there are finitely many independent frequencies), and the quantum expectation value corresponds to averaging over the angles of the quantized invariant torus whose actions are associated with $|n\rangle$ (see e.g. Percival 1977). $C(t)$ is given by a formula similar to (5), in which the ω_{nm} are replaced by (non-zero) integer linear combinations of the N classical frequencies. It then follows from (6) that the moments are zero.

It seems paradoxical that a quantum expectation value can have zero moments while the moments of its classical limit are finite. But the moments we are calculating are constructed to exploit the clash of limits $\hbar \to 0$, $t \to \infty$, because they are dominated by the behaviour of $Q(t)$ and $C(t)$ at large t—precisely where the classical and quantum evolutions disagree. Specifically, for long times $t > \hbar/(\text{mean level spacing}) \sim 1/\hbar^{(N-1)}$, $Q(t)$ is dominated by oscillations associated with the discreteness of the spectrum, while $C(t)$ decays because of the mixing associated with chaos. The essence of quantization is here incompatible with the essence of chaos.

A purely mathematical example illustrating this curious behaviour is provided by the 'quantum' function

$$Q(t) = \hbar \sum_{m=-\infty}^{\infty} m \exp\{-\hbar^2 m^2\} \sin\{m\hbar t\} \tag{15}$$

and its 'classical' limit, in which the sum is replaced by an integral,

$$C(t) = \int_{-\infty}^{\infty} \mathrm{d}x\, x \exp\{-x^2\} \sin\{xt\} = \frac{\sqrt{\pi}}{2}\, t \exp\{-\tfrac{1}{4}t^2\}. \tag{16}$$

(Despite superficial appearances, this is not a model for any kind of harmonic oscillator.) Both are odd functions of t, whose moments are easily calculated to be

$$\begin{aligned} &Q_r = 0 \qquad (\text{all } r) \\ &C_r = \begin{cases} 0 & (r \text{ even}) \\ 2^{r+1}\sqrt{\pi}\,(\tfrac{1}{2}r)! & (r \text{ odd}) \end{cases} \end{aligned} \tag{17}$$

showing the clash of limits.

In this example the mysterious classical appearance of the moments can be traced explicitly, by re-expressing (15) with the aid of the Poisson sum formula: without approximation, we have

$$\begin{aligned} Q(t) &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}x\, x \exp\{-x^2\} \sin\{xt\} \exp\left\{\frac{2\pi i n x}{\hbar}\right\} \\ &= \frac{\sqrt{\pi}}{2} \sum_{n=-\infty}^{\infty} \left(t - \frac{2\pi n}{\hbar}\right) \exp\left\{-\frac{1}{4}\left(t - \frac{2\pi n}{\hbar}\right)^2\right\}. \end{aligned} \tag{18}$$

Thus $Q(t)$ is here a series of copies of $C(t)$, displaced along the t axis by multiples of $2\pi/\hbar$. As $\hbar \to 0$ all these copies recede to $\pm\infty$, leaving $C(t)$ alone at finite t. The moments are derivatives of the Fourier transform of $Q(t)$ at zero frequency ω. Each copy generates a phase-shifted reproduction of the transform of $C(t)$, whose sum involves

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \exp\{2\pi i n\omega/\hbar\} &= 1 + 2\,\mathrm{Re} \sum_{n=1}^{\infty} \exp\{2\pi i n\omega/\hbar\} \\ &= 1 + 2\,\mathrm{Re}\, \frac{\exp\{2\pi i\omega/\hbar\}}{1 - \exp\{2\pi i\omega/\hbar\}} \\ &= 1 - 1 = 0 \end{aligned} \tag{19}$$

(we ignore the delta-function at $\omega = 0$ because this is negated by a zero of the transform of $C(t)$ there). The -1 in (19) represents the contribution of all the copies to Q_r, and cancels C_r.

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The Geometric Phase for Chaotic Unitary Families

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Abstract

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

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1. Introduction

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

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

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

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

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

2. Unitary families

Consider the family of Hamiltonians

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

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

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

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

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

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

it follows that

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

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

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

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

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

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

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

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

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

$$U \to Ue^{-i\hat{K}/\hbar}, \tag{8}$$

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

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

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

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

3. Canonical families

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

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

canonically related to H.

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

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

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

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

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

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

(13) is used several times in what follows.

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

4. Classical limit

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

$$\langle f \rangle_{E\mathbf{R}} = \frac{1}{\partial_E \Omega} \int dz \delta(E - h) f(z, \mathbf{R}); \tag{14}$$

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

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

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

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

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

the classical limits of $\mathbf{A}_n$ and $\mathbf{V}_n$

In RB we derived the general formula

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

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

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

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

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

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

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

$$\langle \dot{\mathbf{g}} \rangle = \langle \nabla h \rangle = \left. \frac{d}{dt} \langle \mathbf{g}_t \rangle \right|_{t=0} = 0, \tag{21}$$

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

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

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

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

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

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

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

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

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

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

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

and $\mathbf{V}^c$ is unchanged.

5. Periodic orbit corrections

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

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

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

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

Here

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

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

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

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

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

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

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

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

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

To establish that (31) agrees with the general result (27), we show in what follows that

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

The periodic orbits $z_j = (q_j, p_j)$ of h depend on parameters through the canonical transformation Φ; explicitly,

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

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

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

Therefore

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

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

6. Closedness of the classical two-form

For canonical families,

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

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

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

and using (12) and (23) obtain

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

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

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

7. Geometric magnetism without dissipation

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

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

$$\ddot{\mathbf{R}} = -\int dz\rho\nabla h, \tag{39b}$$

where ϵ is a small parameter which insures that $\mathbf{R}$ evolves slowly relative to ρ. Within an adiabatic treatment of the reaction forces on the slow system (the fast ensemble is taken to be microcanonical to lowest order), there appears a 'classical Born-Oppenheimer' force $-\langle\nabla h\rangle_{E\mathbf{R}}$ at zeroth order, and at first order a velocity-dependent force $-\epsilon\mathrm{K}\cdot\dot{\mathbf{R}}$, where the tensor K is given by

$$\begin{gathered} K_{ij}(E,\mathbf{R}) = \frac{1}{\partial_E\Omega}\partial_E\left[\partial_E\Omega\int_0^\infty dt\left\langle(\widetilde{\partial_i h})_t\widetilde{\partial_j h}\right\rangle_{E\mathbf{R}}\right], \\ \text{where } \partial_i \stackrel{\text{def}}{=} \partial/\partial R_i, \quad \widetilde{f}(z,E,\mathbf{R}) \stackrel{\text{def}}{=} f - \langle f\rangle_{E\mathbf{R}}. \end{gathered} \tag{40}$$

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

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

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

so that

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

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

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

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

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

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

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

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

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

8. Examples

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

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

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

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

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

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

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

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

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

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

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

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

9. Discussion

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

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

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

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Appendix

The definition of the classical generators,

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

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

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

We try to fix $\mathbf{g}$ uniquely by imposing the z-antiderivative of (A.2),

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

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

To show that (A.3) can be satisfied, first suppose $\mathbf{g}_0$ satisfies (A1) but not (A3), and let

$$\boldsymbol{\alpha} = \nabla\wedge\mathbf{g}_0 - \tfrac{1}{2}\{\mathbf{g}_0,\wedge\mathbf{g}_0\}. \tag{A4}$$

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

$$\begin{aligned}\nabla\cdot\boldsymbol{\alpha} &= -\tfrac{1}{2}\nabla\cdot\{\mathbf{g}_0,\wedge\mathbf{g}_0\} = \{\mathbf{g}_0,\cdot\nabla\wedge\mathbf{g}_0\}\\ &= \{\mathbf{g}_0,\cdot(\tfrac{1}{2}\{\mathbf{g}_0,\wedge\mathbf{g}_0\}+\boldsymbol{\alpha})\} = \tfrac{1}{2}\{\mathbf{g}_0,\cdot\{\mathbf{g}_0,\wedge\mathbf{g}_0\}\}\\ &= \tfrac{1}{2}\sum_{ijk}\epsilon_{ijk}\{g_{0i},\{g_{0j},g_{0k}\}\} = 0,\end{aligned} \tag{A5}$$

where the last equality follows from the Jacobi identity for Poisson brackets. Since $\nabla\cdot\boldsymbol{\alpha} = 0$, $\boldsymbol{\alpha}$ is given (locally at least) by $\nabla\wedge\boldsymbol{\beta}$. Letting $\mathbf{g} = \mathbf{g}_0 + \boldsymbol{\beta}$, one verifies that $\mathbf{g}$ satisfies (A.3).

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