Chaotic classical and half-classical adiabatic reactions: geometric magnetism and deterministic friction

By M. V. Berry and J. M. Robbins
H. H. Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, U.K.

We study the dynamics of a heavy (slow) classical system coupled, through its position, to a classical or quantal light (fast) system, and derive the first-order velocity-dependent corrections to the lowest adiabatic approximation for the reaction force on the slow system. If the fast dynamics is classical and chaotic, there are two such first-order forces, corresponding to the antisymmetric and symmetric parts of a tensor given by the time integral of the force–force correlation function of the fast motion for frozen slow coordinates. The antisymmetric part is geometric magnetism, in which the 'magnetic field' is the classical limit of the 2-form generating the quantum geometric phase. The symmetric part is deterministic friction, dissipating slow energy into the fast chaos; previously found by Wilkinson, this involves the same correlation function as governs the fluctuations and drift of the adiabatic invariant. In the 'half-classical' case where the fast system is quantal with a discrete spectrum of adiabatic states, the only first-order slow force is geometric magnetism; there is no friction. This discordance between classical and quantal fast motion is explained in terms of the clash between the semiclassical and adiabatic limits. A generalization of the classical case is given, where the slow velocity, as well as position, is coupled to the fast motion; to first order, the symplectic form in the lowest-order hamiltonian dynamics is modified.

1. Introduction

Consider a light system, which may be classical or quantal, coupled to a heavy classical system. The evolution of the light system is rapid on the scale of the heavy motion, which can therefore be regarded as slow. Here we will concentrate on this slow classical motion, which is influenced by reactions from the fast system. In the usual 'Born–Oppenheimer' (Messiah 1962) or 'adiabatic averaging' (Arnold *et al.* 1988; Lochak & Meunier 1988) approximation, the energy of the fast motion, calculated for frozen slow variables, acts as a potential in which the slow system moves.

In the next approximation beyond this, there are two additional reaction forces linear in the slow velocities. The first is of magnetic type. The field which generates it (Mead & Truhlar 1979; Jackiw 1988; Berry 1989) is the 2-form that gives the geometric phase in the fast system (Berry 1984*a*; Shapere & Wilczek 1989). Because of the connection with the geometric phase, we call this force 'geometric magnetism'. For examples of the effects of geometric magnetism – and also of the higher-order electric reaction force – see Berry & Robbins (1993) and Aharonov & Stern (1992). The second force was calculated by Wilkinson (1990), and exists when the fast

Proc. R. Soc. Lond. A (1993) **442**, 659–672

Printed in Great Britain

motion is classical and chaotic; it is deterministic friction. We use this term to emphasize that no thermodynamic limit is necessary for this kind of friction, which arises out of the deterministic chaos in low-dimensional fast systems.

Our aim here is to derive these first-order adiabatic reaction forces within a systematic framework. When the light system is classical (§2), we consider the fast motion to be ergodic and mixing. This case has long been problematic. Although the classical limit of the quantum phase 2-form has recently been calculated for chaotic motion (Robbins & Berry 1992*a*), it was not clear how to derive the reaction force it generates on the slow system using purely classical arguments. The reason is that the accuracy of conservation of the adiabatic invariant for chaotic motion (Ott 1979; Brown *et al.* 1987) is much poorer than in an integrable (or a quantum) system. To deal consistently with fluctuations, we use the following physical model: the slow system is coupled to a (microcanonical) ensemble of fast systems (described by a phase-space distribution function), rather than to a single fast trajectory. Deterministic friction emerges as the symmetric part of the tensor producing the velocity-dependent reaction force at first order. The antisymmetric part is geometric magnetism.

When the light system, coupled to the heavy classical one, is quantal (§3), we have a situation which (following a suggestion of Dr J. H. Hannay) we call 'half-classical mechanics' (there being no implication that the light system is semiclassical, i.e. near its classical limit). Then we couple the slow motion to a density matrix representing the fast system. From this formalism emerges geometric magnetism but not friction. This quantum/classical discordance – that friction vanishes in quantum mechanics, for all finite $\hbar$, but it is not zero in the classical limit when the motion is chaotic – is discussed in §4 (for a related instance of it, see Robbins & Berry 1992*b*).

For simplicity of exposition, most of the discussion is restricted to a slow system with three freedoms, described by the motion of a vector

$$\boldsymbol{R} = \{R_i\} = \{X, Y, Z\}. \tag{1}$$

Coupling to the fast motion is through this slow position $\boldsymbol{R}(t)$ (and not through the slow velocity $\boldsymbol{V} \equiv \dot{\boldsymbol{R}}$). The slow acceleration is determined by the reaction force, that is

$$\dot{\boldsymbol{V}} = \boldsymbol{F} \tag{2}$$

and the aim is to determine $\boldsymbol{F}$ in terms of averages over the fast motion, including terms linear in the velocity $\boldsymbol{V}$. It is, however, possible to give a much more general treatment, in which the slow system can have any number of freedoms and coupling can involve the slow velocities as well as coordinates. We show (§5) that in this case geometric magnetism and deterministic friction appear as modifications of the symplectic form generating the slow equations of motion.

2. Classical fast motion

Let the fast system be bound, with D freedoms and $2D$ phase-space variables

$$z = \{\boldsymbol{q}, \boldsymbol{p}\} = \{q_1, \ldots, p_D\} \tag{3}$$

and let the ensemble of fast trajectories be represented by a phase-space distribution function $\rho(z, t)$ which is normalized, i.e.

$$\int \mathrm{d}z\, \rho = 1. \tag{4}$$

Let the time-dependent hamiltonian h generating the fast motion be governed parametrically by the (changing) slow coordinates $\boldsymbol{R}$, i.e. $h = h(z, \boldsymbol{R}(t))$. Thus the evolution of the ensemble ρ is determined by its Poisson bracket with h:

$$\epsilon\dot{\rho}(z,t) = \{h(z,\boldsymbol{R}(t)), \rho(z,t)\}. \tag{5}$$

Here ϵ is an adiabatic parameter whose smallness guarantees that the z motion is indeed fast compared with the $\boldsymbol{R}$ motion; ϵ^2 could for example represent the light/heavy mass ratio, appearing in the form (5) after scaling the equations of motion. The force in (2) is defined as the following average over fast phase space:

$$\boldsymbol{F} = -\int \mathrm{d}z\, \rho\, \nabla h. \tag{6}$$

Here and hereafter gradients ∇ will act on the slow coordinates $\boldsymbol{R}$.

We shall find the first two terms of $\boldsymbol{F}$ in an expansion in powers of ϵ. This requires a formal expansion of the distribution function:

$$\rho \equiv \sum_{r=0}^{\infty} \epsilon^r \rho_r. \tag{7}$$

From (5), the ρ_r are determined by

$$\{h, \rho_0\} = 0, \quad \{h, \rho_r\} = \dot{\rho}_{r-1} \quad (r > 0). \tag{8}$$

Thus ρ_0 is constant on an invariant manifold of the fast dynamics with frozen $\boldsymbol{R}$. For chaotic motion the invariant manifolds are the energy surfaces and, densely distributed over these, the periodic orbits. We choose the normalized microcanonical distribution

$$\rho_0(z,t) = \frac{\delta(E(\boldsymbol{R}) - h(z,\boldsymbol{R}))}{\partial_E \Omega(E(\boldsymbol{R}), \boldsymbol{R})}. \tag{9}$$

Here $\boldsymbol{R} = \boldsymbol{R}(t)$ and Ω denotes the phase volume within the energy surface specified by E and $\boldsymbol{R}$, namely

$$\Omega(E, \boldsymbol{R}) = \int \mathrm{d}z\, \Theta(E - h(z, \boldsymbol{R})), \tag{10}$$

where Θ denotes the unit step. The function $E(\boldsymbol{R})$ determines the energy surfaces visited by ρ_0 as $\boldsymbol{R}$ changes with t. Its form is determined by the adiabatic theorem for ergodic systems (Lochak & Meunier 1988), namely $\Omega = \text{const.}$ for infinitely slow changes. (We invoke the adiabatic theorem at this point as a matter of convenience, as the adiabatic form of $E(\boldsymbol{R})$ actually emerges from the following analysis.)

Now we introduce two useful notations. Averaging over the energy surface E will be denoted by

$$\langle \ldots \rangle_E \equiv \int \mathrm{d}z\, \rho_0(z,t) \ldots = \frac{1}{\partial_E \Omega} \int \mathrm{d}z\, \delta(E - h(z, \boldsymbol{R})) \ldots. \tag{11}$$

The fluctuation of the fast Hamiltonian relative to the adiabatically evolving energy $E(\boldsymbol{R})$ will be denoted by

$$\tilde{h} \equiv h(z, \boldsymbol{R}) - E(\boldsymbol{R}). \tag{12}$$

Adiabaticity then implies

$$\langle \nabla \tilde{h} \rangle_{E(\boldsymbol{R})} = 0. \tag{13}$$

We can write the force (6) as

$$\boldsymbol{F} = -\int \mathrm{d}z\,\rho\nabla h = -\left(\int \mathrm{d}z\,\rho\right)\nabla E - \int \mathrm{d}z(\rho_0 + \epsilon\rho_1 + O(\epsilon^2))\,\nabla\tilde{h}. \tag{14}$$

Since ρ is normalized and $\int \mathrm{d}z\,\rho_0 \nabla\tilde{h} = \langle\nabla\tilde{h}\rangle_{E(\boldsymbol{R})}$ vanishes (cf. (9) and (13)), we have

$$\boldsymbol{F} = -\nabla E(\boldsymbol{R}) + \epsilon\boldsymbol{F}_1 + O(\epsilon^2), \quad \text{where} \quad \boldsymbol{F}_1 \equiv -\int \mathrm{d}z\,\rho_1\nabla\tilde{h}. \tag{15}$$

The leading term $-\nabla E$ is the Born–Oppenheimer force. The focus of interest here is the next term $\epsilon\boldsymbol{F}_1$, which is the desired first-order reaction force. To find it, we need the first correction ρ_1 in the distribution function, which we obtain using arguments of Ott (1979).

According to (8), the corrections to ρ_0 are determined by the solutions of equations of the form

$$\{h,f\} = g, \tag{16}$$

where h and g are given functions of z, and f is to be determined. Because $\langle\{h,f\}\rangle_E = 0$ (microcanonical averages are constant in time), a necessary condition for (16) to have a solution is

$$\langle g\rangle_E = 0. \tag{17}$$

It is shown in Appendix A that a particular solution of (16) is

$$f(z) = -\int_{-\infty}^{0} \mathrm{d}\tau\, g(z_\tau(z)), \tag{18}$$

where $z_\tau(z)$ is the trajectory generated by the hamiltonian h in time τ starting from z. As a function of τ, $g(z_\tau)$ is oscillatory with vanishing time average (as implied by (17) and ergodicity). Thus (18), like the integral of a random function, need not converge, but instead gives f as a distribution, whose averages over phase-space functions do converge. Equation (18) is the causal solution, depending only on the fast motion in the past, rather than the future. We may add to it any solution f_1 of the homogeneous equation $\{h,f\} = 0$, which is necessarily a function of h because energy is the only constant of motion.

Using (8), the first correction can be determined from (18) as

$$\rho_1(z,t) = -\int_{-\infty}^{0} \mathrm{d}\tau\,\partial_t\rho_0[z_\tau(z,\boldsymbol{R}(t)),t] + f_1[h(z,\boldsymbol{R}(t)),t], \tag{19}$$

where $z_\tau(z,\boldsymbol{R})$ is the orbit under the frozen dynamics, and the partial derivative ∂_t acts only on the second argument of ρ_0. Applied to (8), the condition (17) requires that $\langle\partial_t\rho_0\rangle_E = 0$. A short calculation shows that this is true if the average of the fluctuation $\nabla(h - E(\boldsymbol{R}))$ vanishes as in (13), that is if the adiabatic theorem holds (indeed this is one way to derive the adiabatic theorem).

Substituting (9) into (19), we find

$$\rho_1 = \boldsymbol{V}\cdot\frac{1}{\partial_E\Omega}\int_{-\infty}^{0} \mathrm{d}\tau[\partial_E\,\delta(E-h)]\,(\nabla\tilde{h})_\tau + (\ldots) + f_1(h,t), \tag{20}$$

where

$$(\nabla\tilde{h})_\tau = \nabla\tilde{h}(z_\tau(z,\boldsymbol{R}),\boldsymbol{R}) \tag{21}$$

and the term $(\ldots)$ is proportional to $\delta(E-h)$ and will not contribute to the first-order force.

The force produced by the term f_1 is velocity-independent. As shown by Jarzynski (1993), it can be determined by imposing the condition (17) on the second-order ($r = 2$) equation in (8). This force is a correction to the Born–Oppenheimer force (and indeed vanishes when the latter does), because it may be expressed as the gradient of a potential. This potential is however time-dependent and involves the history of the slow motion; therefore Jarzynski's force is a memory effect. From now on we neglect the contribution from f_1, but it is certainly worth exploring.

From (15) and (20) $\boldsymbol{F}_1$ can be written as the time integral of the correlation function, over the fast dynamics with frozen $\boldsymbol{R}$, of the gradients of the fast hamiltonian, that is the force–force correlation function. Thus

$$\boldsymbol{F}_1 = -\boldsymbol{V}\cdot\frac{1}{\partial_E \Omega}\partial_E\left[\partial_E \Omega \int_{-\infty}^{0} \mathrm{d}\tau \langle (\nabla\tilde{h})_\tau \nabla\tilde{h}\rangle_E\right] \tag{22}$$

with $E = E(\boldsymbol{R})$. Changing the sign of τ, and using the invariance of correlation functions to a time shift, we obtain

$$\boldsymbol{F}_1 = -\boldsymbol{V}\cdot\frac{1}{\partial_E \Omega}\partial_E\left[\partial_E \Omega \int_{0}^{\infty} \mathrm{d}\tau \langle \nabla\tilde{h}(\nabla\tilde{h})_\tau\rangle_E\right] = -\boldsymbol{K}\cdot\boldsymbol{V},$$

where
$$K_{ij} \equiv \frac{1}{\partial_E \Omega}\partial_E\left[\partial_E \Omega \int_{0}^{\infty} \mathrm{d}\tau\, C_{ij}(\tau)\right], \tag{23}$$

and
$$C_{ij}(\tau) \equiv \langle (\partial_i \tilde{h})_\tau \partial_j \tilde{h}\rangle_E.$$

For chaotic motion, the correlation function $C_{ij}(\tau)$ vanishes as $\tau \to \infty$, because of mixing, and we assume it decays fast enough for the integral in K_{ij} to converge.

To interpret this result, we separate K_{ij} into symmetric and antisymmetric parts:

$$K_{ij}^{(\mathrm{s})} \equiv \tfrac{1}{2}(K_{ij}+K_{ji}), \quad K_{ij}^{(\mathrm{a})} \equiv \tfrac{1}{2}(K_{ij}-K_{ji}). \tag{24}$$

Consider first the antisymmetric part. The corresponding force $\boldsymbol{F}_1^{(\mathrm{a})}$ is geometric magnetism, since

$$\boldsymbol{F}_1^{(\mathrm{a})} = \boldsymbol{V} \wedge \boldsymbol{B}(\boldsymbol{R}), \tag{25}$$

where the 'magnetic field' is given by

$$\boldsymbol{B}(\boldsymbol{R}) = -\frac{1}{2\,\partial_E \Omega}\partial_E\left[\partial_E \Omega \int_{0}^{\infty} \mathrm{d}\tau \langle (\nabla\tilde{h})_\tau \wedge \nabla\tilde{h}\rangle_E\right]. \tag{26}$$

This is precisely the expression we previously found (Robbins & Berry 1992*a*) as the classical limit of the geometric phase 2-form. We showed that $\boldsymbol{B}$ vanishes when the fast dynamics possesses time-reversal symmetry (the two essential steps of the argument are invariance of the correlation function under time shift, and the existence of pairs of initial phase points z and $\mathrm{T}z$ such that the forward evolution of ∇h from z is the same as its backward evolution from $\mathrm{T}z$). We also gave formal arguments suggesting that $\boldsymbol{B}$ is divergenceless.

The symmetric part of the first-order force is deterministic friction, that is irreversible viscous dissipation of slow energy by the fast chaos (Wilkinson 1990). We emphasize that this phenomenon requires only low-dimensional deterministic chaos: no heat bath has been introduced. To lowest order in ϵ, the dissipated energy is

$$\epsilon \boldsymbol{V}\cdot\boldsymbol{F}_1 = -\epsilon V_i V_j K_{ij}. \tag{27}$$

In calling this dissipation, we are assuming that the tensor K_{ij} in (23) must be positive definite. Wilkinson (1987) shows that

$$\int_0^\infty \mathrm{d}\tau\, C_{ii}(\tau) > 0 \quad (i \text{ not summed}) \tag{28}$$

but dissipation requires more: this quantity times $\partial_E \Omega$ must increase with E. This is true for scaling systems, where the fast hamiltonian h is the sum of kinetic energy and a potential U satisfying

$$U(\alpha \boldsymbol{q}, \boldsymbol{R}) = \alpha^\mu U(\boldsymbol{q}, \boldsymbol{R}) \quad (\mu > 0) \tag{29}$$

since then the quantity in square brackets in K_{ij} in (23) scales as

$$E^{(D+1)(\mu+2)/2\mu}, \tag{30}$$

which increases with E. We cannot give a proof of the positivity of K_{ij} in the general case. Indeed, for certain low-dimensional systems we have found what appear to be counter-examples, although these can all be eliminated by increasing D. However, the inequality (28) is sufficient to guarantee dissipation if the unperturbed distribution ρ_0 is a decreasing function of h, e.g. the Boltzmann distribution or the Fermi–Dirac distribution (Wilkinson 1990), in contrast to the microcanonical ensemble considered here.

Unlike geometric magnetism, this frictional force exists whether or not the fast dynamics possesses time-reversal symmetry. But it does require the dynamics to be chaotic. To see this, consider the integrable case $D = 1$, for which the correlation function is periodic:

$$C_{ij}(\tau) = \sum_{n=1}^{\infty} (S_{ij}(n) \cos n\omega\tau + A_{ij}(n) \sin n\omega\tau), \quad \omega > 0, \tag{31}$$

where S_{ij} is symmetric and A_{ij} is antisymmetric. Only S_{ij} could contribute to the dissipation (cf. (24) and (27)), but its contribution is proportional to

$$\int_0^\infty \mathrm{d}\tau \cos n\omega\tau = \pi\delta(n\omega) = 0. \tag{32}$$

(This argument can be generalized to higher-dimensional integrable systems.) Thus the irreversibility of deterministic friction arises from chaos, together with causality as embodied in the solution (18) of (16).

By assuming that correlations decay exponentially, as in systems with homogeneous chaos, we can obtain useful approximate expressions for the tensors in (23) and (24). We write

$$C_{ij}(\tau) \approx (C_{ij}(0) + \tau \dot{C}_{ij}(0)) \exp\{-\lambda\tau\} = (\langle \partial_i \tilde{h}\, \partial_j \tilde{h} \rangle_E + \tau \langle \{h, \partial_i \tilde{h}\}\, \partial_j \tilde{h} \rangle_E) \exp\{-\lambda\tau\}, \tag{33}$$

where λ is the entropy characterizing the chaos. Thus the tensor K_{ij} is

$$K_{ij} \approx \frac{1}{\partial_E \Omega} \partial_E \left[\partial_E \Omega \left(\frac{\langle \partial_i \tilde{h}\, \partial_j \tilde{h} \rangle_E}{\lambda} + \frac{\langle \{h, \partial_i \tilde{h}\}\, \partial_j \tilde{h} - \{h, \partial_j \tilde{h}\}\, \partial_i \tilde{h} \rangle_E}{2\lambda^2} \right) \right], \tag{34}$$

where in writing the second term we have used the invariance of the average under time shift. The first term is symmetric, and represents deterministic friction, while the second is antisymmetric and represents geometric magnetism. This expression is simple because it requires only the valuation of fixed (that is, not evolved) phase-space quantities, in addition to λ.

The structure (23) of these first-order forces exemplifies linear response theory (Landau & Lifshitz 1990; Kubo *et al.* 1985), with the force $\epsilon \boldsymbol{F}_1$ and the slow velocity $\boldsymbol{V}$ ('cause' and 'effect') being related by the tensor K_{ij}. Note that in the tensor K_{ij} describing 'non-equilibrium' response (changing $\boldsymbol{R}$) there occurs the correlation function C_{ij} describing 'equilibrium' (constant $\boldsymbol{R}$) fluctuations (in ∇h). This is an example of the fluctuation-dissipation theorem. And indeed as shown by Ott (1979) and Brown *et al.* (1987) the same C_{ij} appears in expressions for the secular drift in the adiabatic invariant Ω (which is directly related to dissipation) and the growth rate of fluctuations in Ω.

When the underlying dynamics has time-reversal symmetry, the linear response tensor K_{ij} is symmetric. This is an example of Onsager's relation. When there is no time-reversal symmetry, K_{ij} has an antisymmetric part, which as we have seen corresponds to geometric magnetism. Thus the geometric phase 2-form appears in a new light, as the antisymmetric cousin of friction.

3. Half-classical mechanics

Now let the fast motion be quantum-mechanical, described by a density matrix $\rho(t)$ driven by a hamiltonian $h(\boldsymbol{R})$, which is time-dependent because the (classical) slow position $\boldsymbol{R}$ is changing. h is a hermitian operator, whose spectrum we assume to be discrete and non-degenerate for all $\boldsymbol{R}$. It is well known (Mead & Truhlar 1979; Wilkinson 1984; Berry 1989) that there appear magnetic (and electric) reaction forces at first (and second) order, associated with the geometric phase. Our purpose here is to give a derivation of geometric magnetism which parallels the discussion of §2, to facilitate the comparison of classical and half-classical results in §4.

The evolution of ρ is governed by the commutator

$$\mathrm{i}\hbar\epsilon\dot{\rho}(t) = [h(\boldsymbol{R}(t)), \rho(t)], \quad \mathrm{Tr}\,\rho = 1, \tag{35}$$

where again ϵ is the adiabatic parameter. Equation (35) is the analogue of (4) and (5). The desired force is given by the analogue of (6), namely

$$\boldsymbol{F} = -\mathrm{Tr}\rho\,\nabla h. \tag{36}$$

Consider first the case where ρ is an evolving pure state $|\psi(t)\rangle$:

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \rho(t)^2. \tag{37}$$

As in the classical case, we write ρ as the series (7) in powers of ϵ. The terms ρ_r are determined by the following equations, analogous to (8):

$$[h, \rho_0] = 0, \quad [h, \rho_r] = \mathrm{i}\hbar\dot{\rho}_{r-1} \quad (r > 0). \tag{38}$$

Thus ρ_0 must commute with the frozen fast hamiltonian $h(\boldsymbol{R})$. If we define the adiabatic eigenstates and energy levels by

$$h(\boldsymbol{R})\,|m(\boldsymbol{R})\rangle = E_m(\boldsymbol{R})\,|m(\boldsymbol{R})\rangle, \tag{39}$$

we can choose ρ_0 as one of these states, say the nth. Thus

$$\rho_0(t) = |n(\boldsymbol{R}(t))\rangle\langle n(\boldsymbol{R}(t))|. \tag{40}$$

This is the natural analogue of the microcanonical distribution (9). It depends on time through the changing slow position $\boldsymbol{R}(t)$.

Now we can write the force (36) in a form analogous to (15):

$$\begin{aligned} \boldsymbol{F} &= -\operatorname{Tr}\rho_0 \nabla h - \epsilon \operatorname{Tr}\rho_1 \nabla h + O(\epsilon^2) \\ &= -\nabla E_n(\boldsymbol{R}) + \epsilon \boldsymbol{F}_1 + O(\epsilon^2), \end{aligned} \tag{41}$$

where

$$\boldsymbol{F}_1 \equiv -\operatorname{Tr}\rho_1 \nabla h = -\sum_{k,l} \langle k|\rho_1|l\rangle \langle l|\nabla h|k\rangle. \tag{42}$$

As with (15), the leading term $-\nabla E_n$ (equal to $-\langle n|\nabla h|n\rangle$) is the Born–Oppenheimer force, and the next term is the desired first-order reaction. To find it, we need the first correction ρ_1 in the density matrix.

In the adiabatic basis the off-diagonal elements of the corrections ρ_r are determined by the commutator equations (38) as

$$\langle k|\rho_r|l\rangle = \mathrm{i}\hbar \langle k|\dot{\rho}_{r-1}|l\rangle/(E_k - E_l) \quad (k \neq l). \tag{43}$$

The diagonal elements are determined by the pure-state condition (37). A simple calculation using (43) shows that the first-order correction ρ_1 is

$$\begin{aligned} \langle k|\rho_1|l\rangle &= \mathrm{i}\hbar\, \boldsymbol{V}\cdot\langle k|\nabla l\rangle\,(\delta_{nl} - \delta_{nk})/(E_k - E_l) \quad &(k \neq l) \\ &= 0 &(k = l). \end{aligned} \tag{44}$$

Using

$$\langle l|\nabla h|k\rangle/(E_k - E_l) = \langle l|\nabla k\rangle \quad (k \neq l) \tag{45}$$

we now find the first-order force (42) as

$$\begin{aligned} \boldsymbol{F}_1 &= -\mathrm{i}\hbar \boldsymbol{V}\cdot\sum_{k,l} \langle k\,|\,\nabla l\rangle\,(\delta_{nl} - \delta_{nk})\,\langle l\,|\,\nabla k\rangle \\ &= \mathrm{i}\hbar \boldsymbol{V}\cdot\sum_k (\langle k\,|\,\nabla n\rangle\langle \nabla n\,|\,k\rangle - \langle \nabla n\,|\,k\rangle\langle k\,|\,\nabla n\rangle) \\ &= \mathrm{i}\hbar \boldsymbol{V} \wedge \sum_k \langle \nabla n\,|\,k\rangle \wedge \langle k\,|\,\nabla n\rangle. \end{aligned} \tag{46}$$

This has the form

$$\boldsymbol{F}_1 = \boldsymbol{V} \wedge \boldsymbol{B}(\boldsymbol{R}), \tag{47}$$

where the 'magnetic field' is

$$\boldsymbol{B}(\boldsymbol{R}) = -\hbar \operatorname{Im}\langle \nabla n(\boldsymbol{R})| \wedge |\nabla n(\boldsymbol{R})\rangle \tag{48}$$

(cf. the classical (25) and (26)).

Now we allow ρ to be a mixed state. From (38), the lowest-order approximation must still commute with h, and it follows that ρ_0 must have the form

$$\rho_0(t) = \sum_m c_m(t)\,|m(\boldsymbol{R}(t))\rangle\langle m(\boldsymbol{R}(t))|, \quad \sum_m c_m(t) = 1. \tag{49}$$

In fact the coefficients c_m must be constants; this is a consequence of the second equation in the hierarchy (38), which implies that $\langle m|\dot{\rho}_0|m\rangle = 0$ for all adiabatic states $|m\rangle$. Now the calculation proceeds as for pure states, except that we cannot determine the diagonal elements of the correction ρ_1 (cf. (44)) by using the pure-state condition. However, to order ϵ any such diagonal elements would give a contribution to $\boldsymbol{F}_1$ of the same form as the Born–Oppenheimer force – effectively a renormalization of the coefficients c_m. The result is very similar to that for pure states: geometric magnetism (47), with the magnetic field given by the sum

$$\boldsymbol{B} = -\hbar \operatorname{Im}\sum_m c_m \langle \nabla m| \wedge |\nabla m\rangle \tag{50}$$

rather than (48).

We have therefore found that when the fast dynamics is quantum-mechanical the first-order force on the classical slow system consists entirely of geometric magnetism. The force is entirely antisymmetric, so there is no friction as when the fast system is classical and chaotic. Therefore quantum and classical mechanics are discordant, an interesting situation which we will discuss in the next section. The expression (48) for the magnetic field is familiar as the 2-form generating the geometric phase in the fast system when $\boldsymbol{R}$ is cycled.

As previously noted in connection with the geometric phase (Berry 1984*a*) the magnetic force $\boldsymbol{B}(\boldsymbol{R})$ is divergenceless except for monopole singularities at the degeneracies of the adiabatic spectrum. For typical h, without symmetry, degeneracies have co-dimension 3 and so correspond to points in the space of slow coordinates $\boldsymbol{R}$. The loss of global divergencelessness of $\boldsymbol{B}$ has an interesting consequence for the classical slow dynamics: this is measure-preserving but not globally hamiltonian (although it is locally hamiltonian). When the slow dynamics brings $\boldsymbol{R}$ near one of these monopoles, the orbits will, locally, be conical spirals (Goddard & Olive 1978). These classical effects will however be weak, since the monopole strength is $\pm\frac{1}{2}\hbar$, which vanishes in the classical limit. Moreover, the breakdown of the adiabatic approximation will be greatest at the degeneracies, because of transitions between adiabatic states.

4. Discordance: classical but not quantal friction

In the classical treatment, deterministic friction originates in the symmetric part of the tensor K_{ij} in (23). For quantal fast motion, no symmetric part appeared. The quantal counterpart of the symmetric part of the correlation integral in (23) is

$$I_{ij} = \frac{1}{2}\int_0^\infty \mathrm{d}\tau (C_{ij}(\tau) + C_{ji}(\tau)),$$

where
$$C_{ij}(\tau) = \tfrac{1}{2}[\langle n|(\partial_i \tilde{h}_n)_\tau \partial_j \tilde{h}_n|n\rangle + \langle n|\partial_j \tilde{h}_n(\partial_i \tilde{h}_n)_\tau|n\rangle] \tag{51}$$
and
$$\tilde{h}_n \equiv h - E_n.$$

Here we make use of time-evolved operators:

$$(A)_\tau \equiv \exp\{\mathrm{i}\,\tau h/\hbar\} A \exp\{-\mathrm{i}\,\tau h/\hbar\}. \tag{52}$$

However, this quantum equivalent I_{ij} is zero. A short calculation shows that

$$\tfrac{1}{2}(C_{ij}(\tau) + C_{ji}(\tau)) = \sum_{m\neq n} \mathrm{Re}\,(\langle n|\partial_i h|m\rangle\langle m|\partial_j h|n\rangle)\cos\left\{\frac{\tau}{\hbar}(E_n - E_m)\right\}. \tag{53}$$

This has the same form as (31), so that the time integral I_{ij} vanishes (cf. (32)).

Therefore there really is no quantum friction in this theory, and the discordance with classical mechanics persists. Its origin is the same as that studied in a related, mathematically inspired, example by Robbins & Berry (1992*b*): a clash between the essence of quantization, namely the discrete spectrum of frequencies, and the essence of chaos, namely mixing and a continuous spectrum extending to zero frequency (which make the integrals in (23) converge to finite values).

At first this discordance appears paradoxical, and a violation of the correspondence principle: the I_{ij} vanish for all finite $\hbar$ but are finite for zero $\hbar$. The resolution lies in a careful consideration of the time scales involved in the correlation integrals. To see the quantal I_{ij} converge to zero, the τ integration must include times much longer than the reciprocal of the smallest frequency in the integrand (53). This is proportional to the level spacing, and scales as $\hbar^{D-1}$, so the integration time diverges semiclassically. Therefore the finite values attained by the classical integrals in a finite time (inversely proportional to the entropy characterizing the chaos; cf. (33)) must be cancelled by quantal contributions over times large compared with $\hbar^{-(D-1)}$.

A model 'quantum' correlation function which shows this behaviour, and has the same structure as (53), is

$$C_{\mathrm{qu}}(\tau) = \hbar \sum_{m=1}^{\infty} \exp\{-\hbar^2 m^2\} \cos\{m\hbar\tau\}. \tag{54}$$

Because of the discrete spectrum, the integral of this function from 0 to ∞ is zero. In the classical limit, summation can be replaced by integration, and

$$C_{\mathrm{qu}}(\tau) \to C_{\mathrm{cl}}(\tau) = \int_0^\infty \mathrm{d}x \exp\{-x^2\} \cos\{x\tau\} = \tfrac{1}{2}\sqrt{\pi} \exp\{-\tfrac{1}{4}\tau^2\}, \tag{55}$$

whose integral is not zero but

$$I_{\mathrm{cl}} = \tfrac{1}{2}\pi. \tag{56}$$

To resolve the discordance, we write (54) exactly in an alternative form, obtained by applying the Poisson sum formula, as follows:

$$\begin{aligned} C_{\mathrm{qu}}(\tau) &= \tfrac{1}{2}\hbar \sum_{m=-\infty}^{\infty} \exp\{-\hbar^2 m^2\} \cos\{m\hbar\tau\} - \tfrac{1}{2}\hbar \\ &= \tfrac{1}{2}\hbar \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}m \exp\{-\hbar^2 m^2\} \cos\{m\hbar\tau\} \exp\{2\pi \mathrm{i} mn\} - \tfrac{1}{2}\hbar \\ &= \tfrac{1}{2}\sqrt{\pi} \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{1}{4}\left(\tau - \frac{2\pi n}{\hbar}\right)^2\right\} - \tfrac{1}{2}\hbar \\ &= \sum_{n=-\infty}^{\infty} C_{\mathrm{cl}}\left(\tau - \frac{2\pi n}{\hbar}\right) - \tfrac{1}{2}\hbar. \end{aligned} \tag{57}$$

Thus the 'quantum' correlation function is a sequence of copies of the classical function (55), centred on $\tau = 2\pi n/\hbar$, together with a classically vanishing negative offset $-\frac{1}{2}\hbar$. In the integral over τ, each copy contributes π, except that centred on the origin, which contributes $\frac{1}{2}\pi$. On the average, these are cancelled by the offset, since, for large T,

$$\begin{aligned} I_{\mathrm{qu}}(T) &\equiv \int_0^T \mathrm{d}\tau\, C_{\mathrm{qu}}(\tau) \approx \tfrac{1}{2}\pi + \pi \,\mathrm{Int}\left[\frac{\hbar T}{2\pi}\right] - \tfrac{1}{2}\hbar T \\ &= \pi(\mathrm{Int}[x] + \tfrac{1}{2} - x), \quad \text{where } x = \hbar T/2\pi. \end{aligned} \tag{58}$$

The mean value of the staircase function $\mathrm{Int}[x]$ is $x - \frac{1}{2}$, so that I_{qu} vanishes, as expected.

In emphasizing the discordance between the classical model with friction and the corresponding quantum model without friction, we are of course not asserting that friction cannot be described within a quantum framework. This must be possible, since friction exists and the world is quantum-mechanical. Indeed, there is the well-known quantum formula of Kubo *et al.* (1985) and Greenwood (1958) for the linear transport coefficients of irreversible thermodynamics. (Moreover, these have an antisymmetric part representing, for example, the (non-dissipative) quantum Hall effect (Thouless *et al.* 1982).) Our assertion is simply that friction does not appear as a first-order force when the fast motion is quantal and with a discrete spectrum. The argument for its non-existence breaks down in the thermodynamic limit where the fast system is regarded as infinite, since then the spectrum becomes continuous and the correlation integrals need not vanish.

Even within the adiabatic framework for finite systems, there is dissipation at higher than the first order in ϵ, caused by non-adiabatic transitions at 'avoided crossings', where $\boldsymbol{R}$ passes near degeneracies of the adiabatic spectrum. For a given quantum system, that is with fixed $\hbar$, these transitions are exponentially small for small ϵ, that is 'beyond all orders' in ϵ. If now $\hbar$ is decreased, keeping ϵ fixed, the density of avoided crossings increases, and they can be treated statistically using random-matrix theory. In this régime, envisaged by Hill & Wheeler (1952) and studied in detail by Wilkinson (1988), dissipation arises as the collective effect of those occasional avoided crossings when levels approach closer than $O(\surd\epsilon)$, for which the transitions are not exponentially small. Making $\hbar$ even smaller leads to levels so close and rapidly changing that there are frequent transitions between many levels, and in this quantally non-adiabatic régime Wilkinson obtains the classical result (23) by taking the limit of the Kubo formula. That very different behaviour can occur during classically and quantally adiabatic changes has been pointed out elsewhere (Berry 1984*b*): the adiabatic and semiclassical limits are both singular, and their combination is much more so.

5. Generalization

Here we consider the case where both slow and fast dynamics are classical, and where the fast motion can be coupled to all the slow variables, that is velocities as well as coordinates. Let the slow coordinates and velocities be denoted by $Z = \{Z_\mu\}$, and let the dynamics of the combined system be governed by a hamiltonian $\mathscr{H}(z, Z)$. As in §2, we consider the slow motion to be coupled to an ensemble of fast trajectories, described by a normalized distribution function $\rho(z,t)$ in fast phase space. From Hamilton's equations, the desired generalized force (rate of change of slow phase-space variables) is

$$\omega_{\mu\nu}\dot{Z}_\nu = \int \mathrm{d}z\,\rho\,\partial_\mu \mathscr{H}. \tag{59}$$

This generalization of (6) involves the unit symplectic matrix

$$\omega_{\mu\nu} \equiv \begin{pmatrix} 0 & -\boldsymbol{I} \\ \boldsymbol{I} & 0 \end{pmatrix}, \tag{60}$$

where $\boldsymbol{I}$ is the identity matrix with dimension equal to the number of slow freedoms. The evolution of the distribution function is slaved to $Z(t)$ by the generalization of (5), namely

$$\epsilon\dot{\rho}(z,t) = \{\mathscr{H}(z, Z(t)), \rho(z,t)\} \tag{61}$$

(where of course the Poisson bracket is with respect to z, not Z).

Again we expand ρ in powers of ϵ. The leading term is the microcanonical distribution (cf. (9))

$$\rho_0(z,t) = \delta(\mathscr{E}(Z)-\mathscr{H}(z,Z))/\partial_{\mathscr{E}}\,\Omega(\mathscr{E}(Z),Z), \tag{62}$$

where again Ω denotes the phase volume, now defined as

$$\Omega(\mathscr{E},Z) = \int \mathrm{d}z\,\Theta(\mathscr{E}-\mathscr{H}(z,Z)) \tag{63}$$

and whose constancy defines the adiabatic energy $\mathscr{E}(Z)$. The generalized force is obtained as in (15)

$$\omega_{\mu\nu}\dot{Z}_\nu = \partial_\mu\mathscr{E}(Z)+\epsilon\int \mathrm{d}z\,\rho_1\,\partial_\mu\tilde{\mathscr{H}}+O(\epsilon^2), \tag{64}$$

where (cf. (12))

$$\tilde{\mathscr{H}} \equiv \mathscr{H}-\mathscr{E}(Z). \tag{65}$$

The first term in (64) is the Born–Oppenheimer energy, and the second term, involving the first correction ρ_1 to the distribution function, is the first-order force we are interested in.

The solution of (61) for ρ_1 is obtained by a procedure precisely analogous to that in §2, with the result of (cf. (23) and (24))

$$\omega_{\mu\nu}\dot{Z}_\nu = \partial_\mu\mathscr{E}-\epsilon\mathscr{K}_{\mu\nu}\dot{Z}_\nu+O(\epsilon^2), \tag{66}$$

where

$$\mathscr{K}_{\mu\nu} = -\frac{1}{\partial_{\mathscr{E}}\Omega}\partial_{\mathscr{E}}\left[\partial_{\mathscr{E}}\Omega\int_0^\infty \mathrm{d}\tau\langle(\partial_\mu\tilde{\mathscr{H}})_\tau\,\partial_\nu\tilde{\mathscr{H}}\rangle_{\mathscr{E}}\right]. \tag{67}$$

(Here as above we are neglecting Jarzynski's force, associated with f_1 in equation (20).) Equation (66) can be written

$$\omega'_{\mu\nu}(Z)\,\dot{Z}_\mu = \partial_\nu\mathscr{E}(\mathscr{Z}),\quad \text{where}\quad \omega'_{\mu\nu}(Z)\equiv\omega_{\mu\nu}+\epsilon\mathscr{K}_{\mu\nu}(Z). \tag{68}$$

In this effective slow equation of motion, accurate to order ϵ, the effect of the Born–Oppenheimer (ϵ^0) hamiltonian $\mathscr{E}(Z)$ is modified by altering the symplectic form from ω to ω'. In the case where the fast motion is integrable, this phenomenon was noted by Gozzi & Thacker (1987) and (in the half-classical case) by Littlejohn & Flynn (1991). Because $\mathscr{K}_{\mu\nu}$ incorporates generalized friction through its symmetric part, ω' is no longer symplectic, and the modified equations of motion are no longer hamiltonian. The antisymmetric part of $\mathscr{K}_{\mu\nu}$ embodies a generalization of geometric magnetism.

This more general theory can of course reproduce the results of §2. This follows from the formulae, appropriate to that special case

$$\left.\begin{aligned} Z = (\boldsymbol{R},\boldsymbol{V});\quad \mathscr{H}(Z) = \tfrac{1}{2}|\boldsymbol{V}|^2+h(z,\boldsymbol{R});\\ \mathscr{E}(Z) = \tfrac{1}{2}|\boldsymbol{V}|^2+E(\boldsymbol{R});\quad \mathscr{K}_{\mu\nu} = \begin{pmatrix}K_{ij} & 0\\ 0 & 0\end{pmatrix},\end{aligned}\right\} \tag{69}$$

where K_{ij} is defined in (23).

We thank Professor V. I. Arnold for a suggestion leading to the generalization in §5, and Dr C. Jarzynski for sending us his paper before publication and thereby enabling us to correct an omission. J.M.R. acknowledges support from the NSF (grant no. Int-9203313).

Appendix A. Solution of the Poisson-bracket equation (16)

To show that the expression (18) is a solution, we substitute it into (16):

$$\{h,f\} = -\int_{-\infty}^{0} \mathrm{d}\tau \{h(z), g(z_\tau(z))\} = -\int_{-\infty}^{0} \mathrm{d}\tau \{h(z_\tau(z)), g(z_\tau(z))\}$$

$$= -\int_{-\infty}^{0} \mathrm{d}\tau (\partial_{q_\tau} h \cdot \partial_{p_\tau} g - \partial_{p_\tau} h \cdot \partial_{q_\tau} g) = \int_{-\infty}^{0} \mathrm{d}\tau \frac{\mathrm{d}}{\mathrm{d}\tau} g(z_\tau(z)) = g(z). \qquad \text{(A 1)}$$

The second equality follows from the invariance of h under its own flow, and the third from the invariance of the Poisson bracket under τ translation, because this is a canonical transformation.

A similar argument shows that the 'anticausal' expression

$$f(z) = \int_{0}^{\infty} \mathrm{d}\tau \, g(z_\tau(z)) \qquad \text{(A 2)}$$

is also a solution of (16). If used instead of (18), this correctly gives geometric magnetism according to (25) and (26), but generates antifriction (feeding energy from chaos into the slow motion) instead of friction.

References

Aharonov, Y. & Stern, A. 1992 *Phys. Rev. Lett.* **69**, 3593–3597.

Arnold, V. I., Kozlov, V. V. & Neishtadt, A. I. 1988 *Dynamical systems. III. Mathematical aspects of classical and celestial mechanics. Encyclopedia of mathematical science*, vol. 3. Berlin: Springer.

Berry, M. V. 1984*a* *Proc. R. Soc. Lond.* A **392**, 45–57.

Berry, M. V. 1984*b* *J. Phys.* A **17**, 1225–1233.

Berry, M. V. 1989 The quantum phase, five years after. In Shapere & Wilczek (1989), pp. 7–28.

Berry, M. V. & Robbins, J. M. 1993 *Proc. R. Soc. Lond.* A **442**, 641–658. (Preceding paper.)

Goddard, P. & Olive, D. I. 1978 *Rep. Prog. Phys.* **41**, 1357–1437.

Gozzi, E. & Thacker, W. D. 1987 *Phys. Rev.* D **35**, 2388–2397.

Greenwood, D. A. 1958 *Proc. Phys. Soc.* **71**, 585–596.

Hill, D. A. & Wheeler, J. A. 1952 *Phys. Rev.* **89**, 1102–1045.

Jackiw, R. 1988 *Commun. at. mol. Phys.* **21**, 71–82.

Jarzynski, C. 1993 *Phys. Rev. Lett.* (In the press.)

Kubo, R., Toda, M. & Hashitsume, N. 1985 *Statistical physics. II. Nonequilibrium statistical mechanics.* Berlin: Springer.

Landau, L. D. & Lifshitz, E. M. 1980 *Statistical physics*, Part I, 3rd edn. Oxford: Pergamon Press.

Littlejohn, R. G. & Flynn, W. G. 1991 *Phys. Rev.* A **44**, 5239–5256.

Lochak, P. & Meunier, C. 1988 *Multiphase averaging for classical systems.* New York: Springer.

Mead, C. A. & Truhlar, D. G. 1979 *J. Chem. Phys.* **70**, 2284–2296. (Reprinted in Shapere & Wilczek, 1989.)

Messiah, A. 1962 *Quantum mechanics*, vol. 2. New York: Wiley.

Ott, E. 1979 *Phys. Rev. Lett.* **42**, 1628–1631.

Brown, R., Ott, E. & Grebogi, C. 1987 *J. statist. Phys.* **49**, 511–550.

Robbins, J. M. & Berry, M. V. 1992*a* *Proc. R. Soc. Lond.* A **436**, 631–661.

Robbins, J. M. & Berry, M. V. 1992*b* *J. Phys.* A **25**, 961–965.

Shapere, A. & Wilczek, F. (eds) 1989 *Geometric phases in physics.* World Scientific: Singapore.

Thouless, D., Kohmoto, M., Nightingale, P. & den Nijs, M. 1982 *Phys. Rev. Lett.* **49**, 405–408.

Wilkinson, M. 1984 Ph.D. thesis, Department of Physics, University of Bristol.
Wilkinson, M. 1987 *J. Phys.* A **20**, 2415–2423.
Wilkinson, M. 1988 *J. Phys.* A **21**, 4021–4037.
Wilkinson, M. 1990 *J. Phys.* A **23**, 3603–3611.

Received 13 January 1993; accepted 5 April 1993