

Classical geometric forces of reaction: an exactly solvable model

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We illustrate the effects of the classical ‘magnetic’ and ‘electric’ geometric forces that enter into the adiabatic description of the slow motion of a heavy system coupled to a light one, beyond the Born–Oppenheimer approximation of simple averaging. When the fast system is a spin \mathbf{S} and the slow system is a massive particle whose spatial position \mathbf{R} is coupled to \mathbf{S} with energy (fast hamiltonian) $\mathbf{S} \cdot \mathbf{R}$, the magnetic force is that of a monopole of strength I (= adiabatic invariant $\mathbf{S} \cdot \mathbf{R}/R$) centred at $\mathbf{R} = 0$, and the electric force is inverse-cube repulsion with strength $S^2 - I^2$. Confining the slow particle to the surface of a sphere eliminates the Born–Oppenheimer and electric forces, and generates motion with precession and nutation exactly equivalent to that of a heavy symmetrical top. In the adiabatic limit the nutation is small and the averaged precession is precisely reproduced by the magnetic force. Alternatively, choosing the exactly conserved total angular momentum to vanish eliminates the Born–Oppenheimer and magnetic forces, and generates as exact orbits a one-parameter family of curly ‘antelope horns’ coiling in from infinity, reversing hand, and receding to infinity. In the adiabatic limit the repulsion of the ‘guiding centre’ of these coils is exactly reproduced by the electric force.

A by-product of the ‘antelope horn’ analysis is a determination of the shape of a curve with a given curvature κ and torsion τ in terms of the evolution of a quantum 2-spinor driven by a planar ‘magnetic field’ with components κ and τ .

1. Introduction

When a light system, whose motion is fast, is coupled to a heavy system, that moves slowly, the dynamics can get quite complicated and hard to analyse. A useful approximation is to solve the fast motion for frozen values of the slow coordinates, and then consider the slow dynamics to be influenced by the average energy of the fast motion. This energy depends on the slow coordinates and so its gradient acts as a reaction force on the slow motion. In quantum mechanics the approximation technique is known as the Born–Oppenheimer method (Messiah 1962) and is commonly used to analyse molecules (where the light and heavy systems are the electrons and nuclei respectively). In classical mechanics it is the method of adiabatic averaging (Arnold *et al.* 1988; Lochak & Meunier 1988). We shall call this reaction force the Born–Oppenheimer force.

In recent years it has become clear (Mead & Truhlar 1979; Jackiw 1988; Berry 1989) that in quantum mechanics an improvement of the approximation, more consistent with the adiabatic assumption for the fast motion, should include in the

slow dynamics two extra reaction forces, which have a gauge structure resembling that of electromagnetism, in addition to the Born–Oppenheimer force. These ‘magnetic’ and ‘electric’ reaction forces depend on the geometry of the fast dynamics in the space of frozen slow coordinates. They are related to the geometric phase (Shapere & Wilczek 1989). In the quantum mechanics of molecules, one effect of the magnetic gauge force (associated with degeneracies in the frozen electronic states) is to alter the energy levels of the nuclear motion (Longuet–Higgins *et al.* 1959; Delacrétaz *et al.* 1986).

Our purpose here is to study the analogous *classical* geometric forces in a simple hamiltonian model where they have real and clearly identifiable effects. This is part of a larger programme in which we are exploring the origin and structure of the classical geometric forces. It is not our intention to give the general theory here, but it will be convenient to present some new formulae for the forces. The novelty is twofold. First, the formulae apply when the fast motion is ergodic, and so extend previous related studies (e.g. Hannay 1985; Berry 1985), which have been confined to integrable systems, to cover the case of chaotic motion, thereby resolving a long-standing problem. (In the present example the fast motion is one dimensional, and so the integrable and ergodic categories coincide.) Second, the forces are expressed as integrals along trajectories, and in the integrable case are manifestly independent of action–angle variables, making them easy to interpret and convenient to calculate.

In the model, introduced in §2, the fast system is a spin, and the slow system to whose coordinates it is coupled is a massive particle moving in three dimensions. The fast motion (with frozen slow coordinates as parameters) is integrable. An interesting feature is that the slow motion can be exactly decoupled from the fast motion – that is, independently of the adiabatic approximation – and the resulting equation is not hamiltonian.

In §3 the gauge forces are calculated; the new formulae enable a speedy derivation, although the results are not new (see e.g. Berry 1989). The magnetic force is that of a monopole and the electric force an inverse-cube repulsion. These alter the slow motion in qualitatively different ways.

Section 4 treats the special case where only the magnetic force acts. This leads to a surprising connection with the motion of an ordinary spinning-top, whose precession can be considered as caused by a magnetic gauge monopole describing the reaction of the (fast) spin on the (slow) dynamics of the symmetry axis, averaged over nutation. In a different special case, considered in §5, only the electric force acts; the repulsion describes precisely the slow motion after oscillations are averaged away. In an interesting technicality (Appendix D) the determination of a curve whose curvature and torsion are given functions of arc length is shown to be equivalent to the ‘Landau–Zener’ evolution of a two-state quantum system, which in certain cases, including that of the orbit in §5, enables the exact analytic solution to be found.

Now we present the general formulae. Let the slow system have coordinates $\mathbf{R} = \{R_1, R_2, \dots\}$ and momenta $\mathbf{P} = \{P_1, P_2, \dots\}$ and let the fast system have phase space variables $z = \{\mathbf{q}, \mathbf{p}\} = \{q_1, \dots, p_1, \dots\}$. For the hamiltonian we take

$$H(\mathbf{R}, \mathbf{P}, z) = \frac{1}{2} \sum \sum Q_{ij} P_i P_j + h(z, \mathbf{R}). \quad (1)$$

Here Q is an inverse mass matrix which is small in the adiabatic régime, and h is the fast hamiltonian coupling the fast variables to the slow coordinates. This can describe a classical or a quantum system, depending on whether \mathbf{R} and \mathbf{P} , and \mathbf{q} and

\mathbf{p} , commute. In the improved adiabatic approximation, the slow variables are governed by the effective hamiltonian

$$H_g(\mathbf{R}, \mathbf{P}) = \frac{1}{2} \sum \sum Q_{ij} (P_i - A_i(\mathbf{R})) (P_j - A_j(\mathbf{R})) + E_{\text{BO}}(\mathbf{R}) + \Phi(\mathbf{R}). \quad (2)$$

Corresponding to this are the three reaction forces

$$\left. \begin{aligned} \text{Born-Oppenheimer; } & -\partial_i E_{\text{BO}}(\mathbf{R}), \\ \text{magnetic gauge: } & B_{ij} \equiv \partial_i A_j(\mathbf{R}) - \partial_j A_i(\mathbf{R}), \\ \text{electric gauge: } & -\partial_i \Phi(\mathbf{R}), \end{aligned} \right\} \quad (3)$$

where $\partial_i \equiv \partial/\partial R_i$.

In quantum mechanics, these forces depend on the eigenstate $|n(\mathbf{R})\rangle$ and energy $E_n(\mathbf{R})$ of the fast hamiltonian h , corresponding to the adiabatically preserved state of the fast system. Berry (1989) obtained

$$\left. \begin{aligned} E_{\text{BO}}(\mathbf{R}) &= E_n(\mathbf{R}), \\ B_{ij}(\mathbf{R}) &= i\hbar [\langle \partial_i n | \partial_j n \rangle - \langle \partial_j n | \partial_i n \rangle], \\ \Phi(\mathbf{R}) &= \sum \sum Q_{ij} g_{ij}(\mathbf{R}), \end{aligned} \right\} \quad (4)$$

where $g_{ij} = \frac{1}{2} \hbar^2 \langle \partial_i n | (1 - |n\rangle \langle n|) | \partial_j n \rangle$. Appendix A outlines a slightly different way of getting this well-known result. We remark that the quantities B_{ij} and g_{ij} , which here influence the slow motion, also have significance in the fast motion: B_{ij} is the 2-form whose flux through an \mathbf{R} circuit gives the geometric phase, and g_{ij} is a metric governing the separation of quantum states in \mathbf{R} space (Provost & Vallée 1980; Berry 1989).

It is remarkable that the quantum geometric forces have finite classical limits. We display the new classical formulae for the case where the fast motion is ergodic (this includes the example to follow, which is one dimensional). The phase volume

$$\Omega(E, \mathbf{R}) = \int dz \Theta \{E - h(z, \mathbf{R})\}, \quad (5)$$

where Θ denotes the unit step, is an adiabatic invariant (in one dimension it is the action times 2π). The fast energy $E_{\text{BO}}(\mathbf{R})$ is determined by taking $\Omega(E_{\text{BO}}, \mathbf{R})$ as constant.

Let $Z_t(z, \mathbf{R})$ denote the orbit which starts at z at $t = 0$ and evolves under h with parameters \mathbf{R} , and let

$$(\partial_i h)_t \equiv \partial_i h(Z_t, \mathbf{R}) \quad (6)$$

denote the time-evolved parameter derivative of the fast hamiltonian. Denote averaging over the energy surface in phase space by

$$\langle \dots \rangle_E \equiv \frac{1}{\partial_E \Omega} \int dz \delta(E - h(z, \mathbf{R})) \dots \quad (7)$$

Then the geometric forces are determined by

$$\left. \begin{aligned} B_{ij}(\mathbf{R}) &= -\frac{1}{2\partial_E \Omega} \partial_E \left[\partial_E \Omega \int_0^\infty dt \langle (\partial_i h)_t \partial_j h - (\partial_j h)_t \partial_i h \rangle_E \right], \\ g_{ij}(\mathbf{R}) &= -\frac{1}{2} \int dt \langle (\tilde{\partial}_i h)_t (\tilde{\partial}_j h) \rangle_E, \end{aligned} \right\} \quad (8)$$

where $\tilde{\partial}_i h \equiv \partial_i h - \langle \partial_i h \rangle = \partial_i h - \partial_i E_{\text{BO}}$. (This last equality is the classical analogue of the quantum Hellman–Feynman formula.)

The magnetic force B_{ij} has been derived by Robbins & Berry (1992) as the classical limit of the quantum expression in (4). The formula for the electric potential was found in 1988 by Berry and Wilkinson (unpublished) in the same way. In Appendix B we outline this method. In one dimension the formula for B_{ij} is, despite appearances, equivalent to the classical 2-form discovered by Hannay (1985). Deriving and interpreting these formulae from classical mechanics in the multi-dimensional ergodic case involves subtle questions which we will discuss in later papers.

In a systematic study of the origin of quantum gauge forces, Weigert & Littlejohn (1992) have shown that an additional (LW) term arises in the effective hamiltonian, which typically is of the same order as the electric geometric scalar potential. They have also considered its classical limit for spin problems (personal communication) of which the one considered here is a special case. In §3 we show that in the particular case we study the LW force is smaller than the other forces, and we will not consider it further.

2. Spin model

The hamiltonian (1) is

$$H = \frac{1}{2}P^2 + \mathbf{R} \cdot \mathbf{S}. \quad (9)$$

Here the heavy system is a particle with classical coordinates $\mathbf{R} = \{R_1, R_2, R_3\}$ and momenta $\mathbf{P} = \{P_1, P_2, P_3\}$. The light system \mathbf{S} is a classical spin whose length is fixed and whose direction can be regarded as a hamiltonian system with one freedom (the momentum is the projection of \mathbf{S} onto any fixed axis, and the coordinate is the azimuth angle about that axis). The equations of motion are

$$\dot{\mathbf{R}} \equiv \mathbf{V} = \mathbf{P}; \quad \dot{\mathbf{P}} = -\mathbf{S}; \quad \dot{\mathbf{S}} = \mathbf{R} \wedge \mathbf{S}. \quad (10)$$

Thus H has four freedoms: three slow and one fast. We shall denote the length of \mathbf{R} by R , and its direction by the unit vector \mathbf{r} , i.e. $\mathbf{R} \equiv R\mathbf{r}$. \mathbf{S} is slaved to the particle position \mathbf{R} and precesses about its instantaneous direction with angular velocity R , and \mathbf{S} influences \mathbf{R} by providing the force on the particle.

The adiabatic régime corresponds to R large, so that the spin precession is fast and \mathbf{S} turns many times while the direction \mathbf{r} remains approximately constant. It is not necessary to introduce an explicit adiabatic parameter (for example a large mass) into the hamiltonian (9), because in this case it can be removed by scaling, something not possible in general.

Classical or quantal aspects of the model (9) have been studied by many authors (e.g. Stone 1986; Gozzi & Thacker 1987; Anandan & Aharonov 1989; Berry 1989; Aharonov & Stern 1992; Bulgac & Kusnezov 1992; Littlejohn, personal communication 1992). There are more general variants, in which for example \mathbf{R} is replaced by any vector function of \mathbf{R} , but (9) suffices for the simple point we wish to make, namely that the gauge forces have real effects. It is possible to interpret (9) as describing the motion of a heavy uncharged spinning particle, with a magnetic moment, through a uniform sphere of monopolum (whose magnetic field is proportional to \mathbf{R}). In an alternative interpretation, the ‘particle’ could be a thin spinning molecule with an electric dipole moment along its axis, moving through a uniform sphere of charge.

The coupled motion (10) is apparently non-integrable for most initial conditions.

Nevertheless, it is a remarkable feature of this model that the fast motion can be eliminated without approximation (that is, independently of any adiabatic assumption), using the fact that because of rotational invariance (10) conserves the total angular momentum (orbital plus spin), namely

$$\mathbf{J} \equiv \mathbf{R} \wedge \mathbf{V} + \mathbf{S} = \text{const.} \tag{11}$$

Note that $\mathbf{J} \cdot \mathbf{R} = \mathbf{S} \cdot \mathbf{R}$. Thus (10) gives the acceleration of the slow variables as

$$\dot{\mathbf{V}} = \mathbf{R} \wedge \mathbf{V} - \mathbf{J}. \tag{12}$$

Now the slow motion corresponds to that of a *charged* particle influenced by the Lorentz force inside a uniform sphere of monopolum, and also by a constant ‘gravitational’ force $-\mathbf{J}$. This newtonian equation is measure-preserving in the phase space \mathbf{R}, \mathbf{V} . It is however not hamiltonian, because the ‘magnetic field’ \mathbf{R} has non-vanishing divergence and hence no vector potential exists. Nevertheless, as Professor R. G. Littlejohn has pointed out to us, there is a 2-freedom hamiltonian equivalent of (12), whose four phase-space variables are radial momentum, radius, action (see (17) later) and azimuthal angle of \mathbf{S} relative to \mathbf{R} .

Two quantities conserved by (12) are the energy and length S of spin, namely

$$E = \frac{1}{2}V^2 + \mathbf{J} \cdot \mathbf{R}; \quad S = |\mathbf{J} - \mathbf{R} \wedge \mathbf{V}|. \tag{13}$$

Note that conservation of S implies constancy of the magnitude of the acceleration in (12).

In §§4 and 5 we shall solve (12) exactly in special cases, to assess the effects of the gauge forces whose derivation follows now.

3. Geometric forces

In this model the slow coordinates form a vector in space, so that in (8) it is convenient to replace derivatives ∂_i by gradients ∇ , and regard the magnetic gauge field as a vector \mathbf{B} . The gauge forces depend on the fast motion generated by

$$h = \mathbf{R} \cdot \mathbf{S}, \quad \text{i.e.} \quad \dot{\mathbf{S}} = \mathbf{R} \wedge \mathbf{S} \tag{14}$$

with fixed \mathbf{R} , via the gradient $\nabla h = \mathbf{S}$. This describes precession about \mathbf{r} , which we take temporarily as the z axis, with angular velocity \mathbf{R} . If the initial spin has polar coordinates θ, ϕ , its evolution is

$$\mathbf{S}_t = (S \sin \theta \cos(\phi + Rt), \quad S \sin \theta \sin(\phi + Rt), \quad S \cos \theta). \tag{15}$$

The constant-energy surface for this one-dimensional integrable and ergodic motion is a latitude circle on the spherical phase space $S = \text{const.}$ whose measure, appearing in (8), is

$$\partial_E \Omega = S \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \delta(E - SR \cos \theta) = \frac{2\pi}{R}. \tag{16}$$

This is independent of E and so cancels from the magnetic field in (8). There is an adiabatic invariant (conserved under infinitely slow changes in \mathbf{R}), given by the component of spin along \mathbf{R} :

$$I = \mathbf{S} \cdot \mathbf{r} = S \cos \theta \left(= \frac{1}{2\pi} \Omega = \frac{1}{2\pi} \oint p \, dq \right). \tag{17}$$

Thus the Born–Oppenheimer, magnetic gauge and electric gauge forces are obtained from

$$\left. \begin{aligned} E_{\text{BO}}(\mathbf{R}) &= IR, \\ \mathbf{B}(\mathbf{R}) &= -\frac{1}{2}\partial_E \int_0^\infty dt \langle \mathbf{S}_t \wedge \mathbf{S} \rangle_E, \\ \Phi(\mathbf{R}) &= -\frac{1}{2} \int_0^\infty dt \langle (\mathbf{S}_t - I\mathbf{r}) \cdot (\mathbf{S} - I\mathbf{r}) \rangle_E. \end{aligned} \right\} \quad (18)$$

The averages $\langle \dots \rangle_E$ are integrals round the latitude circle with $\cos \theta = I/S$, and a direct calculation using the orbit (15) gives the known results

$$\mathbf{B}(\mathbf{R}) = -I \frac{\mathbf{r}}{R^2}, \quad \Phi(\mathbf{R}) = \frac{S^2 - I^2}{2R^2}. \quad (19)$$

As previously asserted, the magnetic force is that of a monopole at $\mathbf{R} = 0$, with strength $-I$, and the electric force is an inverse-cube radial repulsion with strength $S^2 - I^2$. From (18) the Born–Oppenheimer force is radial and constant, and attractive or repulsive if $I > 0$ or $I < 0$. This calculation, based on the new formulae (8), is much simpler than the analogous calculation (Berry 1986) of \mathbf{B} from the earlier formalism involving the shift of invariant tori with \mathbf{R} .

Adiabatic theory therefore predicts that the slow motion is determined by the equation of motion generated by the effective hamiltonian (2), namely

$$\dot{\mathbf{V}} = -I\mathbf{r} - I \frac{\mathbf{V} \wedge \mathbf{r}}{R^2} + \frac{(S^2 - I^2)}{R^3} \mathbf{r} \quad (20)$$

in which the acceleration is the sum of Born–Oppenheimer, magnetic and electric terms. This looks very different from the exact equation (12) for the slow motion, and yet we will find that it gives very good approximations to the average of the slow motion. Aharonov & Stern (1992) have derived the geometric forces in (20) by physical arguments involving careful averaging.

In this example the additional term discovered by Weigert & Littlejohn (1992) in the effective slow hamiltonian is

$$H_{\text{LW}} = I|\mathbf{r} \wedge \mathbf{P}|^2/2R^3. \quad (21)$$

To estimate its importance, consider its effect when acting in conjunction with the Born–Oppenheimer and geometric electric forces, that is in the hamiltonian

$$H_{\text{eff}} = \frac{1}{2}P^2 + IR + (S^2 - I^2)/2R^2 + H_{\text{LW}}. \quad (22)$$

Conserved quantities are the angular momentum and energy:

$$\mathbf{L} = \mathbf{R} \wedge \mathbf{P} = \frac{\mathbf{R} \wedge \mathbf{V}}{1 + I/R^3}, \quad 2E = \dot{R}^2 + 2IR + \frac{S^2 - I^2}{R^2} + \frac{L^2}{R^2} + I \frac{L^2}{R^5}. \quad (23)$$

Thus motion is planar, with the LW force contributing an inverse sixth-power repulsive force whose strength depends on L . Since L is proportional to R , this is smaller in the adiabatic régime of large R than the inverse-cube repulsion (inverse-square potential) of the electric gauge force, and from now on we neglect it. (The essential reason for the smallness of the LW force is that the Born–Oppenheimer force is radial.)

4. Magnetic force only

(a) Exact solution

Both the Born–Oppenheimer and electric forces in (20) are radial. To eliminate their effects, and thereby study the case where the only adiabatic effective force is magnetic, we constrain the particle to the surface of a sphere. This can be achieved by replacing the kinetic energy in (9) by

$$P^2 \rightarrow P^2 - (\mathbf{P} \cdot \mathbf{r})^2 \tag{24}$$

because then Hamilton’s equation gives the velocity as

$$\mathbf{V} = \mathbf{P} - \mathbf{P} \cdot \mathbf{r} \mathbf{r}, \quad \text{i.e.} \quad \mathbf{V} \cdot \mathbf{r} = 0. \tag{25}$$

The total angular momentum (11) is still conserved, and the fast variables \mathbf{S} can be exactly eliminated, to give the slow acceleration as (12) together with forces incorporating the constraint:

$$\dot{\mathbf{V}} = \mathbf{R} \wedge \mathbf{V} - \mathbf{J} + \mathbf{J} \cdot \mathbf{r} \mathbf{r} - (V^2/R) \mathbf{r}. \tag{26}$$

In addition to R , this conserves E and S given by (13), and hence the combination

$$K = E + (1/2R^2)(J^2 - S^2) = \mathbf{R} \cdot \mathbf{J} + (\mathbf{r} \wedge \mathbf{V}) \cdot \mathbf{J}/R. \tag{27}$$

To determine the motion of \mathbf{R} on its sphere, we first introduce polar coordinates (θ, ϕ) for \mathbf{r} , with \mathbf{J} as axis, and thus obtain

$$\begin{aligned} E &= \frac{1}{2}R^2[\dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2] + JR \cos \theta, \\ K &= J(\sin^2 \theta \dot{\phi} + R \cos \theta). \end{aligned} \tag{28}$$

Choosing the time origin when $\dot{\theta} = 0$, with $\theta = \theta_0$ and azimuthal speed $\dot{\phi}_0$, we can eliminate E and K :

$$\frac{1}{2}R\dot{\theta}^2 = (c_0 - c) \left\{ -\frac{R^3}{2s^2}(c_0 - c) + \frac{R^2 s_0^2}{s^2} \dot{\phi}_0 + \frac{R s_0^2}{2s^2}(c_0 + c) \dot{\phi}_0^2 + J \right\}, \tag{29}$$

where $c \equiv \cos \theta$, $c_0 \equiv \cos \theta_0$, $s \equiv \sin \theta$, $s_0 \equiv \sin \theta_0$.

This describes precession about the z axis (figure 1), with variable speed $\dot{\phi}$, accompanied by oscillations in θ (nutation) between limits θ_0 and θ_1 where $\dot{\theta} = 0$. Exactly this motion is familiar in the heavy symmetrical top (Arnold 1978) and indeed as we show in Appendix C one form of the equations of motion for the top is precisely (26).

In the adiabatic limit of large R , the amplitude of nutation vanishes. To see this, we find the extreme θ_1 (i.e. $\dot{\theta} = 0$) from the dominant terms in (29). Thus

$$\begin{aligned} \cos \theta_0 - \cos \theta_1 &\approx \frac{2 \sin^2 \theta_0 \dot{\phi}_0^2}{R} \quad \text{if} \quad \dot{\phi}_0 \neq 0, \\ &\approx \frac{2 \sin^2 \theta_0 J}{R^3} \quad \text{if} \quad \dot{\phi}_0 = 0. \end{aligned} \tag{30}$$

Both expressions vanish as $R \rightarrow \infty$ (the second because J is of order R – consistent with (13) for S constant), so that $\theta_1 \rightarrow \theta_0$. This shows the accuracy to which the adiabatic invariant $I = \mathbf{S} \cdot \mathbf{r} = \mathbf{J} \cdot \mathbf{r} = J \cos \theta$ is conserved.

Taking the motion to be pure precession round a circle of latitude, we find the angular velocity $\dot{\phi}$ from (26):

$$\dot{\phi} = [R^2 - \sqrt{(R^4 - 4JR \cos \theta)}] / 2R \cos \theta \rightarrow J/R^2 \quad \text{as} \quad R \rightarrow \infty. \tag{31}$$

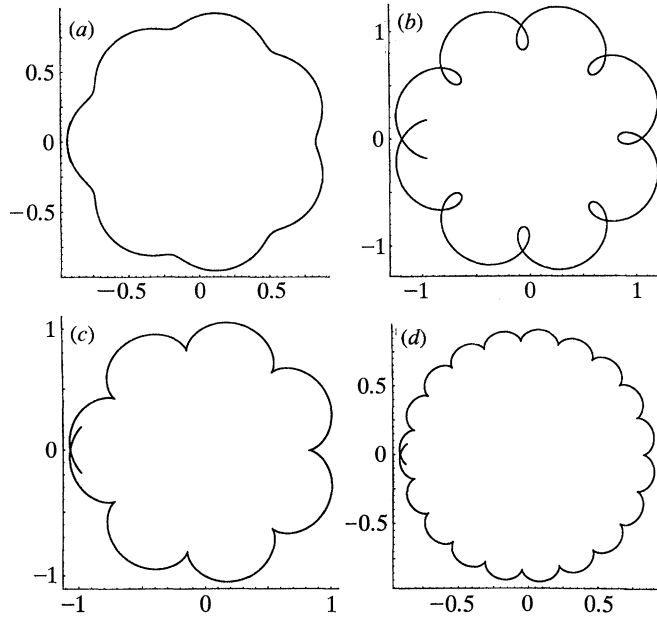


Figure 1. Stereographic (south pole) projection of the motion of the particle when confined to a sphere with radius R , calculated from (26) with (a)–(c): $R = 3, J = 3$; (d): $R = 4, J = 3$, for $\theta(0) = 45^\circ$ and different initial azimuthal velocities. (d) shows the decrease in the amplitude of nutation as R increases and the adiabatic régime is approached.

The speed of this adiabatic precession on the R sphere is

$$V = R \sin \theta \dot{\phi} = \frac{J \sin \theta}{R} = \frac{I \tan \theta}{R}. \tag{32}$$

(b) *Motion under magnetic gauge force*

In the adiabatic gauge model the equation of motion is (20), with the magnetic monopole force included and the two radial forces (Born–Oppenheimer and electric) omitted and replaced by the force constraining the particle to the sphere:

$$\dot{V} = -I(\mathbf{V} \wedge \mathbf{r})/R^2 - (V^2/R)\mathbf{r}. \tag{33}$$

In addition to R this conserves energy and a modified angular momentum incorporating the monopole field:

$$E = \frac{1}{2}V^2 = \text{const.}, \quad \mathbf{Q} \equiv \mathbf{R} \wedge \mathbf{V} + I\mathbf{r} = \text{const.} \tag{34}$$

These imply that $\mathbf{r} \cdot \mathbf{Q} = I$ is constant, so that the particle moves with constant speed in a circle with axis \mathbf{Q} . The angle made by \mathbf{r} with \mathbf{Q} is θ , where, from (34),

$$\tan \theta = |\mathbf{R} \wedge \mathbf{V}|/I = RV/I. \tag{35}$$

Comparing with (32), we see that the magnetic gauge field, from the monopole at $\mathbf{R} = 0$, describes precisely the steady mean precession of the particle on the sphere in the adiabatic limit when the amplitude of nutation is negligible.

Thus the precession from the magnetic gauge force describes the main global feature of the adiabatic dynamics. Note that ordinary Born–Oppenheimer theory, in which this force is omitted, fails completely because it predicts that the particle remains at rest on the sphere.

To see that the result (35) is not trivial, consider the case where the particle is released from rest at polar angle θ_0 . Then from (28) and (29) it follows that $E = K = JR \cos \theta_0$, and the motion is nutation in a series of loops (figure 1) between latitude circles θ_0 and θ_1 , given by

$$\cos \theta_1 = \frac{R^3}{4J} \left(1 - \sqrt{1 - 16 \left(\frac{J \cos \theta_0}{2R^3} - \frac{J^2}{R^6} \right)} \right) \approx \cos \theta_0 - (2J/R^3) \sin^2 \theta_0 \quad \text{for large } R \quad (36)$$

(cf. the second equation in (30)). In the adiabatic régime, the loops are tiny and roughly semicircular. ‘Microscopically’, the motion is far from steady, because the precession stops – that is, $\dot{\phi} = 0$ – every time θ returns to θ_0 . However, a short calculation, which we do not give, shows that (31) still gives the *average* rate of precession over a nutation cycle.

Returning to the analogy with the heavy symmetrical top (Appendix C) we arrive at an unexpected picture of its motion. The fast spin of the top can be regarded as adiabatically transported by the slow motion of the axis, which in turn is driven by the reaction of the spin, in the form of the magnetic force from a monopole centred on the point that is held fixed.

5. Electric force only

(a) Exact solution

Now we remove the constraint that kept R constant, and specialize the model of §2 differently, to eliminate the Born–Oppenheimer and magnetic forces in the adiabatic approximate equations of motion (20) and retain only the electric gauge force. This can be achieved by setting $I = 0$, which we do in a particular way that enables the motion to be solved exactly, namely by demanding that the conserved quantity \mathbf{J} defined by (11) vanishes. Thus $I = \mathbf{S} \cdot \mathbf{r} = \mathbf{J} \cdot \mathbf{r} = 0$, and the adiabatic invariant remains zero not only adiabatically but exactly. Thus from (12) the motion is determined by

$$\dot{\mathbf{V}} = \mathbf{R} \wedge \mathbf{V}. \quad (37)$$

This could describe the motion of a ‘spin’ \mathbf{V} , driven, as is \mathbf{S} , by the position \mathbf{R} , and coupled to it by $\dot{\mathbf{R}} = \mathbf{V}$, or, alternatively, a charged particle in the magnetic field of a uniform sphere of monopolum.

The shape of the orbits is determined by a single parameter. This is because five of the six quantities required to specify a solution of (37) can be eliminated: one by choosing the origin of time as the instant of closest approach; three by rigid rotation about $\mathbf{R} = 0$, possible because of the rotational invariance of (37); and one by the dilation law obeyed by (37), namely that if $\mathbf{R}(t)$ is a solution then so is $\alpha \mathbf{R}(\alpha t)$ for arbitrary α .

In solving (37) exactly, the first step is to note that the speed V is constant. Next, we use

$$\frac{1}{2} \partial_t^2 (R^2) = \frac{1}{2} \partial_t^2 (\mathbf{R} \cdot \mathbf{R}) = \partial_t (\mathbf{R} \cdot \mathbf{V}) = V^2 + \mathbf{R} \cdot \dot{\mathbf{V}} = V^2 = \text{const.} \quad (38)$$

so that the distance from the origin obeys the repulsion law

$$R^2(t) = V^2 t^2 + R_0^2. \quad (39)$$

Corresponding to the ‘spin’ \mathbf{V} is the ‘adiabatic invariant’ $\mathbf{r} \cdot \mathbf{V}$; unlike the analogous quantity I for the original spin \mathbf{S} , this is not constant, but from (38) and (39) varies as

$$\mathbf{r} \cdot \mathbf{V} = (\mathbf{R} \cdot \mathbf{V})/R = Vt/\sqrt{t^2 + R_0^2/V^2}. \quad (40)$$

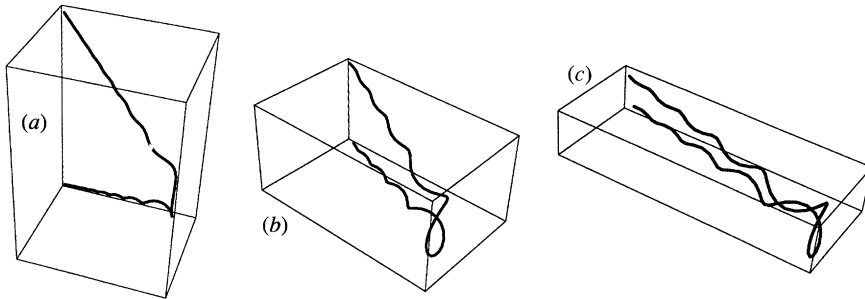


Figure 2. 'Antelope horns' obtained by solving (37) (which corresponds to $J = 0$) for the orbits $\mathbf{R}(t)$, with speed $V = 1$ and distances of closest approach (a): $R_0 = 1$; (b): $R_0 = 1.5$; (c): $R_0 = 2$.

This changes sign at $t = 0$ but has the asymptotically constant values $\pm V$, indicating that the orbits ultimately recede along straight lines.

Without loss of generality we can set $V = 1$, and regard R_0 as the single shape parameter. Adiabatic orbits are those with $R_0 \gg 1$.

With $V = 1$, time equals arc length along the orbit, the velocity \mathbf{V} is the unit tangent vector, and the determination of the orbit can be reduced to a problem in the differential geometry of space curves. The curvature κ of the curve (see e.g. Struik 1950) is the magnitude of the acceleration, which from (37)–(39) is

$$\kappa = \sqrt{(\dot{\mathbf{V}} \cdot \dot{\mathbf{V}})} = \sqrt{[(\mathbf{R} \wedge \mathbf{V}) \cdot (\mathbf{R} \wedge \mathbf{V})]} = \sqrt{[R^2 - (\mathbf{R} \cdot \mathbf{V})^2]} = R_0 = \text{const.} \quad (41)$$

The unit normal \mathbf{n} and binormal \mathbf{b} of the curve are the vectors

$$\mathbf{n} = \frac{\dot{\mathbf{V}}}{R_0} = \frac{\mathbf{R} \wedge \mathbf{V}}{R_0}, \quad \mathbf{b} = \mathbf{V} \wedge \mathbf{n} = \frac{\mathbf{V} \wedge (\mathbf{R} \wedge \mathbf{V})}{R_0} = \frac{\mathbf{R} - t\mathbf{V}}{R_0}. \quad (42)$$

The torsion is

$$\tau = -\dot{\mathbf{b}} \cdot \mathbf{n} = t\dot{\mathbf{V}} \cdot (\mathbf{R} \wedge \mathbf{V})/R_0^2 = t(R^2 - (\mathbf{R} \cdot \mathbf{V})^2)/R_0^2 = t. \quad (43)$$

Thus the orbit is a curve with constant curvature R_0 and changing torsion t . To get a preliminary idea of its shape, note that, for a helix uniformly wound on a cylinder, κ and t are given in terms of the radius a and pitch p (longitudinal distance between coils) by

$$\kappa = \frac{4\pi^2 a}{p^2 + 4\pi^2 a^2}, \quad \tau = \frac{2\pi p}{p^2 + 4\pi^2 a^2}. \quad (44)$$

Thus for large $|t|$, when the torsion can be regarded as locally constant, we expect the orbit to wind about its asymptotes in a coil with shrinking radius and pitch

$$a = \frac{R_0}{R_0^2 + t^2} \rightarrow \frac{R_0}{t^2}, \quad p = \frac{2\pi t}{R_0^2 + t^2} \rightarrow \frac{2\pi}{t}. \quad (45)$$

Since the torsion changes sign at $t = 0$, the negative- t and positive- t asymptotic windings have opposite senses.

Thus each orbit $\mathbf{R}(t)$ resembles a pair of curly antelope horns. Figure 2 shows some of these shapes, for different values of R_0 obtained by solving (37) numerically. It will also be convenient to study the track of the velocity \mathbf{V} on its unit sphere; this is a curve whose speed is the curvature R_0 of $\mathbf{R}(t)$, and whose curvature is the torsion t of $\mathbf{R}(t)$, and which therefore has the shape of a **S** coiling infinitely rapidly into asymptotic directions $\mathbf{V}(\pm \infty)$; figure 3 shows some of these shapes.

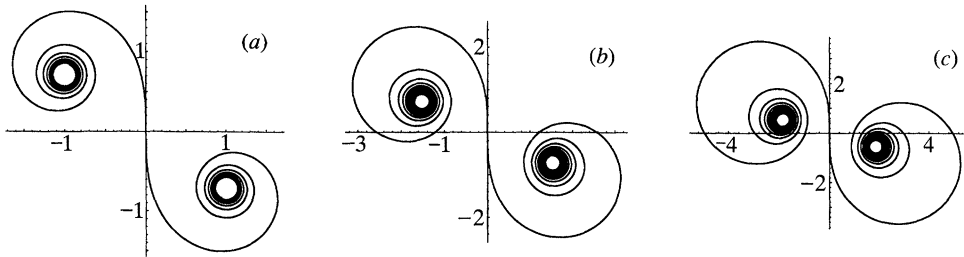


Figure 3. Stereographic (south pole) projection of the velocity V (unit tangent vector) corresponding to the orbits of figure 2.

To compare with adiabatic theory, we need to know the asymptotic opening angle $\theta(R_0)$ of the antelope horns, defined by

$$\cos\{\theta(R_0)\} = \mathbf{r}(-\infty) \cdot \mathbf{r}(+\infty) = -\mathbf{V}(-\infty) \cdot \mathbf{V}(+\infty). \tag{46}$$

Figure 3 indicates that the asymptotic directions $\mathbf{V}(\pm\infty)$ become mutually antipodal as R_0 increases. Since the angle between these directions is $\pi - \theta(R_0)$, we conclude that $\theta = 0$ in the adiabatic limit, so that the horns spiral out in the same direction as they spiralled in, but with opposite torsion. This is confirmed by figure 2. Now we will determine the geometry of the curve exactly from its κ and τ and find the angle $\theta(R_0)$ analytically.

In Appendix D we explain how the triad $\mathbf{V}, \mathbf{n}, \mathbf{b}$ is determined by the solution of a problem in quantum mechanics: the evolution of a complex 2-spinor, describing for example a spin- $\frac{1}{2}$ particle, driven by a ‘magnetic field’ whose x and z components are κ and $-\tau$. As a special case, the velocity in our problem is

$$\begin{aligned} \mathbf{V} &= \left\langle \boldsymbol{\psi} \left| \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right| \boldsymbol{\psi} \right\rangle \\ &= (|\psi_{x+}|^2 - |\psi_{x-}|^2, \quad |\psi_{y+}|^2 - |\psi_{y-}|^2, \quad |\psi_{z+}|^2 - |\psi_{z-}|^2), \end{aligned} \tag{47}$$

where $|\boldsymbol{\psi}\rangle$ denotes the 3-vector of 2-spinors

$$|\boldsymbol{\psi}\rangle \equiv \left\{ \begin{pmatrix} \psi_{x+} \\ \psi_{x-} \end{pmatrix}, \quad \begin{pmatrix} \psi_{y+} \\ \psi_{y-} \end{pmatrix}, \quad \begin{pmatrix} \psi_{z+} \\ \psi_{z-} \end{pmatrix} \right\} \tag{48}$$

each of whose components satisfy the Schrödinger equation

$$i|\dot{\psi}\rangle = \frac{1}{2} \begin{pmatrix} -t & R_0 \\ R_0 & t \end{pmatrix} |\psi\rangle \tag{49}$$

with initial conditions

$$|\psi_x(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\psi_y(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |\psi_z(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{50}$$

Equation (49) defines the Landau–Zener problem of quantum transition theory (Zener 1932). It can be exactly solved via the second-order equation that the components ψ_{\pm} satisfy separately, namely

$$\ddot{\psi}_{\pm} + \left(\frac{1}{4}t^2 + \frac{1}{4}R_0^2 \mp \frac{1}{2}i\right) \psi_{\pm} = 0. \tag{51}$$

These two equations are complex conjugates of each other. We express the $|\psi_j\rangle$ as linear combinations of the standard even and odd solutions y_1 and y_2 with initial conditions

$$y_1(0) = 1, \quad y_1'(0) = 0; \quad y_2(0) = 0, \quad y_2'(0) = 1. \tag{52}$$

In terms of these, (50) fixes the quantum states as

$$\psi_x = \frac{1}{\sqrt{2}} \begin{pmatrix} y_1^* - \frac{1}{2}iR_0 y_2^* \\ y_1 - \frac{1}{2}iR_0 y_2 \end{pmatrix}, \quad \psi_y = \frac{1}{\sqrt{2}} \begin{pmatrix} y_1^* + \frac{1}{2}R_0 y_2^* \\ iy_1 - \frac{1}{2}iR_0 y_2 \end{pmatrix}, \quad \psi_z = \begin{pmatrix} y_1^* \\ -\frac{1}{2}iR_0 y_2 \end{pmatrix}, \quad (53)$$

The velocity of the particle is now seen to be, from (47),

$$V = (R_0 \operatorname{Im} y_1 y_2^*, \quad R_0 \operatorname{Re} y_1 y_2^*, \quad |y_1|^2 - \frac{1}{4}R_0^2 |y_2|^2) \quad (54)$$

To determine the orbit $\mathbf{R}(t)$, integration of $V(t)$ is unnecessary, since from (42)

$$\mathbf{R}(t) = tV(t) + R_0 \mathbf{b}(t) \quad (55)$$

gives the orbit which from (D 12) has initial conditions

$$\mathbf{R}(0) = (-R_0, 0, 0), \quad V(0) = (0, 0, 1). \quad (56)$$

The solutions of (51) are parabolic cylinder functions, and the standard solutions can be expressed in terms of confluent hypergeometric (Kummer) functions. From §§ 19.2, 19.16 and ch. 13 of Abramowitz & Stegun (1964) we identify

$$\begin{aligned} y_1(t) &= \exp\{-\frac{1}{4}it^2\} M(\frac{1}{8}iR_0^2, \frac{1}{2}, \frac{1}{2}it^2), \\ y_2(t) &= t \exp\{-\frac{1}{4}it^2\} M(\frac{1}{8}iR_0^2 + \frac{1}{2}, \frac{3}{2}, \frac{1}{2}it^2). \end{aligned} \quad (57)$$

From the known asymptotic behaviour of these functions we obtain, for the dominant terms,

$$\left. \begin{aligned} y_1(t) &\rightarrow \sqrt{\pi} \frac{\exp\{-\frac{1}{16}\pi R_0^2\}}{\Gamma(\frac{1}{2} - \frac{1}{8}i\pi R_0^2)} \exp\{-\frac{1}{4}i[t^2 + \frac{1}{2}R_0^2 \ln(\frac{1}{2}t^2)]\}, \\ y_2(t) &\rightarrow \sqrt{(\frac{1}{2}\pi)} \frac{\exp\{-\frac{1}{16}\pi R_0^2\}}{\Gamma(1 - \frac{1}{8}i\pi R_0^2)} \exp\{-\frac{1}{4}i[t^2 + \frac{1}{2}R_0^2 \ln(\frac{1}{2}t^2) - \pi]\}, \end{aligned} \right\} \quad (58)$$

as $t \rightarrow +\infty$.

Thus (54) gives the asymptotic velocity

$$V \rightarrow \sqrt{[2 \sinh(\frac{1}{4}\pi R_0^2)]} \exp\{-\frac{1}{8}\pi R_0^2\} (-\sin \gamma, \cos \gamma, 0) + \exp\{-\frac{1}{4}\pi R_0^2\} (0, 0, 1) \quad \text{as } t \rightarrow +\infty \quad (59)$$

where

$$\left. \begin{aligned} \gamma &\equiv \arg \{ \Gamma(\frac{1}{2} - \frac{1}{8}i\pi R_0^2) \Gamma(1 + \frac{1}{8}i\pi R_0^2) \} + \frac{1}{4}\pi \\ &\approx \frac{1}{4}\pi \quad \text{if } R_0 \ll 1. \\ &\approx \frac{1}{2}\pi \quad \text{if } R_0 \gg 1. \end{aligned} \right\} \quad (60)$$

For $t \rightarrow -\infty$, V is given by (59) with the signs of the x and y components reversed. Thus from (46) we obtain the opening angle of the antelope horns as

$$\theta(R_0) = 2 \arcsin \exp\{-\frac{1}{4}\pi R_0^2\}. \quad (61)$$

In the adiabatic limit $R_0 \rightarrow \infty$ this vanishes, confirming our previous conclusion. From (59), the asymptotic direction of the horns in the xy plane makes an angle $\gamma + \frac{1}{2}\pi$ with the x axis, and from (60) this varies from $\frac{3}{4}\pi$ to π as R_0 varies from 0 to ∞ .

An equation resembling (37), but with \mathbf{R} replaced by the field of a monopole, has been obtained by Leinaas (1978) in a model where the spin of a moving particle is constrained to point radially. The orbits are conical spirals.

(b) Motion under electric gauge force

From this lengthy analysis of the exact solution of the model (9) with zero total angular momentum \mathbf{J} , we concluded that in the adiabatic limit the particle spirals in from infinity to a distance R_0 , and then spirals back out along the same direction. Averaged over oscillations, this motion becomes that of a ‘guiding centre’ that is purely radial, with the history of R changing according to the exact formula (39) with $V = 1$. Now we show that precisely this behaviour follows from the adiabatic equations of motion (20).

Since $\mathbf{J} = 0$ implies $I = 0$, (20) reduces to

$$\dot{V} = (S^2/R^3) \mathbf{r}, \quad (62)$$

where, from (11) and the initial conditions,

$$S = |\mathbf{R}(0) \wedge \mathbf{V}(0)| = R_0. \quad (63)$$

Equation (62) describes scattering. The shapes of orbits are determined by energy E and impact parameter b , which we identify from the asymptotic form of the exact orbits of (37). Since $V = 1$, $E = \frac{1}{2}$; and since the orbital angular momentum oscillates about zero ($\mathbf{S} = -\mathbf{R} \times \mathbf{V}$ precesses equatorially about \mathbf{R}), $b = 0$. The corresponding solution of (62) is

$$\mathbf{R}(t) = (-\sqrt{(R_0^2 + t^2)}, 0, 0). \quad (64)$$

This is identical with the exactly calculated radial behaviour (39).

Thus the repulsion from the electric gauge force describes the main global feature of the adiabatic dynamics. Note that ordinary Born–Oppenheimer theory, in which this force is omitted, fails completely because it predicts that the particle remains at rest or moves without acceleration.

6. Concluding remarks

Our main aim has been to show by exact calculation that in classical mechanics the gauge forces of reaction produce real effects. These forces are appealing because of the simple picture they give for the averaged slow motion, and the ease with which they reproduce features that are quite deeply buried in exact solutions (where these are available).

Woven into the exact analysis has been a tissue of spin analogies. In the basic model (9) there is the spin \mathbf{S} , driven by the coordinate \mathbf{R} . In the ‘electric’ special case (§5*a*), the velocity \mathbf{V} appears as a spin, again driven by \mathbf{R} . And in the determination of a curve from its curvature and torsion (Appendix D) each vector in the Frenet frame acts as a spin, driven by the Darboux vector $\boldsymbol{\Omega}$ (Equation (D5)); this is equivalent to the quantum spin states $|\psi_j\rangle$ being driven by the ‘magnetic field’ $\boldsymbol{\Omega}$.

We have deliberately restricted ourselves to exactly solvable special cases of the model (9). On the basis of some numerical exploration of the exact equation (12) governing the slow motion, we anticipate that in the general case there will be very complicated behaviour. For example, according to (20) the Born–Oppenheimer force is radial, and when acting alone (or in conjunction with the much smaller electric gauge force) would generate multiply periodic planar loops around the origin if the force is attractive (i.e. when the adiabatic invariant I is positive), and scattering if the force is repulsive (i.e. when $I < 0$). The effect of the magnetic gauge force is to cause these orbits to swerve out of the plane, and we have observed this (along

with superimposed small non-adiabatic oscillations from the reaction of the spin precession) in the numerical solution of (12). Over long times, the exact motion for 'attractive' initial conditions is observed to consist of non-planar loops with erratically varying radii and inclinations, probably indicating chaos (as also seen in a similar model by Bulgac & Kusnezov (1992)), with substantial changes in the adiabatic invariant near the closest approaches where the precession frequency R is smallest.

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Appendix A. Quantum origin of gauge forces

The evolution operator for the hamiltonian (1), describing the development of quantum states for a finite time t , can be decomposed into the product of infinitesimal operators:

$$U(t) = \exp\left\{-it\frac{H(\mathbf{R}, \mathbf{P}, z)}{\hbar}\right\} = \left[\exp\left\{-i\frac{t}{N}\frac{H(\mathbf{R}, \mathbf{P}, z)}{\hbar}\right\}\right]^N, \quad (\text{A } 1)$$

where N is large. Between each pair of factors we can insert the resolution of unity for the complete set of eigenstates $|n(\mathbf{R})\rangle$ in the fast subspace:

$$U(t) = \sum_{n_0} |n_0(\mathbf{R})\rangle \langle n_0(\mathbf{R})| \prod_{i=1}^N \left[\sum_{n_i} \exp\left\{-i\frac{t}{N}\frac{H(\mathbf{R}, \mathbf{P}, z)}{\hbar}\right\} |n_i(\mathbf{R})\rangle \langle n_i(\mathbf{R})| \right] \quad (\text{A } 2)$$

(of course \mathbf{R} is an operator in the full Hilbert space, but acts as a c-number in the fast subspace).

Now we make the adiabatic assumption that there are no transitions between fast states, so that all the sums can be replaced by the single term corresponding to the initial state, $|n\rangle$ say. Thus the effective evolution operator governing the slow motion becomes

$$\begin{aligned} U_g(t) &= [\langle n(\mathbf{R})| \exp\{-i(t/N)H(\mathbf{R}, \mathbf{P}, z)/\hbar\} |n(\mathbf{R})\rangle]^N \\ &= [\langle n(\mathbf{R})| 1 - i(t/N)H(\mathbf{R}, \mathbf{P}, z)/\hbar |n(\mathbf{R})\rangle]^N \\ &= \exp\{-it\langle n(\mathbf{R})|H(\mathbf{R}, \mathbf{P}, z)|n(\mathbf{R})\rangle/\hbar\} \\ &\equiv \exp\{-itH_g(\mathbf{R}, \mathbf{P})/\hbar\}, \end{aligned} \quad (\text{A } 3)$$

where
$$H_g(\mathbf{R}, \mathbf{P}) = \frac{1}{2}\langle n(\mathbf{R})| \Sigma \Sigma Q_{ij} P_i P_j |n(\mathbf{R})\rangle + E_n(\mathbf{R}). \quad (\text{A } 4)$$

Now the result (4) follows from a double application of

$$P_i |n(\mathbf{R})\rangle = -i\hbar\partial_i |n(\mathbf{R})\rangle + |n(\mathbf{R})\rangle P_i. \quad (\text{A } 5)$$

We do not claim that this argument is rigorous, but it has the merit of suggesting that the gauge forces are part of the lowest-order adiabatic approximation, in the sense that they are a consequence of the assumption that there are no transitions. A similar argument was given by Kuratsuji & Iida (1985), in a study of the effect of the magnetic gauge force on quantization; the electric force did not appear in their analysis.

Appendix B. Classical limit of the quantum gauge forces

Inserting the resolution of the identity into B_{ij} and Φ in (4), and using

$$\langle m|\partial_i n\rangle = \langle m|\partial_i h|n\rangle/(E_n - E_m) \quad (\text{B } 1)$$

(where here and hereafter we do not write the \mathbf{R} -dependences explicitly), we obtain the known formulae

$$\left. \begin{aligned} B_{ij}(\mathbf{R}) &= i\hbar \sum_{m \neq n} \frac{\langle m|\partial_i h|n\rangle \langle n|\partial_j h|m\rangle - \langle m|\partial_j h|n\rangle \langle n|\partial_i h|m\rangle}{(E_n - E_m)^2}, \\ g_{ij} &= \frac{1}{2}\hbar^2 \sum_{m \neq n} \frac{\langle m|\partial_i h|n\rangle \langle n|\partial_j h|m\rangle}{(E_n - E_m)^2}. \end{aligned} \right\} \quad (\text{B } 2)$$

Now we substitute

$$\frac{1}{E^2} = -\frac{1}{\hbar^2} \int_0^\infty dt \exp\left\{\pm i \frac{Et}{\hbar}\right\}. \quad (\text{B } 3)$$

and thereby express the gauge forces as integrals over time:

$$\left. \begin{aligned} B_{ij} &= -\frac{i}{2\hbar} \int_0^\infty dt \langle n | [(\partial_i h)_t, \partial_j h] - [(\partial_j h)_t, \partial_i h] | n \rangle, \\ g_{ij} &= -\frac{1}{2} \int_0^\infty dt \langle n | (\partial_i h - \partial_i E_n)_t (\partial_j h - \partial_j E_n) | n \rangle. \end{aligned} \right\} \quad (\text{B } 4)$$

Here

$$(\partial_i h)_t \equiv \exp\left\{\frac{i\hbar t}{\hbar}\right\} \partial_i h \exp\left\{-\frac{i\hbar t}{\hbar}\right\}. \quad (\text{B } 5)$$

denotes the time-evolved operator, and the diagonal terms in the m -sum, necessary to include in (B 2) to get (B 4), are zero.

Now we can take the classical limit directly from the correspondence principle: the expectation value is replaced by the phase-space average (7) over the classical invariant manifold (here the energy surface) corresponding to the state, and commutators by $i\hbar$ times the Poisson brackets. Thus we immediately obtain the classical formula for g_{ij} in (8); the formula for B_{ij} follows after substituting the identity (Robbins & Berry 1992)

$$\langle \{ (A)_t, B \} \rangle_E = \frac{1}{\partial_E \Omega} \partial_E (\partial_E \Omega \langle \partial_t (A)_t B \rangle_E) \quad (\text{B } 6)$$

and integrating by parts over t .

Appendix C. Analogy with heavy symmetrical top

Let the top have moments of inertia A, B, B about the point of support $\mathbf{R} = 0$, mass m , and axis determined by the unit vector \mathbf{r} , and let gravity $\mathbf{g} = -g\mathbf{e}_z$ act through the centre of mass at $\mathbf{R} = l\mathbf{r}$. Let the axis \mathbf{r} , whose motion we seek, have polar angles θ, ϕ , and let the third Euler angle, describing the spin about \mathbf{r} , be ψ . In an inertial frame (i.e. not in the usual body frame), the angular velocity $\boldsymbol{\Omega}$ and angular momentum \mathbf{L} are

$$\boldsymbol{\Omega} = (\dot{\psi} + \dot{\phi} \cos \theta) \mathbf{r} + \mathbf{r} \wedge \dot{\mathbf{r}}, \quad \mathbf{L} = A(\dot{\psi} + \dot{\phi} \cos \theta) \mathbf{r} + B\mathbf{r} \wedge \dot{\mathbf{r}}. \quad (\text{C } 1)$$

Gravitation determines the motion of \mathbf{L} through the torque

$$\dot{\mathbf{L}} = -mgl\mathbf{r} \wedge \mathbf{e}_z. \quad (\text{C } 2)$$

By symmetry, the components of \mathbf{L} along \mathbf{r} and \mathbf{e}_z are conserved:

$$\left. \begin{aligned} L_\psi &\equiv \mathbf{r} \cdot \mathbf{L} = A(\dot{\psi} + \dot{\phi} \cos \theta) = \text{const.}, \\ L_\phi &\equiv \mathbf{e}_z \cdot \mathbf{L} = L_\psi \mathbf{r} \cdot \mathbf{e}_z + Br \wedge \dot{\mathbf{r}} \cdot \mathbf{e}_z = \text{const.} \end{aligned} \right\} \quad (\text{C } 3)$$

Thus the equation of motion (C 2) becomes

$$L_\psi \dot{\mathbf{r}} + Br \wedge \ddot{\mathbf{r}} = -mgl\mathbf{r} \wedge \mathbf{e}_z, \quad (\text{C } 4)$$

or, since \mathbf{r} is a unit vector,

$$\ddot{\mathbf{r}} = (L_\psi/B) \mathbf{r} \wedge \dot{\mathbf{r}} - (mgl/B) (\mathbf{e}_z - \mathbf{e}_z \cdot \mathbf{r}\mathbf{r}) - |\dot{\mathbf{r}}|^2 \mathbf{r}. \quad (\text{C } 5)$$

Comparing this with (26) and recognizing that $\mathbf{V} = R\dot{\mathbf{r}}$, we see that the top equation is identical with that for the spinning particle constrained to a sphere, provided we make the identifications

$$R = L_\psi/B, \quad \mathbf{J} = (mglL_\psi/B^2) \mathbf{e}_z. \quad (\text{C } 6)$$

The conserved quantity K (equation (27)) is essentially the vertical component of angular momentum, since $K = JL_\phi/B$.

Therefore the adiabatic limit régime of large R corresponds to large L_ψ , that is the top spinning fast. A puzzling feature of this analogy is that there is in the top no obvious physically significant counterpart of the spin \mathbf{S} of the ‘particle’ whose position corresponds to its axis, namely

$$\mathbf{S} = \mathbf{J} - \mathbf{R} \wedge \mathbf{V} = (L_\psi/B^2) [mgl\mathbf{e}_z - L_\psi \mathbf{r} \wedge (\boldsymbol{\Omega} \wedge \mathbf{r})]. \quad (\text{C } 7)$$

Appendix D. Quantum spinor method for finding a curve from its curvature and torsion

That the shape of a space curve is determined by its curvature κ and torsion τ , given as functions of arc length, is the content of the fundamental theorem of differential geometry (Struik 1950). We employ the conventional notation \mathbf{t} , \mathbf{n} , \mathbf{b} for the orthogonal frame comprising the tangent, normal and binormal along the curve, which has arc length s . The curve $\mathbf{R}(s)$ is obtained by finding \mathbf{t} from the Frenet equations (Struik 1950)

$$\mathbf{t}' = \kappa \mathbf{n}, \quad \mathbf{n}' = -\kappa \mathbf{t} + \tau \mathbf{b}, \quad \mathbf{b}' = -\tau \mathbf{n} \quad (\text{D } 1)$$

and then integrating:

$$\mathbf{R}(s) = \int_0^s ds' \mathbf{t}(s'). \quad (\text{D } 2)$$

To solve the nine coupled equations (C 8) we first note that they can be written in the 3×3 matrix form

$$f'_{ij} = \epsilon_{ikl} \Omega_k f_{lj}, \quad (\text{D } 3)$$

where f_{ij} , specifying the frame, is

$$f_{ij} \equiv \begin{pmatrix} -\mathbf{b} \\ \mathbf{n} \\ \mathbf{t} \end{pmatrix} = \begin{pmatrix} -b_x & -b_y & -b_z \\ n_x & n_y & n_z \\ t_x & t_y & t_z \end{pmatrix} \quad (\text{D } 4)$$

and

$$\{\Omega_k\} = (\kappa, 0, -\tau) \equiv \boldsymbol{\Omega} \quad (\text{D } 5)$$

is the angular velocity of the frame (Darboux vector). Note that the indices j are passive in (D 3).

We claim that solutions of (D 3) have the form

$$f_{ij} = 2 \langle \psi_j | \sigma_i | \psi_j \rangle, \tag{D 6}$$

where σ_i denotes the three Pauli matrices

$$\sigma_i = \left\{ \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \equiv \boldsymbol{\sigma} \tag{D 7}$$

and the spinors

$$| \psi_j \rangle = \begin{pmatrix} \psi_{j+} \\ \psi_{j-} \end{pmatrix} \tag{D 8}$$

are any three solutions of the ‘Schrödinger equation’

$$i | \psi' \rangle = \boldsymbol{\Omega} \cdot \boldsymbol{\sigma} | \psi \rangle \tag{D 9}$$

in which the ‘Hamiltonian’ is

$$\boldsymbol{\Omega} \cdot \boldsymbol{\sigma} = \frac{1}{2} \begin{pmatrix} -\tau(s) & \kappa(s) \\ \kappa(s) & \tau(s) \end{pmatrix}. \tag{D 10}$$

To prove this assertion, we differentiate (D 6) and use, successively (D 9) and its conjugate, and the commutation relations for the Pauli matrices:

$$\begin{aligned} f'_{ij} &= 2(\langle \psi'_j | \sigma_i | \psi_j \rangle + \langle \psi_j | \sigma_i | \psi'_j \rangle) \\ &= 2i\Omega_k \langle \psi_j | [\sigma_k, \sigma_i] | \psi_j \rangle \\ &= -2\epsilon_{kij} \Omega_k \langle \psi_j | \sigma_j | \psi_j \rangle \\ &= -2\epsilon_{kij} \Omega_k f_{ij}. \end{aligned} \tag{D 11}$$

By antisymmetry, this is identical with (D 3), which is what we wanted to show.

A convenient choice of initial conditions is that $| \psi_i(0) \rangle$ is the eigenstate of σ_i with eigenvalue $+\frac{1}{2}$, i.e. (50). Then (D 6) fixes the orientation of the reconstructed curve (D 2) by the following initial orientation of the triad:

$$f_{ij}(0) = \delta_{ij}, \quad \text{i.e.} \quad \mathbf{t}(0) = (0, 0, 1), \quad \mathbf{n}(0) = (0, 1, 0), \quad \mathbf{b}(0) = (-1, 0, 0). \tag{D 12}$$

The foregoing argument is equivalent to the reduction of the Frenet equations, by Lie and Darboux (Struik 1950), to a single Riccati equation (this is satisfied by the logarithmic derivative of either component of any of the spinors $| \psi \rangle$).

An interesting duality, which follows from the symmetry of the Frenet equations (D 1), or the ‘hamiltonian’ (D 10), is that once the curve specified by κ and τ is found, the curve with *torsion* κ and *curvature* τ is given by integrating $\mathbf{b}(s)$ rather than $\mathbf{t}(s)$.

When κ and τ are slowly varying functions of s , the Schrödinger equation (D 9) can be solved by the adiabatic approximation. The resulting ‘adiabatic curves’ form a class of helices of which the asymptotic coils of the antelope horns, discussed in the paragraph following (43), are an example.

References

- Abramowitz, M. & Stegun, I. A. 1964 *Handbook of mathematical functions*. Washington, D.C.: National Bureau of Standards.
- Anandan, J. & Aharanov, Y. 1989 *Phys. Rev. Lett.* **38**, 1863–1870.
- Aharonov, Y. & Stern, A. 1992 *Phys. Rev. Lett.* **69**, 3593–3597.
- Arnold, V. I. 1978 *Mathematical methods of classical mechanics*. New York: Springer
- 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. 1985 *J. Phys. A* **18**, 15–27. (Reprinted in Shapere & Wilczek 1989.)
- Berry, M. V. 1986 Adiabatic phase shifts for neutrons and photons. In *Fundamental aspects of quantum theory* (ed. V. Gorini & A. Frigerio), NATO ASI series vol. 144, pp. 267–278. Plenum.
- Berry, M. V. 1989 The quantum phase, five years after. In Shapere & Wilczek 1989, pp. 7–28.
- Bulgac, A. & Kusnezov, D. 1992 *Nucl. Phys. A (Netherlands)* **545**, 549c–560.
- Delacrétaz, G., Grant, E. R., Whetten, R. L., Wöste, L. & Zwanziger, J. W. 1986 *Phys. Rev. Lett.* **56**, 2598–2601. (Reprinted in Shapere & Wilczek 1989.)
- Gozzi, E. & Thacker, W. D. 1987 *Phys. Rev. D* **35**, 2398–2406.
- Jackiw, R. 1988 *Commun. at. molec. Phys.* **21**, 71–82.
- Hannay, J. H. 1985 *J. Phys. A* **18**, 221–230. (Reprinted in Shapere & Wilczek 1989.)
- Kuratsuji, H. & Iida, S. 1985 *Phys. Lett. A* **111**, 220–222.
- Leinaas, J. M. 1978 *Physica Scripta* **17**, 483–486.
- Lochack, P. & Meunier, C. 1988 *Multiphase averaging for classical systems*. New York: Springer.
- Longuet-Higgins, H. C., Öpik, U., Pryce, M. H. L. & Sack, R. A. 1959 *Proc. R. Soc. Lond. A* **244**, 1–16.
- 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.
- Provost, J. P. & Vallée, G. 1980 *Commun. math. Phys.* **76**, 289–301.
- Robbins, J. M. & Berry, M. V. 1992 *Proc. R. Soc. Lond. A* **436**, 631–661.
- Shapere, A. & Wilczek, F. (eds) 1989 *Geometric phases in physics*. Singapore: World Scientific.
- Stone, M. 1986 *Phys. Rev. D* **33**, 1191–1194. (Reprinted in Shapere & Wilczek 1989.)
- Struik, D. J. 1950 *Lectures on classical differential geometry*. Reading, MA: Addison-Wesley.
- Weigert, S. & Littlejohn, R. G. 1992 *Phys. Rev. A*. (Submitted.)
- Zener, C. 1932 *Proc. R. Soc. Lond. A* **137**, 696–702.

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