

QUANTUM, CLASSICAL AND SEMICLASSICAL ADIABATICITY

M.V. Berry

H.H. Wills Physics Laboratory, Tyndall Avenue
 Bristol BS8 1TL, U.K.

Adiabatic theorems are reviewed, and an asymptotic connection established between quantum and classical anholonomy properties of systems whose Hamiltonians contain parameters that are slowly varied round a cycle. The quantum property is a geometrical phase accompanying transport of an eigenstate round the cycle; the classical property is a shift in phase-space torus angle variables. Examples are given. Starting from the geometrical phase, different classes of quantum system are seen to have different degeneracy properties. Sometimes, quantum tunnelling causes discordance between the adiabatic and semiclassical limits; for these cases a uniform semiclassical adiabatic approximation can be found, encompassing both limits.

INTRODUCTION

Consider a dissipationless mechanical system with N freedoms executing bound motion under the action of forces that may be time-dependent. The evolution is governed by a Hamiltonian $H(q, p; X(t))$, where $q \equiv \{q_1, \dots, q_N\}$ and $p \equiv \{p_1, \dots, p_N\}$ are the coordinates and conjugate momenta [1, 2] and $X(t) \equiv \{X_1(t), X_2(t), \dots\}$ are parameters controlling the forces. If the system is classical, q and p are ordinary variables; if it is quantum-mechanical, q and p are operators with the commutation law [3]

$$[q_i, p_j] = i\hbar \delta_{ij} \quad (1)$$

where \hbar is Planck's constant, leading to a Hermitian Hamiltonian operator H (after applying factor ordering conventions if necessary). This framework is very general and encompasses not only quantum and classical mechanics but also physical and geometrical optics and linear theories of acoustic, elastic and water waves and their ray approximations. Those less familiar with quantum mechanics might prefer to think in terms of wavevector k and frequency Ω , related to p and H by

$$\left. \begin{aligned} k &= p/\hbar \quad (\text{de Broglie relation}) \\ \Omega(q, k; X(t)) &= \frac{1}{\hbar} H(q, p; X(t)) \quad (\text{dispersion relation}) \end{aligned} \right\} \quad (2)$$

with wave equations constructed by regarding q as an ordinary variable and k as the operator $-i\partial/\partial q$ (a choice which satisfies (1)).

The asymptotics of two limiting situations is particularly interes-

ting and important. First, there is the semiclassical limit $\hbar \rightarrow 0$, corresponding (cf. (2)) to high frequency $\bar{\Omega}$ or short wavelength $2\pi/k$. Second, there is the adiabatic limit $dX/dt \rightarrow 0$, corresponding to slow change of the parameters. These limits can be very subtle and complicated because quantities often turn out to depend nonanalytically on \hbar and dX/dt . My purpose here is to give an informal account of the two limits and describe how they may be sometimes concordant, sometimes discordant.

ADIABATIC THEOREMS

For physicists, adiabatic theory began around 1910, with the embryonic quantum mechanics inspiring a result in classical mechanics: for a one-dimensional harmonic oscillator (e.g. a pendulum) whose frequency ω (now considered as the parameter X) is slowly changed (e.g. by altering the length of the string), what is conserved is not the energy E but the ratio E/ω . The argument was that for fixed ω the energies are restricted by quantum mechanics to values we would now write as

$$E_n = (n + \frac{1}{2})\hbar\omega \quad (n=1, 2, \dots), \quad (3)$$

and n , being integer, cannot vary continuously, so as ω is changed E_n must change proportionately, thus conserving E_n/ω which ought to be conserved classically too because it does not involve \hbar . Thus a classical adiabatic invariant (E/ω) has been derived from an (implied) quantal adiabatic theorem (persistence of state labelled n) via an (implied) semiclassical connection (the quantum state n is associated with the classical motion whose energy is E_n). In the succeeding years these ingredients of the adiabatic argument were made more precise and generalized as follows.

The quantal adiabatic theorem [4] concerns states $|\Psi(t)\rangle$ satisfying the time-dependent Schrödinger equation

$$H(q,p;X(t))|\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle, \quad (4)$$

and asserts that in the adiabatic limit of infinitely slow variation of the parameters $X(t)$ there are states, labelled $|\Psi_n(t)\rangle$, which cling to the eigenstates $|n;X\rangle$ of the instantaneous Hamiltonians. These eigenstates, and their energies $E_n(X)$, are defined by

$$H(q,p;X)|n;X\rangle = E_n(X)|n;X\rangle, \quad (5)$$

and the adiabatic assertion is

$$|\Psi_n(t)\rangle = e^{i\phi_n(t)}|n;X(t)\rangle, \quad (6)$$

where $\phi_n(t)$ are phases to be discussed in the next section. Non-adiabatic behaviour, measured in terms of the amplitudes for transitions to states other than n , can be extremely small (of order $\exp\{-|dX/dt|^{-1}\}$) if X varies analytically with t [5,6], even if the total change in the X is large.

The classical adiabatic theorem [1,2,7] does not have the generality of the quantal theorem, because it is restricted to Hamiltonians which for constant X support quasiperiodic motion, that is motion where orbits explore N -dimensional tori in the $2N$ -dimensional phase space of the variables q,p . Such tori fill phase space when $N=1$ and also when $N>1$ for integrable systems, that is systems with

N constants of motion. Generically, however, phase space has some regions where motion is chaotic [2,8,9] and orbits explore regions of dimensionality greater than N which in the extreme case of ergodicity consist of the entire energy surface $H=\text{constant}$, whose dimensionality is $2N-1$. For nonchaotic motion, then, the theorem asserts that for slow variations of X the orbit clings to that torus which preserves the values of the N actions $I=\{I_1 \dots I_N\}$. These quantities, which are thus the adiabatic invariants, are defined as the line integrals

$$I_j \equiv \frac{1}{2\pi} \oint_{\Gamma_j} p_i(q;X) dq_i \tag{7}$$

around the irreducible cycles Γ_j of the torus. The succession of tori thus selected will, in general, have different energies whose instantaneous values are given by the Hamiltonian in 'action' representation, namely

$$E_I(t) = H(I;X(t)) . \tag{8}$$

For $N>1$, application of the adiabatic theorem to nonintegrable systems depends on the continuing existence of the torus with actions I during the variation of the parameters X. Generically, however, the torus will be repeatedly disrupted near resonance zones where the ratios of its frequencies

$$\omega = \{\omega_j(X) \equiv \frac{\partial H(I;X)}{\partial I_j}\} \tag{9}$$

are close to rational. Nevertheless, there are some nontrivial cases where a torus can remain nonresonant - for example when an external force field is rigidly rotated or translated.

The semiclassical connection that the two adiabatic theorems strongly suggest, and which is confirmed by asymptotic analysis [10,11], is an association, valid as $\hbar \rightarrow 0$, between the quantum state labelled by quantum numbers $n \equiv \{n_1 \dots n_N\}$ and the classical torus with actions I. The association is

$$I_j(n) = (n_j + \alpha_j) \hbar \tag{10}$$

where the indices α_j depend on how the torus is embedded in phase space [2,10]. The energy of the asymptotic state $|n;X\rangle$ is then given by

$$E_n(X) = H(I(n);X) . \tag{11}$$

Preservation of the association between $|n\rangle$ and the torus I as X varies is guaranteed by the two adiabatic theorems. Although (11) does generalize the quantum-mechanical WKB approximation, it is of course restricted to systems whose classical motion lies on tori. For these systems, however, the method is very useful in practice for calculating energy eigenvalues, especially in quantum chemistry [12-18].

For classically chaotic motion, there seem to be no adiabatic invariants (except for systems very close to integrable ones [51]) and no asymptotic semiclassical relation giving (for example) the energies of the quantum states, except for the limiting case of ergodic motion. In this case [19] there is a single adiabatic invariant,

namely the phase-space volume within the energy surface, defined by

$$\text{Vol}(E) \equiv \int d^N q \int d^N p \theta(E - H(q, p; X)) \quad (12)$$

where θ denotes the unit step function. Thus, when X varies slowly, the energy changes in accordance with

$$\text{Vol}(E(X(t))) = \text{Vol}(E(X(0))). \quad (13)$$

This suggests that for classically ergodic systems the quantum states are labelled by a single quantum number n in terms of which the energy levels are given asymptotically by

$$\text{Vol}(E_n) = (2\pi\hbar)^N (n + \frac{1}{2}). \quad (14)$$

As an expression of the old idea [11] that one quantum state 'occupies' a volume $(2\pi\hbar)^N$ of classical phase space, this approximation (augmented by asymptotic correction terms) gives surprisingly good agreement with the trend of exact quantal energy curves $E_n(X)$ for a range of parameters X (see fig.5 of ref [20]). (Superimposed on this trend are small-scale fluctuations whose statistics seem to be universal [21,22,40], and also larger-scale fluctuations connected with classical closed orbits [11,23,24,50].)

ADIABATIC ANHOLONOMY

For each of the two adiabatic theorems just described, a question is left unanswered. In the quantum case, the question is: what is the phase ϕ_n (eq.6) associated with the adiabatic convection of the eigenstate $|n\rangle$? In the classical case, the question is: how do the angle variables $\theta \equiv \{\theta_1, \dots, \theta_N\}$ (conjugate to the actions, and describing positions on the N tori [2,8]) evolve as the orbit clings adiabatically to the torus I ? Because of the arbitrariness in the definition of the phase of the eigenstate $|n\rangle$ and of the origin with respect to which angles are measured on each torus I , these questions only have invariant meaning if the parameter variation consists of a circuit C in the space X . We imagine this circuit to be traversed over a (long) time T , after which $X(T) = X(0)$, the Hamiltonian has returned to its original form, the state $|\Psi_n(t)\rangle$ returns to the original eigenstate $|n(0)\rangle$ (up to a phase) and the classical orbit returns to the same torus I .

When thus posed, the two questions have immediate naive answers, both wrong. In the quantal case, the naive answer is that the phase change between $t=0$ and $t=T$ is the 'dynamical' increase of the phase associated with the instantaneous eigenstate, namely

$$\frac{1}{\hbar} \int_0^T dt E_n(X(t)). \quad (15)$$

The correct answer [25] is that the states before and after the circuit are related by

$$|\Psi_n(T)\rangle = \exp\left\{\frac{i}{\hbar} \int_0^T dt E_n(X(t)) + i\gamma_n(C)\right\} |\Psi_n(0)\rangle \quad (16)$$

where $\gamma_n(C)$ is a geometrical phase depending, in a manner soon to be explained, on the circuit C in parameter space and the transported state $|n\rangle$, but not on the time T taken to traverse C . Thus $\gamma_n(C)$ is small in comparison with the dynamical phase but does not vanish in

the adiabatic limit. In the classical case, the naive answer is that the increments in the angles θ are given by

$$\int_0^T dt \omega(X(t)) \tag{17}$$

where $\omega(X)$ are the frequencies (9) with which the orbit whirls around the cycles Γ of the instantaneous I-torus at the parameter-space point X . The correct answer [26,27] is that the angles before and after the circuit are related by

$$\theta(T) = \theta(0) + \int_0^T dt \omega(X(t)) + \Delta\theta(I;C), \tag{18}$$

where $\Delta\theta(I;C) \equiv \{\Delta\theta_i\}$ are classical adiabatic angles depending only on the circuit C and the action I of the torus being transported, but not on T .

Each of the quantities $\gamma_n(C)$ and $\Delta\theta(I;C)$ is naturally expressed as an integral in parameter space, over any surface A spanning C , that is: as the flux of a 2-form through C . Quantally, it can be shown [25] by analysis of the time-dependent Schrödinger equation (4) that

$$\gamma_n(C) = - \int_{\partial A=C} V(N;X) \tag{19}$$

where the phase 2-form V is

$$V(n;X) = \text{Im} \langle dn | \wedge | dn \rangle \tag{20}$$

and d refers to displacement (of the state $|n;X\rangle$) in parameter space. Classically, it can be shown [26,27] by analysis of Hamilton's equations that

$$\Delta\theta(I;C) = - \frac{\partial}{\partial I} \int_{\partial A=C} W(I;X) \tag{21}$$

where the angle 2-form is given in terms of

$$W(I;X) = \frac{1}{(2\pi)^N} \oint d^N\theta \, dp \wedge dq, \tag{22}$$

and the integral is of parameter-space-displacements of the p 's and q 's, and over the I-torus at X .

Both γ_n [28] and $\Delta\theta$ can be regarded as exemplifying anholonomy, that is closure failure under parallel transport, and the two-forms correspond to curvatures (analogous to those of spacetime in general relativity [29]). What turns mathematical connection phenomena into potentially observable physical phenomena is the fact that the Schrödinger and Hamilton equations induce precisely those connections which are mathematically natural.

The geometrical phase $\gamma_n(C)$ is a completely general feature of quantum mechanics. Its applicability is not restricted to the semiclassical limit or even to systems with classical analogues. But when $|n\rangle$ does have a classical analogue which moreover corresponds to quasiperiodic motion, the phase 2-form V , given by (20), can be shown [27] to be semiclassically related to the 2-form W , given by (22), by

$$V(n;X) = -\frac{1}{\hbar} W(I;X) \quad (23)$$

so that the classical adiabatic angles are given by

$$\Delta\theta_j(I;C) = -\hbar \frac{\partial \gamma_n}{\partial I_j}(C) = -\frac{\partial \gamma_n}{\partial n_j}(C) \quad (24)$$

where the association (10) enables the quantum numbers n to be treated as continuous variables.

Now we make two remarks which help in interpreting and evaluating the quantal formulae (19) and (20). Firstly, if there are three parameters, these can be regarded as components of a vector \tilde{X} , d becomes the gradient ∇ in \tilde{X} space, and \wedge becomes the cross product of ordinary vector analysis. If in addition the state $|n;X\rangle$ is expressed in position representation in terms of the wavefunction $\psi_n(q;\tilde{X}) \equiv \langle q|n;X\rangle$, then the geometrical phase can be written as

$$\gamma_n(C) = -\text{Im} \int_{\partial A=C} d^N q \int \tilde{A} \cdot \nabla \psi_n^*(q;\tilde{X}) \wedge \nabla \psi(q;\tilde{X}). \quad (25)$$

Secondly, if the Hamiltonian operator can be represented (non-classically) as a 2×2 Hermitian matrix, written in the general form

$$H(X) = \frac{1}{2} \begin{pmatrix} w(X) & u(X) - iv(X) \\ u(X) + iv(X) & -w(X) \end{pmatrix} \quad (26)$$

then the phase 2-form for the upper and lower eigenstates $|\pm\rangle$ can be calculated to be

$$V_{\pm} = \mp \frac{u \, dv \wedge dw + v \, dw \wedge du + w \, du \wedge dv}{2(u^2 + v^2 + w^2)^{3/2}}. \quad (27)$$

Physically, $\gamma_n(C)$ could be observed by the interference produced when the state that has been transported round C is superposed with a state which has evolved under a constant Hamiltonian (fixed X). A feasible realization of this idea employs a beam of polarized nuclei in a spin- n eigenstate of an external magnetic field B . The beam is split into two beams, one of which passes through a region of constant B while the other passes through a region where the vector B is taken round a cycle C (in magnetic field space which is the X space in this case); then the cycled beam can be shown [25] to have acquired a phase $\gamma_n(C) = n\Omega(C)$, where $\Omega(C)$ is the solid angle subtended by C at $\underline{B}=0^n$, and this phase difference can be revealed as a fringe shift when the two beams are recombined.

The phase anholonomy embodied in $\gamma_n(C)$ is not confined to quantum mechanics but can be expected whenever Hermitian matrices arise in physics. One such area is the optics of anisotropic media [30], where the two polarization states of electromagnetic waves which propagate unchanged with wavevector \underline{k} are the eigenvectors of the 2×2 transverse part of the inverse of the dielectric tensor. If the medium is both uniaxially birefringent and gyrotropic (i.e. the plane of polarization rotates) with both optic axes coinciding, and this common axis is made to turn once in a cone of semiangle θ about \underline{k} , then [31] the two eigenpolarizations experience a phase shift

$$\gamma_{\pm}(\theta) = \pm 2\pi \left(1 - \frac{\sigma \cos \theta}{(\sin^4 \theta + \sigma^2 \cos^2 \theta)^{1/2}} \right) \quad (28)$$

where σ is a constant involving the ratio of the strengths of the gyrotropy and birefringence. One way to produce this effect would be to employ a liquid with an external magnetic field (giving rise to gyrotropy via the Faraday effect) and, in the same direction, an electric field (giving rise to birefringence via the Kerr effect).

As an example of the classical anholonomy embodied in $\Delta\theta$, consider a particle sliding freely with speed v round a noncircular planar hoop with area A and perimeter L . Now let the hoop be slowly rotated in its own plane and in the same sense as the particle so that it makes a complete turn in time T . The distance it has travelled round the hoop is not vT but $vT + \Delta s$, where [26,27]

$$\Delta s = \frac{L\Delta\theta}{2\pi} = -L + L\left(1 - \frac{4\pi A}{L^2}\right). \tag{29}$$

The first term is the expected slippage through one turn; the second term is the anholonomy effect, and is always positive by the isoperimetric inequality. This is related to the Sagnac effect [32] which is the basis of the navigationally important ring gyroscopes [33].

DEGENERACY

Let us study the phase 2-form $V(n;X)$ more closely, by enquiring where it can have singularities. For this purpose a form more transparent than (20) is the sum [25]

$$V(n;X) = \text{Im} \sum_{m \neq n} \frac{\langle n | dH | m \rangle \wedge \langle m | dH | n \rangle}{[E_m(X) - E_n(X)]^2} \tag{30}$$

over all states $|m\rangle$ other than that being transported. The denominators indicate that V has singularities at those parameter values X^* where $|n\rangle$ is degenerate with the state immediately above or below it in energy, and large phase changes $\gamma_n(C)$ can be expected for circuits near X^* .

In the neighbourhood of X^* , only the state $|m\rangle = |n+1\rangle$ or $|n-1\rangle$ with which $|n\rangle$ degenerates contributes (in the simplest case of an eigenvalue with multiplicity two at X^*) to the sum (30). Thus $H(X)$ can be represented by a 2×2 matrix, for which a convenient normal form, involving three parameters $\tilde{X} = (X, Y, Z)$, is

$$H(\tilde{X}) = \frac{1}{2} \begin{pmatrix} Z & X - iY \\ X + iY & -Z \end{pmatrix}, \tag{31}$$

where the degeneracy X^* has been chosen as origin. The two eigenvalues are

$$E_{\pm}(\tilde{X}) = \pm \frac{1}{2} (X^2 + Y^2 + Z^2)^{\frac{1}{2}}. \tag{32}$$

This shows that the degeneracy is isolated at X^* , illustrating the old result [34] that for families of Hermitian matrices without symmetry degeneracies have codimension 3.

By comparing (31) and (26), the result (27) can be used to show that near \tilde{X}^* the phase 2-form is

$$\tilde{V}(\pm; \tilde{X}) = \pm \frac{X}{2} (X^2 + Y^2 + Z^2)^{3/2} \tag{33}$$

so the singularity is that of a monopole with strength $\pm\frac{1}{2}$. This leads to the result that with the normal coordinates as in (31) the geometrical phase is

$$\gamma_{\pm}(C) = \mp \Omega(C)/2 \quad (34)$$

where $\Omega(C)$ is the solid angle subtended by C at X^* .

Now let us concentrate on the important special case where H is real symmetric instead of Hermitian; this includes for example all of wave theory and quantum mechanics in the absence of external influences which are chiral or not invariant under time-reversal. In (31) this corresponds to restriction to the parameter plane $Y=0$, and (32) now illustrates the known result [34,2] that for families of real symmetric matrices degeneracies are of codimension 2.

A circuit enclosing such a degeneracy subtends the solid angle of a hemisphere, namely 2π , so (34) predicts $\gamma=\pm\pi$, implying eigenvectors of a real symmetric matrix will change sign when transported around a degeneracy. This has long been known in a special case: the index is $\pm 1/2$ for generic singularities of tensor fields such as disclinations in liquid crystals [35] (around which molecules reverse) and umbilic points on surfaces [36] (around which lines of curvature reverse). In quantum mechanics it arises in the theory of molecular spectra, in the approximation where the coordinates of nuclei can be considered as parameters on which the states of electrons depend [37-39]. The sign change has been seen in computations [20] of the spectra of families of vibrating membranes whose boundaries are triangular (with the two independent angles taken as the parameters X).

Equation (32) shows that in E, X space the connection between surfaces $E=E_n(X)$ and $E=E_{n+1}(X)$ at a degeneracy X^* has the form of a double cone (in the real symmetric case) or hypercone (in the Hermitian case); this association between diabolos and degeneracies suggests the term diabolical point [20] to describe the connection. Diabolical points are degeneracies occurring in generic cases, that is without symmetry, and are therefore what physicists have called 'accidental'. But, as with traffic accidents, an event that is accidental for an individual (i.e. a degeneracy between levels of a given Hamiltonian) becomes almost inevitable when a population is considered (i.e. two- or three-parameter families of Hamiltonians). Variation of a single parameter will not, in these generic cases, produce degeneracies, because a line in parameter space will miss the diabolical points; of course, close encounters with diabolical points may occur, causing the curves of E_n versus parameter to show hyperbolic avoided crossings. The existence of these avoided crossings in one-parameter families of spectra has now been established by calculations for a variety of quantal systems [41-44,20], whose classical counterparts have varying degrees of chaos but share the feature of nonintegrability.

This leads to the conjecture that those families of quantal systems with the generic property that their spectra display diabolical points will have classical limits whose motion is nonintegrable. Such behaviour differs strikingly from that of separable systems, or integrable systems whose levels are approximated by the torus quantization formula (11): in these cases, when $N>1$, degeneracies occur when a single parameter is varied (because, from (11), levels correspond to intersection of constant-energy surfaces with points n in the N -dimensional lattice of quantum numbers, and variation of a

parameter will cause the surface through a given n to turn and repeatedly intersect additional points).

In the semiclassical limit, energy levels are very close together and it becomes meaningful to speak of the statistics of the levels near a given energy E and set of parameters X , with X regarded as parameterising an ensemble of spectra. A useful statistic is the probability distribution $P(S)$ of the spacings between neighbouring levels E_{n+1} and E_n ; it is convenient to measure S in terms of the average level spacing, which is of order \hbar^N [24]. A simple geometrical argument [11,40,41] shows that the different codimensions $K=3,2,1$ of degeneracies of families of generic Hermitian, generic real symmetric, and torus-quantized Hamiltonians imply different behaviour of $P(S)$ in the limit $S \rightarrow 0$ of small spacings (which is determined by behaviour close to degeneracies):

$$P(S) \propto S^{K-1} \text{ as } S \rightarrow 0. \tag{35}$$

For the nonintegrable cases ($K=3$ or $K=2$), $P(S)$ is therefore predicted to vanish as $S \rightarrow 0$. This phenomenon, called level repulsion, has been observed in many calculations [20,41,44] for $K=2$ but to my knowledge no such calculations have been performed for the Hermitian case $K=3$. For separable systems, or integrable systems with torus quantization, $K=1$ and $P(S)$ is predicted to have a finite limit as $S \rightarrow 1$, indicating level clustering; a detailed study [45] of (11) shows that in fact $P(S) = \exp(-S)$ for generic integrable Hamiltonians $H(I)$, and computational tests abundantly confirm this result. Therefore classically integrable and nonintegrable systems can show striking differences in the fine structures of their quantal spectra.

QUANTUM AND CLASSICAL ADIABATIC DISCORDANCE [46]

Sometimes, the semiclassical and adiabatic limits can come into conflict in the sense that they lead to opposite predictions for the evolution of a system, rather than being complementary as in the examples given so far. Such discordance can arise when there are regions of phase space that are classically separated but which may be quantally connected by tunnelling.

The simplest case in which this occurs is the one-dimensional Hamiltonian

$$H(q,p;X) = \frac{p^2}{2m} + V(q;X), \tag{36}$$

describing a particle of mass m moving along the q axis in a potential V consisting of two potential wells separated by a barrier. As the single parameter X increases, the left-hand well (L) gets shallower and the right-hand well (R) gets deeper.

Attention will be restricted to energies below the barrier top. Then classical orbits must always be confined to L or R, which correspond to disconnected sets of loops (tori) in the phase plane q,p . For fixed X , the simplest semiclassical theory, based on (11), predicts that the quantum energy eigenstates are similarly localized in L or R. And indeed for most values of X the exact eigenstates are indeed localized (with accuracy $\exp\{-1/\hbar\}$) in L or R. But close to 'semiclassical degeneracies', i.e. when X is such that an approximate eigenstate in L has energy differing from that of an approximate eigenstate in R by an amount of order $\exp\{-1/\hbar\}$ (small in comparison with the mean spacing which is of order \hbar) then simple semiclassical

theory breaks down [47] and the eigenstates are shared by both wells (the extreme case is the symmetric double-well (L and R identical), for which the true states are, to a close approximation, even and odd superpositions of the simple semiclassical single-well states). As X varies, the energy level curves $E_n(X)$ do not cross as (11) would predict, but are smooth curves with exponentially small splittings instead of degeneracies; as X varies across a semiclassical degeneracy, the state corresponding to $E_n(X)$ transfers from one well to the other. All this is well known.

The adiabatic-semiclassical discordance arises as follows. Suppose H is made time-dependent by slowly increasing X across a semiclassical degeneracy at X^* , starting at t_i and ending at t_f , and semiclassical conditions prevail so that the wells are deep (i.e. supporting many states) and the barrier high (i.e. with exponentially small penetration). If the initial quantum state (at t_i) is chosen to be an eigenstate localized in L, what is the state at t_f ? Because $dX(t)/dt$ and \hbar are small, it is natural to attempt predictions using adiabatic and semiclassical theory. Because classical particles remain in L throughout the change, the semiclassical theory leads to the expectation that at t_f the system will again be in an L-localized eigenstate. But because the exact quantum state which is initially localized in L transfers smoothly (albeit rapidly) to R as X passes X^* , the quantum adiabatic theorem leads to the expectation that the system will cling to this eigenstate and so be localized in R at t_f .

To resolve this paradox it is necessary to make a detailed study [46] of the evolution as determined by the time-dependent Schrödinger equation, which governs the probability amplitudes $a_L(t), a_R(t)$ for finding the system in L, R, the initial condition being

$$a_L(t_i) = 1; \quad a_R(t_i) = 0 \quad (37)$$

(of course $|a_L(t)|^2 + |a_R(t)|^2 = 1$ for all t). The aim is to find $|a_L(t_f)|^2$, which is the probability of finding the system in L after passage through the semiclassical degeneracy.

The result is a uniform asymptotic formula for $|a_L(t_f)|^2$, involving a single quantity Q , incorporating both the semiclassical and adiabatic limits. Semiclassical smallness is governed by the energy splitting Δ of the quantum states at the semiclassical degeneracy, given by standard WKB theory [47] as

$$\Delta = \frac{\hbar}{\pi} (\omega_L \omega_R)^{\frac{1}{2}} \exp\left\{-\frac{1}{\hbar} \int_{q_L^+}^{q_R^-} dq [2m(V(q)-E^*)]^{\frac{1}{2}}\right\} \quad (38)$$

where ω_L and ω_R are the frequencies of classical motion in the wells, E^* is the energy of the semiclassical degeneracy, and q_L^+ and q_R^- are the inner limits (turning points) of classical motion in the wells. Adiabatic smallness is governed by the rate at which the difference between the wells changes, i.e. by

$$dX(t)/dt, \quad \text{where } X(t) = E_L(t) - E_R(t), \quad (39)$$

E_L and E_R being the semiclassical well energies given by (11). The uniform asymptotic formula is given [46] by

$$|a_L(t_f)|^2 = \exp\{-Q\}$$

$$\text{where } Q = \frac{\pi\Delta^2}{2\hbar|\dot{X}(t^*)|} = \frac{\hbar\omega_L\omega_R \exp\{-\frac{2}{\hbar}\int_{q_L^+}^{q_R^-} dq [2m(V(q)-E^*)]^{1/2}\}}{2\pi|\frac{d}{dt}(E_L(t^*)-E_R(t^*))|} \quad (40)$$

The two discordant limits are easily recovered from this 'exponential of an exponential': in the semiclassical limit, $\hbar \rightarrow 0$, so that $Q \rightarrow 0$ and $|a_L(t_f)|^2 \rightarrow 1$, as predicted; in the adiabatic limit, $d(E_L - E_R)/dt \rightarrow 0$ so that $Q \rightarrow \infty$ and $|a_L(t_f)|^2 \rightarrow 0$ and the system switches to R, as predicted. There is no inconsistency in these limits being different, but it is important to notice that the quantum adiabatic limit is achieved not when the parameter speed dX/dt is small in comparison with the frequency of classical motion in each well, but when it becomes negligible in comparison with the much smaller frequency of tunnelling between the wells. Otherwise, the system jumps the energy gap and remains, classically, in L.

The simplicity of (40) for the final probability conceals considerable complexity in the evolution for times between t_i and t_f , involving parabolic cylinder functions of complex order and complex argument [48].

One feature of this simple system that is particularly worthy of emphasis, because it is likely to occur more widely, is the qualitatively different asymptotic behaviour associated with different degrees of adiabatic slowness. It might, for example, account for the difficulty in finding classical adiabatic invariants for quasi-integrable systems [52], where tori repeatedly dissolve into chaos as changes in parameters X take them through resonant zones: if dX/dt is not too slow, the orbit might hardly notice the chaos, and emerge from resonance onto a torus with the same actions as before; if dX/dt is very slow (and $N > 2$), the orbit might 'forget' its adiabatic invariants whilst exploring the chaos, and emerge onto a torus with quite different actions (for systems whose closeness to integrability is measured by a small parameter ϵ , the time for such forgetting is exponentially long in $1/\epsilon$ [51]). In the analogous quantal problem, the system might, if dX/dt is not too small, jump the avoided level crossings [40-43] associated with classical resonances and so continue to be associated with semiclassical torus states as given by (11). These considerations might explain the accuracy of a calculation [49] of approximate quantum levels of non-integrable systems, based on a classical calculation of orbits of a system whose Hamiltonian is slowly changed from integrable to nonintegrable, together with the assumption that the association (11) holds, even though in these calculations no attention was paid to classical resonances or quantal avoided crossings.

REFERENCES:

[1] Landau, L.D. and Lifshitz, E.M. Mechanics (Vol.1 of Course of Theoretical Physics) (3rd Ed. Pergamon: Oxford 1976)

[2] Arnol'd, V.I. Mathematical Methods of Classical Mechanics (Springer: New York 1978)

- [3] Dirac,P.A.M.,The Principles of Quantum Mechanics (Oxford: Clarendon Press, 1947)
- [4] Messiah,A.,Quantum Mechanics (North-Holland: Amsterdam 1962)
- [5] Peierls, R.E.,Surprises in Theoretical Physics (New Jersey: Princeton University Press 1979)
- [6] Hwang,J-T and Pechukas,P.,J.Chem.Phys. 67 (1977) 4640-4653
- [7] Born,M.,The Mechanics of the Atom (Frederick Ungar:New York 1960)
- [8] Berry,M.V., Regular and Irregular Motion,in:Topics in Nonlinear Mechanics (S.Jorna,ed.) Am.Inst.Phys.Conf.Proc. 46 (1978) 16-120.
- [9] Lichtenberg,A.J. and Liberman,M.A., Regular and Stochastic Motion (Springer: New York 1983)
- [10] Maslov,V.P. and Fedoriuk,M.V., Semiclassical Approximation in Quantum Mechanics (D.Reidel: Dordrecht 1981)
- [11] Berry,M.V., Semiclassical Mechanics of Regular and Irregular Motion,in:Chaotic Behavior of Deterministic Systems (Les Houches Lectures XXXVI, eds.G.Iooss,R.H.G.Helleman and R. Stora (North-Holland: Amsterdam 1983) pp171-271
- [12] Noid,D.W. and Marcus,R.A., J.Chem.Phys. 67 (1977)559-567
- [13] Eastes,W and Marcus,R.A., J.Chem.Phys. 61 (1974) 4301-4306
- [14] Noid,D.W. and Marcus,R.A., J.Chem.Phys. 62 (1975) 2119-2124
- [15] Noid,D.W., Koszykowski,M.L., and Marcus,R.A., J.Chem.Phys. 71 (1979) 2864-2873
- [16] Percival, I.C. and Pophrey,N., Mol.Phys. 31 (1976) 97-114
- [17] Jaffe,C. and Reinhardt,W.P., J.Chem.Phys. 71 (1979) 1862-1869
- [18] Chapman,S., Garrett,B. and Miller,W.H., J.Chem.Phys. 64 (1976) 502-509
- [19] Kahan,Th., Physique Theoreique,Vol.II (Paris: Presses Universitaires de France (1960))
- [20] Berry,M.V. and Wilkinson,M., Proc.Roy.Soc.Lond. A392 (1984) 15-43
- [21] Bohigas,O., Giannoni,M.J. and Schmit,C., Phys.Rev.Lett. 52 (1984) 1-4.
- [22] Pechukas,P., Phys.Rev.Lett. 51 (1983) 943-946
- [23] Balian,R. and Bloch,C., Ann.Phys. (N.Y) 69 (1972) 76-160
- [24] Berry,M.V., Structures in Semiclassical Spectra: a Question of Scale,in:The Wave-Particle Dualism (ed.S.Diner, D.Fargue,

- G.Lochak and F.Selleri) (D.Reidel: Dordrecht 1984) 231-252.
- [25] Berry, M.V., Proc.Roy.Soc.Lond. A392 (1984) 45-57.
- [26] Hannay, J.H., (1984) Submitted to J.Phys.A.
- [27] Berry, M.V., (1984) Submitted to J.Phys.A.
- [28] Simon, B., Phys.Rev.Lett. 51 (1983) 2167-2170.
- [29] Misner, C.W., Thorne, K.S. and Wheeler, J.A., Gravitation (Freeman: San Francisco, 1973).
- [30] Landau, L.D. and Lifshitz, E.M., Electrodynamics of continuous media (Vol.8 of course of Theoretical Physics) (Pergamon: Oxford, 1960).
- [31] M.V.Berry. In preparation.
- [32] Post, E.J., Revs.Mod.Phys. 39 (1967) 475-493.
- [33] Forder, P.W., J.Phys.A. 17 (1984) 1343-1355.
- [34] Von Neumann, J. and Wigner, E., Phys.Z. 30 (1929) 467-470.
- [35] Frank, F.C., Disc.Far.Soc. 25 (1958) 19-28.
- [36] Berry, M.V. and Hannay, J.H., J.Phys.A. 10 (1977) 1809-1821.
- [37] Herzberg, G. and Longuet-Higgins, H.C., Disc.Far.Soc., 35 (1963) 77-82.
- [38] Longuet-Higgins, H.C., Proc.Roy.Soc.Lond. A344 (1975) 147-156.
- [39] Mead, C.A., Chem.Phys.(Netherlands) 49 (1980) 23-32, 33-38.
- [40] Berry, M.V., Aspects of Degeneracy, in: Proc.Como Conference on Quantum Chaos (G.Casati, ed) (Plenum: London, 1984). In press.
- [41] Berry, M.V., Ann.Phys.(N.Y) 131 (1981) 163-216.
- [42] Noid, D.W., Koszykowski, M.L., Tabor, M. and Marcus, R.A., J.Chem.Phys. 72 (1980) 6167-6175.
- [43] Marcus, R.A., in: Nonlinear Dynamics (ed.R.H.G.Helleman) Ann N.Y.Acad.Sci. 357 (1980) 169-182.
- [44] Richens, P.J. and Berry, M.V., Physica 1D (1981) 495-512.
- [45] Berry, M.V. and Tabor, M., Proc.Roy.Soc.Lond. A356 (1977) 375-394.
- [46] Berry, M.V., J.Phys.A. 17 (1984) 1225-1233.
- [47] Fröman, N., Fröman, P.O., Myhrman, U. and Paulsson, R., Ann.Phys.(N.Y) 74 (1972) 314-323.

- [48] Zener, C., Proc. Roy. Soc. Lond. A137 (1932) 696-702.
- [49] Solov'ev, E. A., Sov. Phys. JETP 48 (1978) 635-639.
- [51] Hannay, J. H. and Ozorio de Almeida A. M., J. Phys. A. (1984).
In Press.
- [52] Nekhoroshev, N. N., Russ. Math. Surv 32 (1977) 1-65.
- [53] Arnold, V. I., Geometrical Methods in the Theory of Ordinary
Differential Equations (Springer: New York, 1983).