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# The adiabatic limit and the semiclassical limit

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**Abstract.** The evolution  $|\Psi(t)\rangle$  of a system with slowly-varying Hamiltonian  $\hat{H}(\Omega t)$  depends not only on the slowness parameter  $\Omega$  but also on Planck's constant  $\hbar$ . For systems with two (or more) classically separated phase-space regions which are quantumly connected by tunnelling, the curves of instantaneous energy levels display hyperbolic near-degeneracies rather than crossings. In such cases the limits  $\Omega \rightarrow 0$  ( $\hbar$  fixed and small) and  $\hbar \rightarrow 0$  ( $\Omega$  fixed and small) lead to opposite behaviour of  $|\Psi(t)\rangle$ . As an illustration, the uniform semiclassical adiabatic behaviour ( $\Omega$  and  $\hbar$  small,  $\Omega/\hbar$  arbitrary) is calculated exactly for a double-well potential for which one well gets shallower as the other gets deeper.

## 1. Introduction

The adiabatic limit is the limit of slow change, and has given rise to two theorems, one for classical systems and one for quantal systems. In its simplest form, the classical adiabatic theorem (Arnol'd 1978) concerns integrable Hamiltonians  $H(q_i, p_i; R_k(\Omega t))$  as  $\Omega \rightarrow 0$ , that is Hamiltonians depending on parameters  $R_k$  which vary slowly with time, as well as on  $N$  coordinates and momenta  $q_i$  and  $p_i$ , and whose orbits for fixed  $R_k$  are confined to  $N$ -tori in the  $2N$ -dimensional phase space. The theorem states that the action integrals  $I_j$  around the  $N$  irreducible cycles  $\gamma_j$  of the tori, defined as

$$I_j \equiv \frac{1}{2\pi} \oint_{\gamma_j} p_i dq_i, \quad (1)$$

are conserved in slow changes of the parameters  $R_k$ . The quantal adiabatic theorem (Messiah 1962) concerns evolution under the time-dependent Hamiltonian operator  $\hat{H}(R_k(t)) \equiv H(\hat{q}_i, \hat{p}_i; R_k(\Omega t))$  and states that a system which starts at  $t=0$  in an eigenstate of  $\hat{H}(R_k(0))$  will remain for all  $t$  in the corresponding eigenstate of  $\hat{H}(R_k(t))$ , provided the  $R_k(t)$  change slowly ( $\Omega \rightarrow 0$ ) and the state is never degenerate.

It is natural to seek to connect these two theorems by means of the semiclassical limit, i.e.  $\hbar \rightarrow 0$ , and indeed such attempts played an important part in the development of quantum mechanics (Born 1960) by leading to the suggestion that (for integrable systems) the classical objects which correspond to quantum stationary states are phase-space tori. A strong form of this connection has been asserted by Hwang and Pechukas (1977), who claimed that the asymptotic limits  $\hbar \rightarrow 0$  and  $\Omega \rightarrow 0$  are equivalent. Their argument is based on scaling: in the Schrödinger equation

$$i\hbar \partial|\Psi\rangle/\partial t = \hat{H}(R_k(\Omega t))|\Psi\rangle, \quad (2)$$

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$\Omega$  can be eliminated from  $\hat{H}$  by defining  $\Omega t = \tau$ , leading to the replacement of  $\hbar$  by  $\Omega\hbar$  on the left-hand side. This argument is ill-founded because the notation  $\hat{H}$  conceals an  $\hbar$ -dependence (whose explicit form is different for different representations) which persists after  $t$ -scaling, leaving an equation depending on  $\hbar$  as well as  $\Omega\hbar$ .

My purpose here is to point out that there is even a class of systems for which the semiclassical limit and the adiabatic limit flatly contradict each other. These systems involve pairs of quantum states associated with classical trajectories in separate regions of classical phase space, which are connected quantumly by *tunnelling*. A simple model for such systems is set up in § 2 and solved in § 3. Some generalisations, and also possible implications for the difficult problem of semiclassical quantisation of non-integrable systems are discussed in § 4.

## 2. The changing double-well potential

Consider a particle of mass  $m$  moving in one dimension with energy  $E$  in the time-dependent potential  $V(q, t)$ , illustrated in figure 1, whose left-hand well (called L) gets shallower and whose right-hand well (R) gets deeper as shape parameters  $R_k(t)$  change slowly. Only energies  $E$  less than the energy of the barrier top will be considered. Thus there are two distinct classical motions with each  $E$ , and two actions  $I_L$  and  $I_R$ , which may be considered to be the parameters  $R_k(t)$  and which are given (cf (1)) by

$$I_L(E, t) = \frac{1}{\pi} \int_{q_{L-}}^{q_{L+}} dq [2m(E - V(q, t))]^{1/2},$$

$$I_R(E, t) = \frac{1}{\pi} \int_{q_{R-}}^{q_{R+}} dq [2m(E - V(q, t))]^{1/2},$$
(3)

where the limits of integration are the classical turning points (figure 1).

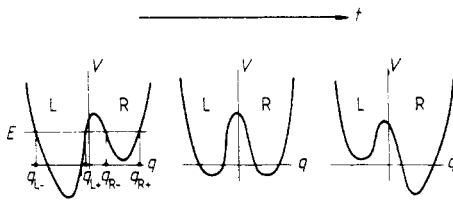


Figure 1. Changing double-well potential.

In the simplest semiclassical approximation, each well supports separate families of localised quantum stationary states  $|\phi_L^m\rangle$  and  $|\phi_R^n\rangle$  with quantum numbers  $n$  and  $m$ ; the exponential tails leaking out of each well may be neglected. The energies  $E_{L,m}(t)$ ,  $E_{R,n}(t)$  of the states are given by the Bohr-Sommerfeld rule

$$I_L(E_{L,m}(t), t) = (m + \frac{1}{2})\hbar \left. \right\}$$

$$I_R(E_{R,n}(t), t) = (n + \frac{1}{2})\hbar \left. \right\}. \quad (4)$$

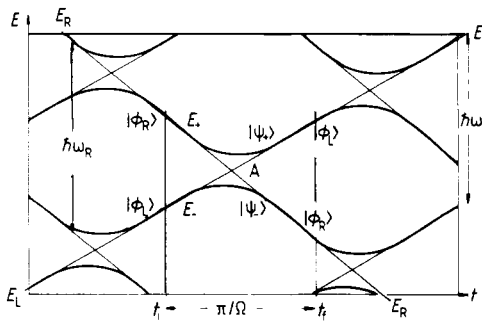
Successive levels in each family are separated by  $\hbar\omega_L$  and  $\hbar\omega_R$ , where  $\omega = (\partial I / \partial E)^{-1}$  is the frequency of classical motion in each well. As  $I_L$  and  $I_R$  change, the energies

of successive pairs of quantised tori, labelled  $m$  and  $n$ , will become equal and these Bohr–Sommerfeld levels (fine lines in figure 2) will cross.

Of course the true quantal levels (heavy lines in figure 2) will not cross, because the Bohr–Sommerfeld degeneracies will be split by barrier penetration. In the neighbourhood of the near-crossings the stationary states will not be localised in one of the wells but will be linear combinations of  $|\phi_L\rangle$  and  $|\phi_R\rangle$ . Near the point A in figure 2, for example, the stationary states will be

$$|\psi_{\pm}\rangle = \alpha_{\pm}|\phi_L\rangle + \beta_{\pm}|\phi_R\rangle, \tag{5}$$

where  $+$  and  $-$  denote the states of higher and lower energy  $E_+$  and  $E_-$  and where the values of  $\alpha_{\pm}$  and  $\beta_{\pm}$  depend on  $t$ .



**Figure 2.** Fine lines: Bohr–Sommerfeld levels  $E_L(t), E_R(t)$  corresponding to localised approximate states  $|\phi_L\rangle, |\phi_R\rangle$ . Heavy curves: true quantal energies  $E_{\pm}(t)$ , corresponding to exact quantal stationary states  $|\psi_{\pm}\rangle$ .

Now comes the central question, which concerns the evolution  $|\Psi(t)\rangle$  of a state which initially, at  $t_1$ , is entirely in (say) a left-well localised state  $|\phi_L\rangle$  (i.e.  $|\psi_-$ ), cf figure 2). What will be the state of the system much later, at  $t_2$ , if a near-degeneracy has intervened at  $t = (t_1 + t_2)/2$ ? We define the duration of the change as

$$t_2 - t_1 = \pi/\Omega, \tag{6}$$

where  $2\pi/\Omega$  is the time for the unperturbed energy splitting  $E_L(t) - E_R(t)$  to change by a mean single-well level spacing, i.e.

$$\Omega = \frac{2\pi}{\hbar(\omega_L\omega_R)^{1/2}} \frac{d}{dt}(E_L(t) - E_R(t)). \tag{7}$$

$\Omega$  is the adiabatic parameter in this problem, and will always be chosen to satisfy

$$\Omega \ll \omega_L, \quad \Omega \ll \omega_R, \tag{8}$$

thus guaranteeing single-well quantal adiabaticity, i.e. ensuring that the state will not undergo transitions to any of the other states localised in the same well.

There are two contrary predictions for the final state  $|\Psi(t_2)\rangle$ . The first, suggested by the classical adiabatic theorem, is that the evolving state will continue to be associated with the same torus and will remain localised in the left-hand well; thus  $|\Psi(t_2)\rangle$  will be proportional to  $|\phi_L\rangle$ , and so will have switched to the eigenstate  $|\psi_+\rangle$  (figure 2) by jumping the gap. The second prediction, suggested by the quantal adiabatic theorem,

is that  $|\Psi(t)\rangle$  will cling to the same instantaneous eigenstate, i.e.  $|\psi_{\pm}\rangle$ , and so will have switched wells and be in  $|\phi_R\rangle$  at  $t_f$ . What in fact happens depends delicately on the value of  $\Omega$  in comparison with  $\hbar$ , as will be shown in the next section.

The possibility of switching or not switching between modes of weakly-coupled systems is well known in electromagnetic theory. The two potential wells correspond to parallel waveguides carrying microwaves (Louisell 1955, Cook 1955 and Fox 1955) or light (Snyder and Love 1983). Time corresponds to distance along the waveguides, and the changes in the shapes of the wells correspond to opposite tapers in the two waveguides. In molecular physics, energy curves such as those in figure 2 are also well known, and correspond to the energies of electrons, which change as the nuclei move; of the many papers dealing with these curve-crossing problems, I will need to cite only the early work by Zener (1932). In the context of this extensive and varied literature the only (minor) novelty of the present work lies in the explicit treatment within one framework of the effects of the two small parameters  $\Omega$  and  $\hbar$ .

### 3. Calculation of final state

Because of the single-well adiabatic condition (8), the state  $|\Psi(t)\rangle$  for  $t_i \leq t \leq t_f$  can be expressed as a linear combination of the two localised states  $|\phi_L\rangle$  and  $|\phi_R\rangle$ , namely

$$|\Psi(t)\rangle = a_L(t) \exp\left(-i \int_0^t E_L(t') dt'/\hbar\right) |\phi_L\rangle + a_R(t) \exp\left(-i \int_0^t E_R(t') dt'/\hbar\right) |\phi_R\rangle \quad (9)$$

with

$$a_L(t_i) = 1, \quad a_R(t_i) = 0. \quad (10)$$

We seek  $a_L(t_f)$  and  $a_R(t_f)$ ; of course these are linked by  $|a_L|^2 + |a_R|^2 = 1$ . In this basis the Hamiltonian  $\hat{H}$  is just the two-state operator

$$\hat{H} = \begin{pmatrix} E_L(t) & \Delta(t)/2 \\ \Delta(t)/2 & E_R(t) \end{pmatrix} \quad (11)$$

whose diagonalisation gives the two eigenstate energies  $E_{\pm}(t)$  as

$$E_{\pm}(t) = \frac{1}{2}(E_L(t) + E_R(t)) \pm \frac{1}{2}[(E_L(t) - E_R(t))^2 + \Delta^2(t)]^{1/2}, \quad (12)$$

thus identifying  $\Delta(0)$  as the energy gap if the unperturbed crossing ( $E_L = E_R$ ) is considered to occur at  $t=0$ .

The Schrödinger equation (2), together with (9), now gives, as the equations determining the multipliers  $a_L(t)$  and  $a_R(t)$ ,

$$\left. \begin{aligned} \frac{da_L(t)}{dt} &= \frac{\Delta(t)a_R(t)}{2i\hbar} \exp\left(\frac{i}{\hbar} \int_0^t dt' (E_L(t') - E_R(t'))\right) \\ \frac{da_R(t)}{dt} &= \frac{\Delta(t)a_L(t)}{2i\hbar} \exp\left(\frac{-i}{\hbar} \int_0^t dt' (E_L(t') - E_R(t'))\right) \end{aligned} \right\} \quad (13)$$

An equivalent pair of coupled evolution equations could have been obtained by using as basis the instantaneous eigenstates  $|\psi_{\pm}\rangle$  instead of the localised states  $|\phi_L\rangle$  and  $|\phi_R\rangle$ , but these equations turn out to be less amenable to a direct solution.

The Bohr-Sommerfeld conditions (4) determine the unperturbed levels  $E_L$  and  $E_R$ , but to find the splitting  $\Delta(0)$  a more accurate semiclassical theory is needed. This

is provided by the WKB method (Berry and Mount 1972), whose connection formulae lead to

$$\cot\left(\frac{\pi I_L(E, t)}{\hbar}\right) \cot\left(\frac{\pi I_R(E, t)}{\hbar}\right) = \frac{1}{4} \exp\left(\frac{-2K(E, t)}{\hbar}\right) \quad (14)$$

where  $K$  denotes the barrier integral (figure 1)

$$K(E, t) \equiv \int_{q_{L-}}^{q_{R-}} dq [2m(V(q, t) - E)]^{1/2}. \quad (15)$$

A careful derivation and discussion of (14) is given by Fröman (1966), Fröman and Myhrman (1970) and Fröman *et al* (1972).

The tunnelling exponential on the right-hand side of (14) is exceedingly small. If it is neglected, the Bohr-Sommerfeld conditions (4) result. But it is not difficult to prove that the energies satisfying (14) can never degenerate as  $t$  varies, and that the splitting  $\Delta(0)$  at the instant  $t = 0$  at which two unperturbed levels  $E_{L,m}$  and  $E_{R,n}$  would degenerate at energy  $E$  is

$$\Delta(0) = (\hbar/\pi)(\omega_L\omega_R)^{1/2} \exp(-K(E, 0)/\hbar). \quad (16)$$

This is far smaller than the single-well splittings  $\hbar\omega_L$  and  $\hbar\omega_R$ , so that the interaction between  $|\phi_L\rangle$  and  $|\phi_R\rangle$  is confined to a tiny fraction of the time interval  $t_f - t_i$ . During this interaction time  $\Delta$  is essentially constant and  $E_L - E_R$  is essentially the linear function (cf 7).

$$E_L(t) - E_R(t) = \hbar(\omega_L\omega_R)^{1/2}\Omega t/2\pi. \quad (17)$$

On changing variables from  $t$  to  $T$ , defined by

$$T \equiv \frac{1}{2}\Omega e^{K/\hbar}t, \quad (18)$$

the evolution equations (13) now become

$$\left. \begin{aligned} \frac{da_L}{dT} &= -\frac{i}{\lambda} a_R \exp(+iT^2/\lambda) \\ \frac{da_R}{dT} &= -\frac{i}{\lambda} a_L \exp(-iT^2/\lambda) \end{aligned} \right\} \quad (19)$$

where the parameter  $\lambda$  is defined as

$$\lambda \equiv \pi\Omega e^{+2K/\hbar}/(\omega_L\omega_R)^{1/2}. \quad (20)$$

As  $t$  varies from  $t_i$  to  $t_f$ , the phases  $T^2/\lambda$  of the oscillatory coefficients in (19) vary from  $\pi(\omega_L\omega_R)^{1/2}/16\Omega$  to zero and back to  $\pi(\omega_L\omega_R)^{1/2}/16\Omega$ ; this follows from (6), (18) and (20). The adiabatic conditions (8) imply that these phase changes are large, so that  $t_i$  and  $t_f$  can be considered to lie in the asymptotic regions of (19), which may therefore be integrated from  $T = -\infty$  (with the initial condition (10)) to  $T = +\infty$ . This integration was carried out exactly by Zener (1932) (for him, (19) was not asymptotically exact, as it is here, but was an approximate model treating unperturbed molecular electron energy curves crossing linearly and interacting with constant strength). Zener's technique was to differentiate the first of equations (19), thereby obtaining for  $a_L$  alone a second-order differential equation, whose exact solution is a parabolic cylinder function of complex order and argument. Standard asymptotic forms of these functions

can then be employed to connect the probabilities at  $T = \pm\infty$ , with the result

$$\begin{aligned} |a_L(-\infty)|^2 = 1 & \longleftrightarrow |a_L(+\infty)|^2 = \exp\{-\pi/\lambda\} \\ |a_R(-\infty)|^2 = 0 & \longleftrightarrow |a_R(+\infty)|^2 = 1 - \exp\{-\pi/\lambda\}. \end{aligned} \quad (21)$$

The main result of this paper, written as an explicit form for the probability that the state has remained localised in the left-hand well at  $t$ , is

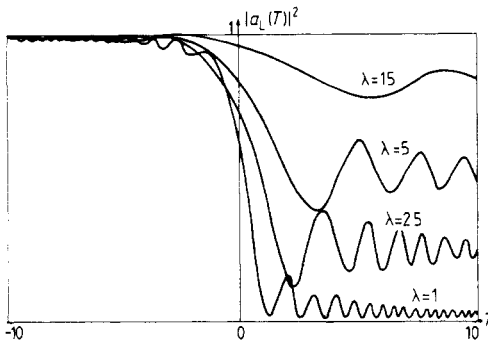
$$|a_L(+\infty)|^2 = \exp\{-[(\omega_L \omega_R)^{1/2}/\Omega] \exp(-2K/\hbar)\}. \quad (22)$$

From this uniform semiclassical adiabatic formula it is easy to extract the semiclassical limit and the adiabatic limit as two extremes, namely

$$|a_L(+\infty)|^2 \begin{cases} \nearrow 1 & \text{as } \hbar \rightarrow 0 \text{ (semiclassical)} \\ \searrow 0 & \text{as } \Omega \rightarrow 0 \text{ (adiabatic)} \end{cases}. \quad (23)$$

These limits accord with intuition: for the change to be quantally adiabatic, i.e. for the state to remain in the instantaneous eigenstate  $|\psi_{-}\rangle$  and so switch wells, the parameter  $\lambda$  must be small, so that  $\Omega$  must not only be small in comparison with  $\omega_L$  and  $\omega_R$  (cf 8) but also small in comparison with the energy splitting, which involves the tunnelling factor  $\exp(-K/\hbar)$  (cf 16); in the semiclassical limit, on the other hand, this factor vanishes and  $\lambda$  is large, so that even changes satisfying (8) appear fast and the state jumps eigenstates from  $|\psi_{-}\rangle$  to  $|\psi_{+}\rangle$  while remaining in the left-hand well.

The behaviour of  $|a_L(T)|^2$  for intermediate times can be quite complicated, with strong and rapid oscillations (which depend on  $\lambda$ ) accompanying the approach to the asymptotic values (21). This is illustrated by figure 3 which shows computed solutions of equation (19) for four values of  $\lambda$ .



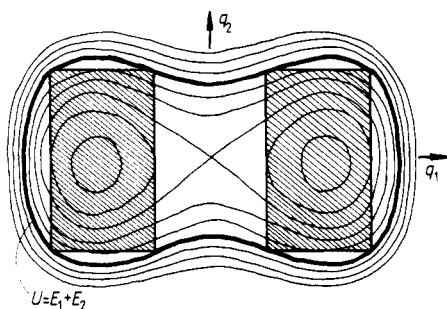
**Figure 3.** Solutions of the Schrödinger equation (19) giving the probability  $|a_L(T)|^2$  that the state remains in the left-hand well, for the indicated values of the parameter  $\lambda$  defined by (20).

#### 4. Discussion

The main conclusion of this paper is that the adiabatic and semiclassical limits lead to opposite behaviour when two levels in a slowly-changing system pass a near-degeneracy resulting from tunnelling between separated classical orbits. This conclusion has wider applicability than the double-well model employed to illustrate it. In particular, the

classical separation of the two orbits need not be enforced by real-space potential barriers.

One way to see this is to imagine the double-well potential  $V(q_1)$  augmented by addition of a single-well potential  $W(q_2)$  depending on a perpendicular coordinate  $q_2$ . For fixed values of well parameters, motion in the combined potential  $U(q_1, q_2) = V + W$  (whose contours are shown in figure 4) is separable classically and quantally, with the  $q_1$  and  $q_2$  energies  $E_1$  and  $E_2$  separately conserved and separately quantised. If  $E_1$  is below the top of the barrier between the wells of  $V(q_1)$ , all the avoided-crossing and quantal evolution discussed in this paper will occur. If in addition  $E_2$  is large enough, then the classically allowed region  $U(q_1, q_2) < E_1 + E_2$  is a single connected region, with no potential barrier restricting its exploration. Nevertheless, the classical orbits do not fill this region: they are restricted by constants of motion to occupy two rectangles within it, as illustrated in figure 4.



**Figure 4.** Fine curves are contours of potential  $U(q_1, q_2) = V(q_1) + W(q_2)$ , where  $V$  has a double well and  $W$  a single well. The heavy curve bounds the classically allowed region for an energy  $E_1 + E_2$  greater than that of the potential saddle. The rectangles bound the regions to which the classical orbits are restricted by the separate constancy of  $E_1$  and  $E_2$ .

Alternatively, the classical orbits may be separated by a potential barrier in momentum space. This can happen in one dimension for rotators, for which the coordinate  $q$  is periodic so that phase space  $q, p$  is a cylinder; the two orbits correspond to opposite rotations with the same actions.  $H(q, p, t)$  may not be a symmetric function of  $p$ , because this would imply *permanent* Bohr–Sommerfeld degeneracies split by momentum tunnelling (provided the  $q$ -dependence is non-trivial), whereas the phenomena described in this paper require *crossing* of Bohr–Sommerfeld levels. One system with a suitable non-symmetric Hamiltonian is a bead sliding on a rotating non-circular hoop whose shape, area or angular velocity is slowly changed.

In conclusion I wish to give a brief discussion of the extent to which adiabatic ideas might be useful in quantising systems whose classical motion is not integrable. Solovév (1978) suggests that the classical adiabatic theorem does apply to such systems, and invokes the correspondence principle to assert that the energy of a state with given quantum numbers, for a non-integrable Hamiltonian  $\hat{H}(t)$ , can be obtained by starting with an exactly-soluble Hamiltonian  $\hat{H}(t)$  which slowly evolves to  $\hat{H}(t)$ , and following the classical trajectory which initially lies on the quantised torus with the same quantum numbers. He illustrates this method by obtaining very accurate values for the energy levels of anharmonically perturbed two-dimensional coupled oscillators.



By labelling states with quantum numbers proportional to the actions of classical tori, Solovev is assuming that tori exist. And indeed for the (quasi-integrable) systems he employs as examples, the KAM theorem (Berry 1978, Arnol'd 1978) guarantees the survival of most tori during perturbation from  $H(\iota_1)$  to  $H(\iota_2)$ . But not all tori survive perturbation; as is well known, the tori near *resonance*, i.e. those whose frequencies are close to commensurability, are destroyed and replaced by phase-space regions of small measure, intricately filled with orbits some of which are chaotic. As a particular torus, labelled by its actions, is followed whilst  $H$  changes, the frequencies must change and so will pass infinitely often through resonance. Therefore there will be many brief intervals between  $\iota_1$  and  $\iota_2$  where the torus will be temporarily lost. Moreover, it is precisely at resonances that Bohr–Sommerfeld quantisation would predict level crossings (Berry 1984), which do not exist quantum-mechanically because splitting will turn them into avoided crossings (Ramaswamy and Marcus 1981).

Therefore neither the tori nor the quantum states will evolve in the way that Solovev assumes. Why then does his method work so well? My opinion is that this is probably because the changes in  $H$ , while slow in comparison with the torus frequencies, are neither so slow as to ensure thorough explorations of the chaotic zones during passage through resonance nor so slow as to ensure that the quantum state would cling to an eigenstate through an avoided crossing and so emerge on a different torus. In other words, in addition to the adiabatic parameter  $\Omega$  there is a non-integrability parameter  $\varepsilon$ , which together with  $\hbar$  will affect the quantal level splitting; if  $\Omega$  is not small in comparison with  $\varepsilon$ , the classical orbit jumps the chaos gap and conserves actions through the resonance, and the quantum state jumps the energy gap and thus continues to be associated with the same torus.

It is worth remarking that the Bohr–Sommerfeld degeneracies associated with resonance involve tori which are neighbours (in action space) and not ones which are separated (as in the double-well example), so that the quantal level splitting depends on tunnelling in a more complicated way and involves  $\varepsilon$  as well as  $\hbar$  (Ozorio de Almeida 1984).

Of course, if the multidimensional system remains integrable between  $\iota_1$  and  $\iota_2$  (unlike generic coupled anharmonic oscillators), there is no torus destruction and the effects of resonance are confined to instants (albeit densely distributed). In this case it was shown by Dirac (1925) that the adiabatic invariants are conserved in slow changes. If in addition the system remains separable, then at the instants of resonance there are true crossings of the quantum energy levels. One example of such a system is a particle in a two-dimensional rectangular box whose side ratio is varied.

Finally, consider an extreme of non-integrability, where there are no tori at all. This corresponds to a one-parameter family of ergodic systems. There are no actions to be conserved and so no consistent labelling of states by corresponding sets of quantum numbers. There is, however, one adiabatic invariant, namely the volume of the energy shell. (It is a curious fact, easily confirmed by examples, that this volume is not an adiabatic invariant for non-ergodic—e.g. separable—systems.) This suggests the quantisation law

$$\frac{1}{(2\pi\hbar)^N} \int \dots \int_{E > H(q,p)} d^N q d^N p = n + \frac{1}{2} \quad (24)$$

for ergodic systems, and indeed Berry and Wilkinson (1984) show that this formula

(augmented by an asymptotic correction) gives accurately the average behaviour of the energy levels of triangles whose angles are varied. Superposed on the average are of course very interesting oscillations and fluctuations (Berry 1984) which lead to level spacings less regular than (24) would predict. (These departures from regularity are much greater in the case of integrable systems, for which (24) retains meaning because its left-hand side is a general asymptotic formula valid for any system, giving the number of levels with energies below  $E$ .)

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