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Semiclassical study of particle motion in two-dimensional and three-dimensional elliptical boxes: I

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Abstract. We compare three problems of quantum mechanics (or more generally of wave mechanics) which reduce to the same problem in classical mechanics and which can also be treated semiclassically by the Einstein, Brillouin and Keller semiquantisation rules. The free particle motion in an ellipsoidal oblate or prolate cavity (a deformed nucleus) is compared to that in a plane elliptical billiard box. Separation of variables is performed in appropriate coordinate systems. The presence of a separatrix in phase space is exhibited, which is connected to a potential barrier that is different for each problem. The uniform approximation is used to calculate WKB phase rules appropriate to each symmetry. An important difference results between the prolate and the oblate systems.

1. Introduction

In classical mechanics a particle moving in any plane trajectory does not distinguish whether the dimension of the space is really two or higher. In quantum mechanics the wave equation may contain, in the system of coordinates appropriate to the symmetry, terms which depend explicitly on the dimension and symmetry. Consequently, the dynamical properties are affected and change significantly. We want to discuss in this paper three different quantum mechanical realisations of a single problem of classical mechanics which enlighten the preceding statements.

Let us consider a particle free to move in a two-dimensional domain with an elliptic boundary of semi-axis $R_>$ and $R_<$ and focal distance $2f$ and let us assume that the boundary is a perfect reflector. Let us call this problem that of the elliptical 'billiard'. We now embed the 'billiard' into a prolate or oblate ellipsoidal cavity. The corresponding quantum mechanical realisations are the study of all the eigenmodes of an elliptical membrane and those of prolate and oblate cavities which are associated with a zero angular momentum projection on the axis of symmetry. The classical dynamics of the elliptic 'billiard' was described by Berry (1981). The semiclassical quantisation of its eigenmodes was discussed by Keller and Rubinow (1960) according to the WKB rules conveniently modified by Keller (1959) for multidimensional systems. These rules are sometimes called primitive because of their severe shortcomings in the description of barrier effects. It is then necessary to use the uniform semiclassical approximation which was developed by Ford *et al* (1959), Miller (1968) and Child (1974). We will use this uniform approximation to complement the work of Keller and Rubinow on the membrane eigenmodes. Moreover, we will also adapt this approximation to the cases of prolate and oblate ellipsoids. These modifications are absolutely necessary to understand the differences between the spectra of our three systems and the role played by the symmetry of the embedding.

A common property of our three systems is the presence of potential barriers which can be found in systems of coordinates suited to the symmetries. The presence of these barriers leads to a division of the phase space into two regions which have already been described by Keller and Rubinow and by Berry. It is simpler to classify classical trajectories by their caustics which are either ellipses or hyperbola homofocal to the elliptic boundary. These families of trajectories are separated by a separatrix which corresponds to the summit of the barrier. We will show that it is a common feature of our three systems that the semiclassical eigenmodes perform the same type of evolution when the deformation is varied. For a zero deformation the caustics are circles, they become ellipses for small enough deformation, and then become hyperbolic. For a specific deformation a semiclassical state stands on the sepatrix. We will derive a very simple rule which enables us, in the frame of the uniform approximation, to determine this deformation in each type of system.

Contrary to the cases of spherical nuclear potential which were studied earlier by Carbonell *et al* (1985), the topology of our systems is not monotonic because of this barrier crossing effect. A barrier crossing which is topologically similar to the one described above has been found by Carbonell (1983) and Carbonell *et al* (1984) in the analysis of the plane trajectories in a deformed Woods–Saxon-type potential. Therefore we feel that the results of this paper form a background which may explain, in a simple way, the important differences in the spectra of prolate and oblate potentials and are relevant in understanding the single particle spectra of deformed nuclei.

The numerical applications of this work are presented in Arvieu and Ayant (1987). The extensions to non-planar orbits will be discussed separately elsewhere.

2. 'Billiard' problem

In this true two-dimensional problem (in the quantum sense) the Hamilton Jacobi and the Schrödinger equations are separable in elliptical coordinates η and ξ defined by

$$x = f \cos \xi \cosh \eta \tag{1}$$

$$y = f \sin \xi \sinh \eta \tag{2}$$

with

$$0 \leqslant \eta < \infty \qquad 0 \leqslant \xi < 2\pi. \tag{3}$$

From the Hamilton Jacobi equation we are led to the following values of the classical momenta p_η and p_ξ:

$$p_\eta^2 = k^2 f^2 \cosh^2 \eta - E \tag{4}$$

$$p_\xi^2 = E - k^2 f^2 \cos^2 \xi. \tag{5}$$

The energy is denoted as

$$W = k^2/2m \tag{6}$$

and the separation constant as E.

If the wavefunction is written as

$$\Psi = G(\eta)F(\xi) \tag{7}$$

we find that G and F obey the Mathieu and associated Mathieu equations respectively:

$$\mathrm{d}^2G/\mathrm{d}\eta^2 + (k^2f^2\cosh^2\eta - E)G = 0 \tag{8}$$

$$\mathrm{d}^2F/\mathrm{d}\xi^2 + (E - k^2f^2\cos^2\xi)F = 0. \tag{9}$$

For each variable there is a potential barrier, the same in the classical and in the quantum problems. These barriers are complementary: when the turning point disappears for one variable a turning point appears for the other one.

(i) If $k^2f^2 < E$ the classical motion occurs in the interval

$$\eta_0 \leqslant \eta \leqslant \eta_1 \tag{10}$$

with

$$\eta_0 = \cosh^{-1}(\sqrt{E}/kf) \tag{11}$$

$$\eta_1 = \cosh^{-1}(R_>/f) \tag{12}$$

and

$$0 \leqslant \xi < 2\pi. \tag{13}$$

(ii) If $k^2f^2 > E$ the limits of variation become

$$0 \leqslant \eta \leqslant \eta_1 \tag{14}$$

$$\xi_0 \leqslant \xi \leqslant \pi - \xi_0 \qquad \pi + \xi_0 \leqslant \xi \leqslant 2\pi - \xi_0 \tag{15}$$

with

$$\xi_0 = \cos^{-1}(\sqrt{E}/kf). \tag{16}$$

(ii) The value $k^2f^2 = E$ defines the separatrix. It can be seen that the trajectory always crosses one focus, then after one reflection the other, etc (Berry 1981).

The wavefunction Ψ is seen to possess two parities. To the reflection with respect to Ox is associated the parity π_x, and similarly π_y is related to the reflection with respect to Oy. F and G are now seen to be of the same parity if we perform $\eta \to -\eta$ and $\xi \to -\xi$. On the other hand, the wavefunction is either even or odd in π_y, i.e. we have either

$$F(\tfrac{1}{2}\pi) = 0 \tag{17a}$$

or

$$(\mathrm{d}F/\mathrm{d}\xi)(\tfrac{1}{2}\pi) = 0. \tag{17b}$$

We call the cases where $\pi_x = +1$ symmetric and the cases where $\pi_x = -1$ antisymmetric.

The WKB solutions of equations (8) and (9) can be written, within constants of normalisation,

$$G(\eta) = c' p_\eta^{-1/4} \cos\left(\int_{\eta_0}^{\eta} p_\eta \,\mathrm{d}\eta - \beta_\eta\right) \tag{18}$$

$$F(\xi) = c' p_\xi^{-1/4} \cos\left(\int_{\xi_0}^{\xi} p_\xi \,\mathrm{d}\xi - \beta_\xi\right) \tag{19}$$

where p_η and p_ξ are the positive roots of (4) and (5) and where η_0 is either 0 or is defined by (11), while ξ_0 is either defined by (16) or is zero. Our purpose is now to find the phases β_η and β_ξ in the uniform approximation.

Let us define the classical actions as

$$I_\eta = \frac{1}{\pi}\int_{\eta_0}^{\eta_1} p_\eta \,\mathrm{d}\eta \tag{20}$$

$$I_\xi = \frac{1}{\pi}\int_{\xi_0}^{\pi-\xi_0} p_\xi \,\mathrm{d}\xi \tag{21}$$

in terms of which we write the quantisation conditions (with $\hbar = 1$) as

$$I_\eta = n_\eta + \tfrac{1}{2} + \beta_\eta/\pi \tag{22}$$

while for the ξ variable we must distinguish the cases according to π_y.

If $\pi_y = 1$

$$(\mathrm{d}F/\mathrm{d}\xi)(\tfrac{1}{2}\pi) = 0 \tag{23}$$

$$\frac{1}{\pi}\int_{\xi_0}^{\pi/2} p_\xi \,\mathrm{d}\xi = n_\xi + \beta_\xi/\pi \tag{24}$$

$$I_\xi = 2n_\xi + 2\beta_\xi/\pi. \tag{25}$$

If $\pi_y = -1$

$$F(\tfrac{1}{2}\pi) = 0 \tag{26}$$

$$\frac{1}{\pi}\int_{\xi_0}^{\pi/2} p_\xi \,\mathrm{d}\xi = n_\xi + \tfrac{1}{2} + \beta_\xi/\pi \tag{27}$$

$$I_\xi = (2n_\xi + 1) + 2\beta_\xi/\pi. \tag{28}$$

In order to determine the phases β_η and β_ξ we will concentrate mostly on the case $k^2f^2 \approx E$ which allows us to expand the potentials up to second order in η and ξ so that the equations become well approximated by

$$\mathrm{d}^2G/\mathrm{d}\eta^2 + (k^2f^2\eta^2 + k^2f^2 - E)G = 0 \tag{29}$$

$$\mathrm{d}^2F/\mathrm{d}\xi^2 + (E - k^2f^2 + k^2f^2\xi^2)F = 0 \tag{30}$$

which are both of the parabolic cylinder type:

$$\mathrm{d}^2y/\mathrm{d}x^2 + (\tfrac{1}{4}x^2 - \alpha)y = 0. \tag{31}$$

We obtain this equation if we use the variable $x = (2kf)^{1/2}\eta$ instead of η and if we define α by

$$\alpha = (E - k^2f^2)/2kf. \tag{32}$$

With a similar change of variable, $x = (2kf)^{1/2}\xi$, we obtain the same equation for ξ but we must modify the definition of α by a change of sign.

We now concentrate on (31). It is known that the asymptotic forms of its solutions are (Abramowitz and Stegun 1972)

$$y_1(x) = (c'/\sqrt{x})[\cos\phi(x) - \theta] \qquad \text{if } y \text{ is even} \tag{33}$$

$$y_2(x) = (c'/\sqrt{x})[\cos\phi(x) + \theta] \qquad \text{if } y \text{ is odd} \tag{34}$$

with

$$\phi(x)=\tfrac{1}{4}x^2-\alpha\log x+\tfrac{1}{4}\pi+\tfrac{1}{2}\arg(-\tfrac{1}{2}+\mathrm{i}\alpha)! \tag{35}$$

$$\theta=\tan^{-1}[(1+\mathrm{e}^{2\pi\alpha})^{1/2}+\mathrm{e}^{\pi\alpha}]. \tag{36}$$

The expressions (35) and (36) are compatible with the WKB for solution (31) which can be written generally as

$$y_1^{\mathrm{WKB}}(x)=\frac{c'}{(\tfrac{1}{4}x^2-\alpha)^{1/4}}\cos\left(\int_{x_0}^{x}(\tfrac{1}{4}x'^2-\alpha)^{1/2}\,\mathrm{d}x'-\beta\right) \tag{37}$$

since one has

$$\int_{x_0}^{x}(\tfrac{1}{4}x'^2-\alpha)^{1/2}\,\mathrm{d}x' \underset{x\to\infty}{=} \tfrac{1}{4}x^2-\alpha\log x-\tfrac{1}{2}\alpha+\tfrac{1}{2}\alpha\log|\alpha|. \tag{38}$$

This allows us to determine β to be

$$\beta=\theta-\tfrac{1}{4}\pi+\tfrac{1}{2}\alpha\log|\alpha|-\tfrac{1}{2}\alpha-\tfrac{1}{2}\arg(-\tfrac{1}{2}+\mathrm{i}\alpha)!. \tag{39}$$

For the odd case, as can be seen from (34), we should simply replace θ by $-\theta$ or better by $\pi-\theta$.

In this way we obtain two subsets of functions β, for η and ξ respectively, using α defined in (32) or its opposite value. Let β_{S} be defined by equation (39) and β_{A} by (39) where θ has been replaced by $\pi-\theta$. We must then use the following functions in (22), (25) and (28) (using the definition (32) for α):

for the symmetric states

$$\beta_\eta=\beta_{\mathrm{S}}(\alpha) \tag{40}$$

$$\beta_\xi=\beta_{\mathrm{S}}(-\alpha) \tag{41}$$

for the antisymmetric states

$$\beta_\eta=\beta_{\mathrm{A}}(\alpha) \tag{42}$$

$$\beta_\xi=\beta_{\mathrm{A}}(-\alpha). \tag{43}$$

The functions $\beta(\alpha)$ are represented in figure 1(a). The following values are interesting to consider:

$$\alpha\to+\infty \qquad \beta_{\mathrm{S}},\beta_{\mathrm{A}}\to\tfrac{1}{4}\pi \tag{44}$$

$$\alpha=0 \qquad \beta_{\mathrm{S}}=\tfrac{1}{8}\pi, \qquad \beta_{\mathrm{A}}=\tfrac{3}{8}\pi \tag{45}$$

$$\alpha\to-\infty \qquad \beta_{\mathrm{S}}\to0 \qquad \beta_{\mathrm{A}}\to\tfrac{1}{2}\pi. \tag{46}$$

Since we have $\beta_{\mathrm{S}}=\beta_{\mathrm{A}}=\tfrac{1}{4}\pi$ for $\alpha\to+\infty$, i.e. when $\eta_0\neq0$ (elliptic caustic), the symmetric and the antisymmetric states are in general degenerate. The only states which are not are the states with $I_\xi=0$. When α decreases the symmetric and the antisymmetric states split, a well known pairing effect first discussed by Ford *et al* (1959). The case $\alpha=0$ corresponds to the situation where one is exactly at the top of the barrier.

The limits (44) and (46) given above correspond to the usual values of the WKB method. The disadvantages of strictly using these constant values ((44) for the case when the classical caustic is elliptic and (46) when it is hyperbolic) are well known and have been discussed in Ford *et al* (1959). Let us discuss them for our problem.

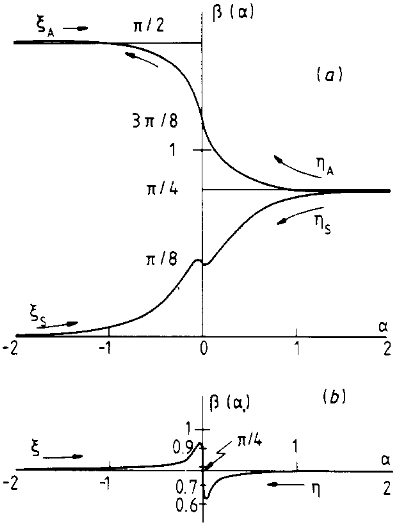

Figure 1. Phases of the WKB wavefunctions defined in equations (18) and (19) plotted as a function of α. (a) The elliptic 'billiard' discussed in § 2. There the phases are different for symmetric (S) and antisymmetric (A) states. The arrows indicate the sense in which the phases β_η, β_ξ evolve as a function of α. A change in the sign of α occurs between η and ξ (see equations (40)–(43)). (b) The prolate ellipsoid with similar conventions.

(i) As long as the caustic is elliptic, equation (44) holds and the states are degenerate, contrary to the quantum case. This is an old problem of barrier penetration which is solved by the use of the phases β which allow the degeneracy to split slowly when one crosses the barrier.

(ii) The discontinuity in the actions which is created when one uses (46) instead of (44) needs to be compensated for by some dynamical change of the deformation. It can be shown (see § 5) that there is a domain of deformation in which one of two situations holds.

(a) There are no solutions of equation (22), neither with (44) nor with (46).

(b) There is one solution using both (44) and (46) and the same quantum numbers.

The use of the variable β completely removes these difficulties. In the limit of a circular billiard the motion described by η corresponds to a purely radial motion. Therefore in this limit $n_\eta \to n$, the radial quantum number. On the other hand, the motion described by ξ corresponds to purely angular motion and the quantum number n_ξ tends to l, the angular momentum quantum number.

All the physical effects of the billiard problem can be summarised in the following way: in the limit $\alpha = +\infty$ the semiclassical state has an elliptic caustic and every state, except for states with $l = 0$, is doubly degenerate. When the summit of the barrier is approached and crossed the symmetric and the antisymmetric states built from a state n, l correspond to phase space cells which slowly go apart. The maximum slipping of each action cell is defined by ΔI_η, ΔI_ξ such that

$$\Delta I_\eta = -\tfrac{1}{4} \qquad \Delta I_\xi = +\tfrac{1}{2} \qquad \text{for the symmetric states}$$

$$\Delta I_\eta = +\tfrac{1}{4} \qquad \Delta I_\xi = -\tfrac{1}{2} \qquad \text{for the antisymmetric states.}$$

The states $l = 0$ are all associated with symmetric states. This situation is represented in figure 2(b).

3. Prolate cavity

In this case it is convenient to use a system of prolate spheroidal coordinates (Strutinsky *et al* 1977):

$$x = f \sinh \eta \sin \xi \cos \phi \tag{47}$$

$$y = f \sinh \eta \sin \xi \sin \phi \tag{48}$$

$$z = f \cosh \eta \cos \xi \tag{49}$$

with

$$0 \leqslant \eta < \infty \qquad 0 \leqslant \xi \leqslant \pi \qquad 0 \leqslant \phi < 2\pi.$$

The canonical momenta are then $p_\phi = L_z$, the z component of the angular momentum, and p_η, p_ξ given by

$$p_\eta^2 = k^2 f^2 \cosh^2 \eta - p_\phi^2/\sinh^2 \eta - E \tag{50}$$

$$p_\xi^2 = E - k^2 f^2 \cos^2 \xi - p_\phi^2/\sin^2 \xi. \tag{51}$$

Although we will only study the cases with $p_\phi = 0$, the formulae are given for arbitrary p_ϕ.

For $L_z = 0$, we obtain the same expressions as (4) and (5) but we now have $0 \leqslant \xi \leqslant \pi$. Similarly, after writing the wavefunction as

$$\psi(\eta, \xi, \phi) = \frac{\mathscr{F}(\xi)}{(\sin \xi)^{1/2}} \frac{\mathscr{G}(\eta)}{(\sin h\eta)^{1/2}} \mathrm{e}^{\mathrm{i} p_\phi \phi} \tag{52}$$

the wave equation separates into

$$\frac{\mathrm{d}^2 \mathscr{G}}{\mathrm{d}\eta^2} + \left(k^2 f^2 \cosh^2 \eta - (E + \tfrac{1}{4}) - \frac{p_\phi^2 - \frac{1}{4}}{\sinh^2 \eta} \right) \mathscr{G} = 0 \tag{53}$$

$$\frac{\mathrm{d}^2 \mathscr{F}}{\mathrm{d}\xi^2} + \left((E + \tfrac{1}{4}) - k^2 f^2 \cos^2 \xi - \frac{p_\phi^2 - \frac{1}{4}}{\sin^2 \xi} \right) \mathscr{F} = 0. \tag{54}$$

For $p_\phi = 0$ we do not recover the classical values of the potential terms since we have the additional *centripetal* terms $\frac{1}{4} \sinh^2 \eta$ and $\frac{1}{4} \sin^2 \xi$. We must therefore modify the discussion of the WKB phase.

We note that there are three systems of turning points (points where $(1/\mathscr{G})(\mathrm{d}^2\mathscr{G}/\mathrm{d}\eta^2) = 0$ or $(1/\mathscr{G})(\mathrm{d}^2\mathscr{F}/\mathrm{d}\xi^2) = 0$), changing $E + \frac{1}{4}$ into E'.

(i) If $kf(kf - 1) < E'$ there is a turning point in the equation for η.

(ii) If $kf(kf + 1) > E'$ there is a turning point in the equation for ξ.

(iii) If $kf(kf - 1) < E' < kf(kf + 1)$ the turning points disappear.

The presence of the centripetal terms completely changes the discussion for the top of the barrier. On the other hand, it is also necessary to consider the cases of wavefunctions even under σ_h, the reflection with respect to the plane Oxy, i.e. $(\mathrm{d}\mathscr{F}/\mathrm{d}\xi)(\frac{1}{2}\pi) = 0$, and also those which are odd, with $\mathscr{F}(\frac{1}{2}\pi) = 0$.

We now write (53) and (54) for $\eta \sim 0$ and $\xi \sim 0$ as

$$\mathrm{d}^2\mathscr{F}/\mathrm{d}\xi^2 + (E' - k^2 f^2 + k^2 f^2 \xi^2 + 1/4\xi^2)\mathscr{F} = 0 \tag{55}$$

$$\mathrm{d}^2\mathscr{G}/\mathrm{d}\eta^2 (k^2 f^2 - E' + k^2 f^2 \eta^2 + 1/4\eta^2)\mathscr{G} = 0. \tag{56}$$

These equations can be reduced to the following form:

$$\mathrm{d}^2 y/\mathrm{d}x^2 + (2 - 4\beta - x^2 + 1/4x^2)y = 0 \tag{57}$$

for which it is known that a solution is

$$y \sim e^{-x^2/2} F(\beta, 1; x^2) \tag{58}$$

with F defined as a confluent hypergeometric function. Indeed, the change of variable $x = (ikf)^{1/2}\xi$ transforms (55) into (57) with

$$\beta = \tfrac{1}{2}(1 - i\alpha) \tag{59}$$

and

$$\alpha = (k^2f^2 - E')/2kf. \tag{60}$$

The same applies for equation (56), but we must define β by changing the sign of α. The asymptotic behaviour of $\mathscr{F}(\xi)$ for $\xi \gg 1$ is now written as (Abramowitz and Stegun 1972)

$$\mathscr{F}(\xi)_{\xi \gg 1} = \xi^{-1/2} \cos[\tfrac{1}{2}kf\xi^2 - \alpha \log \xi - \tfrac{1}{4}\alpha \log \xi - \tfrac{1}{4}\pi + \arg(-\tfrac{1}{2} + i\tfrac{1}{2}\alpha)!]. \tag{61}$$

Let us now write the WKB solution of (54) for $p_\phi = 0$ and ξ large enough:

$$\mathscr{F}_{\text{WKB}}(\xi) = c'(E' - k^2f^2 + k^2f^2 \sin^2 \xi)^{-1/4} \times \cos\left(\int_{\xi_0}^{\xi} (E' - k^2f^2 + k^2f^2 \sin^2 \xi')^{1/2}\, d\xi' - \beta_\xi\right). \tag{62}$$

It is possible to identify (62) with (61) in the two following limits, which is sufficient for our purpose:

$$E' > k^2f^2 \qquad E' - k^2f^2 \ll k^2f^2 \qquad \xi_0 = 0 \tag{63}$$

$$E' < k^2f^2 \qquad k^2f^2 - E' \ll k^2f^2 \qquad \xi_0 \simeq (k^2f^2 - E')/k^2f^2. \tag{64}$$

In both cases, which correspond to situations where one is near the top of the barrier, the phase of the cosine in (62) becomes identical to that of (61) if one takes

$$\beta_\xi = \tfrac{1}{4}\pi + \tfrac{1}{2}\alpha(\log \tfrac{1}{2}|\alpha| - 1) + \arg(-\tfrac{1}{2} + i\tfrac{1}{2}\alpha)!. \tag{65}$$

A similar expansion of equation (56) for the variable η leads to a phase β_η similar to (65), but with α replaced by $-\alpha$ and $\eta_0 = 0$ if $k^2f^2 > E'$ and $\eta_0 = \arg\sinh(E' - k^2f^2)/kf]$ if $k^2f^2 < E'$.

The quantisation condition of the action I_η is now written, using (20), as

$$I_\eta = n_\eta + \tfrac{1}{2} + \beta_\eta/\pi \tag{66}$$

while for the action I_ξ we obtain the following, using (21).

If Ψ is even under σ_h,

$$I_\xi = 2n_\xi + 2\beta_\xi/\pi. \tag{67}$$

If Ψ is odd under σ_h,

$$I_\xi = 2n_\xi + 1 + 2\beta_\xi/\pi. \tag{68}$$

The function $\beta(\alpha)$ defined by (65) is plotted in figure 1(b). We have the three interesting limits

$$\alpha \to +\infty \text{ or } -\infty \qquad \beta \to \tfrac{1}{4}\pi \qquad \text{and} \qquad \alpha = 0 \qquad \beta = \tfrac{1}{4}\pi. \tag{69}$$

While there is a significant change in the Maslov indices for the 'billiard' problem, the present values of β deviate little from $\frac{1}{4}\pi$. Therefore the quantisation conditions for almost every α can be written

$$I_\eta = n + \tfrac{3}{4} \tag{70}$$

$$I_\xi = l + \tfrac{1}{2} \tag{71}$$

where $l = 2n_\xi$ or $2n_\xi + 1$.

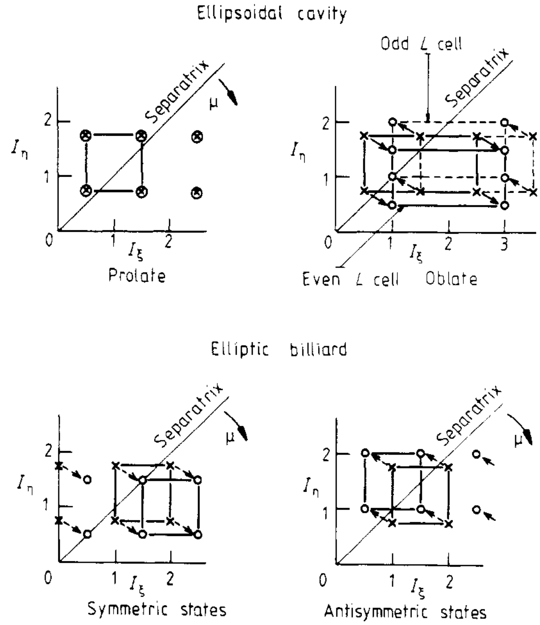

Figure 2. The lattices of quantisation of the three systems discussed in the text. Crosses and circles are points of the quantisation lattice associated to elliptic and hyperbolic caustics respectively in the primitive WKB approximation. The arrows indicate how the points should be connected through the uniform approximation. The line denoted separatrix indicates the actions of trajectories lying on the separatrix for an arbitrary deformation $\mu = R_>/R_<$. When μ increases the line rotates around the origin, as shown by an arrow. The slipping of the action cells is to be noted, if present.

Thus the summit of the barrier is crossed in a particularly smooth way in the prolate case. Numerical calculations reported in Arvieu and Ayant (1987) confirm this smooth behaviour.

We have written the quantum numbers in equations (70) and (71) as n and l because the action I_η tends to the radial action in the spherical limit while I_ξ tends to the angular action which obeys the well known rule $l+\frac{1}{2}$. We note that it is the same function β_ξ, defined by equation (65), which allows the quantisation for the even as well as the odd values of l.

If we summarise the physical effect in the same way as at the end of § 2 we say that there is a *very tiny oscillation of the phase space cell* around the values (70) and (71) when we follow a state as a function of α. These constant values are represented in the upper part of figure 2.

4. Oblate cavity

The oblate spheroidal coordinate system is now appropriate (the difference from equations (47)-(49) is that we must interchange $\sinh \eta$ with $\cosh \eta$). The expressions for p_η and p_ξ are now written

$$p_\eta^2 = k^2 f^2 \cosh^2 \eta + p_\phi^2/\cosh^2 \eta - E \tag{72}$$

$$p_\xi^2 = E - k^2 f^2 \sin^2 \xi - p_\phi^2/\sin^2 \xi. \tag{73}$$

After defining the wavefunction as

$$\Psi(\eta,\xi,\phi)=\frac{\mathcal{F}(\xi)}{(\sin\xi)^{1/2}}\frac{\mathcal{G}(\eta)}{(\cosh\eta)^{1/2}}\,e^{ip_\phi\phi} \tag{74}$$

we obtain the coupled wave equations

$$\frac{d^2\mathcal{G}}{d\eta^2}+\left(k^2f^2\cosh^2\eta-(E+\tfrac{1}{4})+\frac{p_\phi^2-\frac{1}{4}}{\cosh^2\eta}\right)\mathcal{G}=0 \tag{75}$$

$$\frac{d^2\mathcal{F}}{d\xi^2}+\left((E+\tfrac{1}{4})-k^2f^2\sin^2\xi-\frac{p_\phi^2-\frac{1}{4}}{\sin^2\xi}\right)\mathcal{F}=0. \tag{76}$$

Again, for $p_\phi=0$ we obtain a centripetal term for the variable ξ and an additional term $-\frac{1}{4}\cosh^2\eta$ in equation (75) which produces a slight change in the potential barrier for $\eta\sim 0$. The potential barriers in equation (75) and (76) complement each other exactly since (still for $p_\phi=0$)

(i) for $k^2f^2<E+\frac{1}{2}$ there is a turning point in the equation for η (75),
(ii) for $k^2f^2>E+\frac{1}{2}$ there is a turning point in the equation for ξ (76), and
(iii) for $k^2f^2=E+\frac{1}{2}$ this value defines the separatrix.

Equation (76) is the most complex. The pseudopotential $k^2f^2\sin^2\xi-1/4\sin^2\xi$ combines a maximum at $\xi=\frac{1}{2}\pi$ with a singularity for $\xi=0$ and π. The restriction of equation (76) to small values of ξ leads to the equation (we use again $E'=E+\frac{1}{4}$)

$$d^2\mathcal{F}/d\xi^2+(E'-k^2f^2\xi^2+1/4\xi^2)\mathcal{F}=0 \tag{77}$$

which also has a solution written in terms of a confluent hypergeometric function (defined below within a normalisation constant)

$$\mathcal{F}(\xi)=c'\exp(-kf\xi^2/2)\sqrt{\xi}F(\beta,1;kf\xi^2) \tag{78}$$

with

$$\beta=\tfrac{1}{2}-E'/4kf. \tag{79}$$

We can now use the asymptotic properties of F to prove the very simple result that if $W\xi^2\ll E'$ and for any E' and k^2f^2 then

$$\mathcal{F}_{\mathrm{WKB}}(\xi)\sim c'\cos(\sqrt{E'}\xi-\tfrac{1}{4}\pi). \tag{80}$$

Thus the line of singularity along the axis Oz creates a phase of $-\frac{1}{4}\pi$ only in the WKB solution.

The discussion for the wavefunction near $\xi=\frac{1}{2}\pi$ is very similar to that given in § 2. The total wavefunction ψ should be even or odd with respect to σ_h, which corresponds to the operation $\xi\to\pi-\xi$. If $\xi\approx\frac{1}{2}\pi$ we have, using $\xi'=\frac{1}{2}\pi-\xi$ and $\xi_0'=\frac{1}{2}\pi-\xi_0$,

$$d^2\mathcal{F}/d\xi'^2+(E'+\tfrac{1}{4}-k^2f^2+k^2f^2\xi'^2)\mathcal{F}=0 \tag{81}$$

which is of the parabolic cylinder type equation (30).

Its WKB solution can be written in obvious notation as

$$\mathcal{F}(\xi')=c'(p_{\xi'})^{-1/4}\cos\left(\int_{\xi_0'}^{\xi'}p_{\xi''}\,d\xi''-\beta_\xi\right) \tag{82}$$

with β_ξ given by (39) if the wavefunction is even under σ_h, or by (39) with $\theta\to\pi-\theta$ if it is odd. We must use the value of α given by

$$\alpha=[k^2f^2-(E+\tfrac{1}{2})]/2kf. \tag{83}$$

The identification of (80) and (82) leads to

$$\int_{\xi_0'}^{\pi/2} p_\xi \, d\xi - \beta_\xi - \tfrac{1}{4}\pi = n_\xi \pi \tag{84}$$

$$I_\xi = \frac{2}{\pi}\int_0^{\xi_0} p_\xi \, d\xi = 2(n_\xi + \beta_\xi/\pi + \tfrac{1}{4}). \tag{85}$$

For the variable η we have, near $\eta = 0$,

$$d^2\mathscr{G}/d\eta^2 + [k^2f^2 - (E' + \tfrac{1}{4}) + k^2f^2\eta^2]\mathscr{G} = 0. \tag{86}$$

Therefore we must again use

$$\alpha = (E + \tfrac{1}{2} - k^2f^2)/2kf \tag{87a}$$

and we have the same results as in § 2 for the action integral I_η:

$$I_\eta = n_\eta + \tfrac{1}{2} + \beta_\eta/\pi. \tag{87b}$$

According to the parity, under σ_h the phases β_η and β_ξ are $\beta_\eta = \beta_S(\alpha)$, $\beta_\xi = \beta_S(-\alpha)$ for the even parity and $\beta_h = \beta_A(\alpha)$, $\beta_\xi = \beta_A(-\alpha)$ for the odd parity, where α is given by (87).

In the limit $\alpha \to +\infty$ we obtain

$$I_\eta = n_\eta + \tfrac{3}{4} \tag{88}$$

$$I_\xi = 2n_\xi + \tfrac{1}{2} \qquad \text{when } \psi \text{ is even under } \sigma_h \tag{89a}$$

$$I_\xi = 2n_\xi + 1 + \tfrac{1}{2} \qquad \text{when } \psi \text{ is odd under } \sigma_h. \tag{89b}$$

In the limit of a spherical cavity, the motion described by η becomes the radial motion while the motion described by ξ becomes the angular motion. There the quantisation condition, (88) and (89), becomes

$$I_\eta = n + \tfrac{3}{4} \qquad I_\xi = l + \tfrac{1}{2} \tag{90}$$

where l is the quantum number associated with the angular momentum. The states which are even under σ_h are identified with the even l states and the odd states under σ_h are identified with the odd l states.

Using the notation n, l let us now write the limit $\alpha \to -\infty$. If l is even, then

$$I_\eta = n + \tfrac{1}{2} \qquad I_\xi = l + 1. \tag{91}$$

If l is odd, then

$$I_\eta = n + 1 \qquad I_\xi = l. \tag{92}$$

When α goes from $+\infty$ to $-\infty$, i.e. when we cross the separatrix, there is a slipping of the action cell from (90) to (91) for l even, and from (90) to (92) for l odd, i.e. for even l

$$\Delta I_\eta = -\tfrac{1}{4} \qquad \Delta I_\xi = +\tfrac{1}{2} \tag{93}$$

and for odd l

$$\Delta I_\eta = +\tfrac{1}{4} \qquad \Delta I_\xi = -\tfrac{1}{2}. \tag{94}$$

This slipping corresponds to a different rate of crossing the top of the barrier. The very top is obtained when the change in the action cell is exactly half that predicted by (93) and (94). Again, this slipping is represented in figure 2, along with the situation described in §§ 2 and 3.

5. Action surface

There is a last step which must be cleared up in order to disclose the common classical skeleton of the three problems: the existence of a common energy-action surface.

Let us return to the billiard problem where the action integrals I_η and I_ξ are defined by equations (20) and (21). Using (4), (5), (11), (12) and (16) they can be put in the general form

$$I_\eta = kf\mathcal{J}_\eta(e, e_0) \tag{95}$$

$$I_\xi = kf\mathcal{J}_\xi(e, e_0) \tag{96}$$

where $\mathcal{J}_\eta$ and $\mathcal{J}_\xi$ are definite integrals which depend only on the eccentricity e of the elliptic boundary and that of the caustic e_0. Equations (95) and (96) provide a parametric representation of the relation between the energy $k^2/2m$ and the actions that we write as

$$E = E(I_\eta, I_\xi, e) \tag{97}$$

the parameter being e_0. This defines the energy-action surface of the problem. The precise forms of $\mathcal{J}_\eta$ and $\mathcal{J}_\xi$ are given by Keller and Rubinov (1960) in terms of elliptic integrals. The semiclassical values of the energy of the 'billiard' problem are given by the values of E for which the actions satisfy equations (22), (25) or (28). We note that for the prolate problem we can also use this surface, but with equations (66)–(68). Finally, for the oblate problem we can use again this surface but with the rules (87) and (85).

We are therefore able to associate the surface with the classical motion common to the three problems but we must use a different lattice of quantisation for each one. Moreover, as described at the end of §§ 2-4, each of these lattices moves in a specific way when we increase the deformation.

We now meet the important problem of finding when a classical motion with specific actions is found on the separatrix. The equations to be solved (for kf and e) are

$$I_\eta = kf\mathcal{J}_\eta(e, 1) \tag{98}$$

$$I_\xi = kf\mathcal{J}_\xi(e, 1). \tag{99}$$

We find the very simple integrals for $e_0 = 1$

$$I_\eta = \frac{1}{\pi}\int_0^{\eta_1} kf \sinh\eta \, d\eta = \frac{1}{\pi} k(R_> - f) \tag{100a}$$

$$I_\xi = \frac{1}{\pi}\int_0^{\pi} kf \sin\xi \, d\xi = \frac{2}{\pi} kf. \tag{100b}$$

From equations (100) we deduce the value e_S of the eccentricity of the cavity and the value k_s of k for which a state is found on the separatrix:

$$e_S = I_\xi/(2I_\eta + I_\xi) \tag{101}$$

$$k_s f = \pi/2I_\xi. \tag{102}$$

Equation (102) and

$$\frac{I_\eta}{I_\xi} = \frac{1 - e_s}{2e_s} \tag{103}$$

define a plane in the space E, I_η, I_ξ which intersects the energy-action surface on a line which separates the surface into two regions. It can easily be seen that if

$$\frac{I_\eta}{I_\xi} > \frac{1-e_s}{2e_s} \qquad e_0 < 1 \tag{104}$$

this part is associated to motion with elliptic caustic, while that with hyperbolic caustic is found whenever

$$\frac{I_\eta}{I_\xi} > \frac{1-e_s}{2e_s} \qquad e_0 > 1. \tag{105}$$

The line $(1-e_s)/2e_s$ is shown for an arbitrary e_s in figure 2. Equation (103) shows that this line rotates around the origin. In the limit $e_s = 0$ all the caustics are circles and the line is vertical; when e_s increases the caustics become elliptic in general and those associated with motion with small angular momentum and high radial action are the first to cross the separatrix. The higher the angular momentum, the larger the eccentricity e_s needed to cross the separatrix.

This picture is purely classical. The specific contribution of the semiclassical quantisation is to tie specific values to the actions through a quantisation lattice which also moves in the plane I_η, I_ξ according to the rules defined above. The slipping of the lattice is either in the same sense as the rotation of the separatrix, which indicates a delay in crossing this singularity (like the symmetric states in the 'billiard', or as the even l states of the oblate ellipsoid) or else in the opposite direction (like the antisymmetric states in the billiard and the odd l states of the prolate ellipsoid, which indicates an advance for the crossing. These differences are observed in the quantum spectrum, as is shown in Arvieu and Ayant (1987), and they bring about marked differences in the spectrum of an oblate spheroid compared to that of the prolate spectrum. All this will be discussed later.

References

Abramowitz M and Stegun I 1972 *Handbook of Mathematical Functions* (New York: Dover) p 693
Arvieu R and Ayant Y 1987 *J. Phys. A: Math. Gen.* **20** to be published
Berry M V 1981 *Eur. J. Phys.* **2** 91-102
Carbonell J 1983 *Thèse de 3ème cycle* Université de Grenoble
Carbonell J, Brut F, Arvieu R and Touchard J 1984 *J. Physique Coll.* C6 **45** 371-8
—— 1985 *J. Phys. G: Nucl. Phys.* **11** 325-42
Child M S 1974 *J. Mol. Spectrosc.* **53** 280-93
Ford K W, Hill D L, Wakano M and Wheeler J A 1959 *Ann. Phys., NY* **7** 239-58
Keller J B 1958 *Ann. Phys., NY* **4** 180-8
Keller J B and Rubinow S I 1960 *Ann. Phys., NY* **9** 24-75
Miller W H 1968 *J. Chem. Phys.* **48** 1651-8
Strutinsky, V M, Magner A G, Ofengenden S R and Dossing T 1977 *Z. Phys.* A **283** 269-82