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WKB method for integrable but non-separable Hamiltonians

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Abstract. A recently proposed extension of the WKB method to integrable but non-separable Hamiltonian systems, based on the construction of global solutions of Dirichlet problems for the Hamilton–Jacobi equation, is applied to the construction of semiclassical wavefunctions for the Barbanis Hamiltonian. The wavefunctions obtained are compared with those generated for the same system, by means of the coherent Gaussian method, by Davis and Heller. It is shown that when the caustics are smooth curves, there is no energy degeneration, and the semiclassical wavefunctions obtained by the extended WKB method agree with those by Davis and Heller. But if internal caustics are present and to the same semiclassical energy level correspond, not simply to one as in the coherent Gaussian method, but several (four in the example investigated) WKB wavefunctions, they differ in the regions inside the internal caustics.

1. Introduction

The semiclassical quantization of generic, non-separable, Hamiltonians, is an old problem, whose interest has been renewed by the study of the so-called quantum chaos [1]. In this framework, a new method has been recently proposed [2], which extends the WKB scheme and is suitable for the tori quantization of integrable or near integrable but non-separable systems. This generalization depends on the explicit construction of global solutions of Dirichlet boundary value problems for the Hamilton–Jacobi (HJ) equation, and exploits recent achievements in this field. For separable Hamiltonians, the solutions have been found to reduce to the usual WKB solutions. In [2] the method has been applied to the well known Henon–Heiles Hamiltonian, getting lists of energy levels and some wavefunctions. When the comparison is possible, the energy eigenvalues obtained moderately agree with those computed by means of different approaches.

In [2], the method's applications were confined to the simplest cases, in which the caustics, which envelope the families of classical trajectories, are smooth curves, without self-intersections, and there are no internal caustics. In the present paper these more complex cases are also investigated, and the method is applied to a different Hamiltonian, i.e. the so-called Barbanis system.

In order to make the paper self-contained, in section 2 the method is briefly resumed; for simplicity, the two-dimensional case is discussed, the extensions being obvious. The results and some details about the numerical procedure are collected in section 3.

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2. WKB method for non-separable Hamiltonians

As is well known, the ordinary WKB method [3] can only be applied to one-dimensional or separable multi-dimensional Hamiltonians. In order to extend it to a generic integrable or near integrable non-separable system, we start as usual by searching for stationary states' wavefunctions of the form $\Psi(\boldsymbol{q}) = \exp(\frac{\mathrm{i}}{\hbar}\sigma(\boldsymbol{q}))$ where the phase σ is written as an asymptotic series in $\hbar$

$$\sigma(\boldsymbol{q}) = W(\boldsymbol{q}) + \frac{\hbar}{\mathrm{i}}\sigma_1(\boldsymbol{q}) + \cdots \tag{1}$$

The zero order term W is a solution of the time-independent HJ equation

$$\tfrac{1}{2}(\nabla W)^2 + V = E \tag{2}$$

where $V(\boldsymbol{q})$ is the potential and E is the particle's total energy.

Let us consider one of the Liouville or KAM phase space tori [4] of the system: its projection on the coordinate space is bounded by caustics, i.e. envelopes of trajectories' families, which delimit the configuration space region allowed for these trajectories. See for example figure 1, where one of these projections is reported, which refers to a family of trajectories for the Barbanis Hamiltonian

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + \tfrac{1}{2}(\omega_x x^2 + \omega_y y^2) + \lambda x^2 y. \tag{3}$$

The equipotential line at the same energy is also reported. The caustics touch this line in four points, which we will call vertices. At first, let us suppose that all the caustics' arcs are smooth curves, without self-intersections. In each caustics' point (x_c, y_c), the momentum

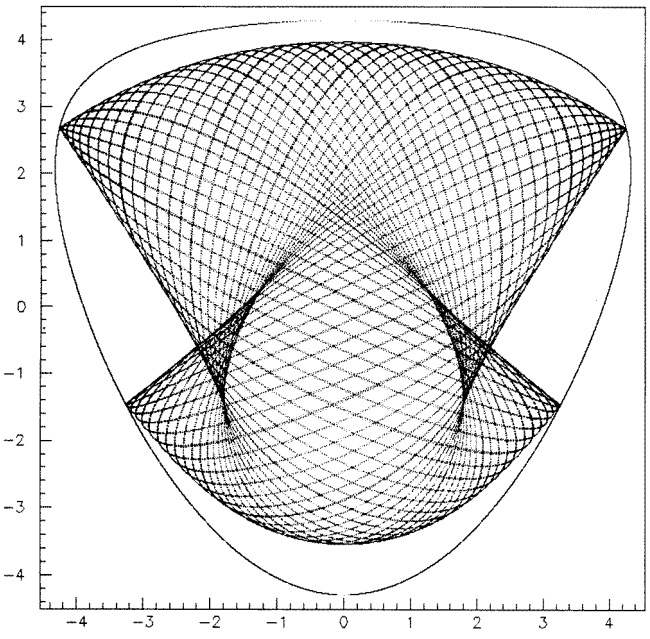

Figure 1. The initial parts of a trajectories' family for the Barbanis Hamiltonian (3), with the energy $E = 9.211$. The equipotential line is also reported.

$\boldsymbol{p}$ is uniquely defined, apart from the sign being that of the trajectory through the point. Starting from a vertex i ($i = 1 \ldots 4$), it is therefore possible to compute the function

$$w_i(x_c, y_c) = \int_i^{x_c, y_c} \boldsymbol{p}\, \mathrm{d}\boldsymbol{q} \tag{4}$$

where the integration is done along the caustics' arcs, coming out the vertex i. The function $w_i(x_c, y_c)$ is then used as boundary data of a Dirichlet problem for the HJ equation (2), in which a solution $W_i(\boldsymbol{q})$ inside the region bounded by the caustics is searched, knowing its values on the boundary. This solution, i.e. the Hamilton characteristic function or (reduced) action, is obtained in two steps: first, according to the characteristic curves' method, for each internal point $\boldsymbol{q}$ the following quantities are (in principle) computed [4, 5]

$$W_i(\boldsymbol{q}) = w_i(x_c, y_c) + \int_{x_c, y_c}^{q} \boldsymbol{p}\, \mathrm{d}\boldsymbol{q} \tag{5}$$

where the integrations are done along all the family's trajectories connecting $\boldsymbol{q}$ to some caustics' points (x_c, y_c). As well known, configuration space trajectories in general intersect, so that equation (5) provides a multivalued solution of the given boundary value problem. However, as shown by Benton [6], it is possible to extract from (5) a global one-valued solution, by taking into account, for each point $\boldsymbol{q}$, only the trajectory which gives the minimum value of $W_i(\boldsymbol{q})$ with respect to the other trajectories meeting there; the elimination of the superfluous trajectories is the second step of our procedure. When the caustics are smooth, the $W_i(\boldsymbol{q})$ so generated are continuous, while they have lines of discontinuity if the caustics present self-intersections. The Benton's method gives a criterion to cover all the classical region with non-intersecting trajectories, i.e. by means of vector fields $\boldsymbol{p}_i = \nabla W_i$. This criterion is not unique, and in the presence of internal caustics which are generated by foldings of the original phase space torus, it has to be relaxed, in order to obtain all the fundamental branches of the action through equation (5) (see below).

The solutions can be continued outside the classical region, by integration in equation (5) along the imaginary trajectories which correspond to complex-values solutions of the Hamilton equations [7]; since at the first order in the expansion (1), $W_i(\boldsymbol{q})$ is the phase of the semiclassical wavefunction, the oscillating or exponential or oscillating–exponential behaviour of the wavefunctions is in this way recovered.

The Benton's approach, based on the classical trajectories, in the framework of the semiclassical mechanics is preferable to the other recently discovered method to generate global solutions of Cauchy or boundary problems for the HJ equation, i.e. the (vanishing) viscosity method [8].

By changing the vertex i in the previous construction, one obtains the four branches $W_i(\boldsymbol{q})$ of a multivalued action $W(\boldsymbol{q})$; each pair W_i, W_{i+2}, where $i = 1, 2$, obtained by starting the construction from a vertex and its opposite, uses the same trajectories, run in both ways, and the two actions are simply related each other. Instead, each pair ($W_1(\boldsymbol{q})$, $W_4(\boldsymbol{q})$) or ($W_2(\boldsymbol{q})$, $W_3(\boldsymbol{q})$), represents a pair of independent global solutions of the HJ equation in the same region of the configuration space. Incidentally, their knowledge, assumed by De Leon and Heller [9], allows us to introduce the nodal coordinates discussed there. For our purposes, the $W_i(\boldsymbol{q})$ permits us to generate the semiclassical wavefunction which, at the first order of the expansion (1) can be written as

$$\sum_j A_j(\boldsymbol{q}) \exp\left(\frac{\mathrm{i}}{\hbar} W_j(\boldsymbol{q})\right) \tag{6}$$

where the coefficients A_j near the vertices, can be determined as in [10], by matching the semiclassical solutions with the solutions of the Schroedinger equation, which are there the

product of two Airy functions.

As shown by Keller [11], these semiclassical wavefunctions can be quantized, by imposing the usual EBK conditions to the two irreducible loops of the originary phase space torus; otherwise, by projecting down from the phase space, as shown in [10], the quantization conditions can be equivalently written in the configuration space, as for instance,

$$\int_1^2 \boldsymbol{p}_1 \, \mathrm{d}\boldsymbol{q} = \overline{h}\pi[n + \tfrac{1}{2}] \tag{7}$$

$$\int_1^4 \boldsymbol{p}_1 \, \mathrm{d}\boldsymbol{q} = \overline{h}\pi[m + \tfrac{1}{2}] \tag{8}$$

where $\boldsymbol{p}_1 = \nabla W_1$, m and n are integers, and the line integrals are done on any arc connecting the contiguous vertices $(1, 2)$, and $(1, 4)$.

A more complex case occurs when the caustics have self-intersections, so that part of them are internal, as in figure 1. This is due to folds of the original phase space manifold. In this case, the boundary data $w_i(x_c, y_c)$ are constructed as before, on the external caustics, but at the discontinuity points, where the momentum $\boldsymbol{p}$ suddenly changes its direction, also the boundary values $w_i(x_c, y_c)$ have a jump Δw_i; this can be seen by considering the results of integrating the form $\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}$ along the originary phase space curve which projects on that caustic's arc.

Moreover, as seen from the figure, in this case, each point $\boldsymbol{q}$ inside the internal caustics is crossed not by two, but by four trajectories, belonging to four families, which are equal in pairs in the two-sheeted region, and differ in the four-sheeted region. A possible choice for them is reported in the figures 2(*a*)–(*d*). Each trajectory starts from the external caustics and ends on it or on a side of the internal caustics, and each family covers the classical region without intersection. Other choices are possible, by combining the trajectories differently in the four-sheeted regions, but this would not change the wavefunctions. In this case the Benton's criterion would generate only the strictly minimal branch of the action and has to be relaxed: in order to construct, through equation (5), all the fundamental branches of the multivalued Hamilton's characteristic function, each of these trajectories' families has to be used. It is clear that by means of equation (5), all the other branches of the action can be generated, but their values in each point $\boldsymbol{q}$ will differ from the fundamental ones only by the addition of multiple integers of the action variables $\boldsymbol{I}$. Each trajectories' family can be run in both ways, and, therefore, generates two actions $W_{i,j}(\boldsymbol{q})$, $W_{i+2,j}(\boldsymbol{q})$ where $i = 1, 2$, $j = 1 \ldots 4$, the first index labelling the vertex, and the second the chosen trajectories family. The various actions $W_{i,j}(\boldsymbol{q})$ so generated are discontinuous along different sides of the internal caustics. In order to obtain a semiclassical wavefunction, the two actions corresponding to a given family have to be combined as in (6) with the two actions corresponding to another family, different from the first in the two-sheeted regions. In this case therefore, four semiclassical wavefunctions, corresponding to the same degenerate energy level, can be generated: they coincide in the two-sheeted part of the classical region, and differ in the four-sheeted ones; moreover, they are discontinuous along two or three sides of the internal caustics. This degeneration is purely semiclassical and it is absent when one considers the quantum wavefunction. Indeed, in order to restore a one-to-one correspondance between the semiclassical approximation and the quantum wavefunction, the average of the four WKB functions can be taken, but its introduction tends to mask the connection between the quantum state, in the limit $\overline{h} \to 0$, and the underlying classical trajectories.

When the amplitudes $A_i(\boldsymbol{q})$ are computed by numerically integrating the continuity equation for the probability flux, it is found that all these WKB wavefunctions diverge on

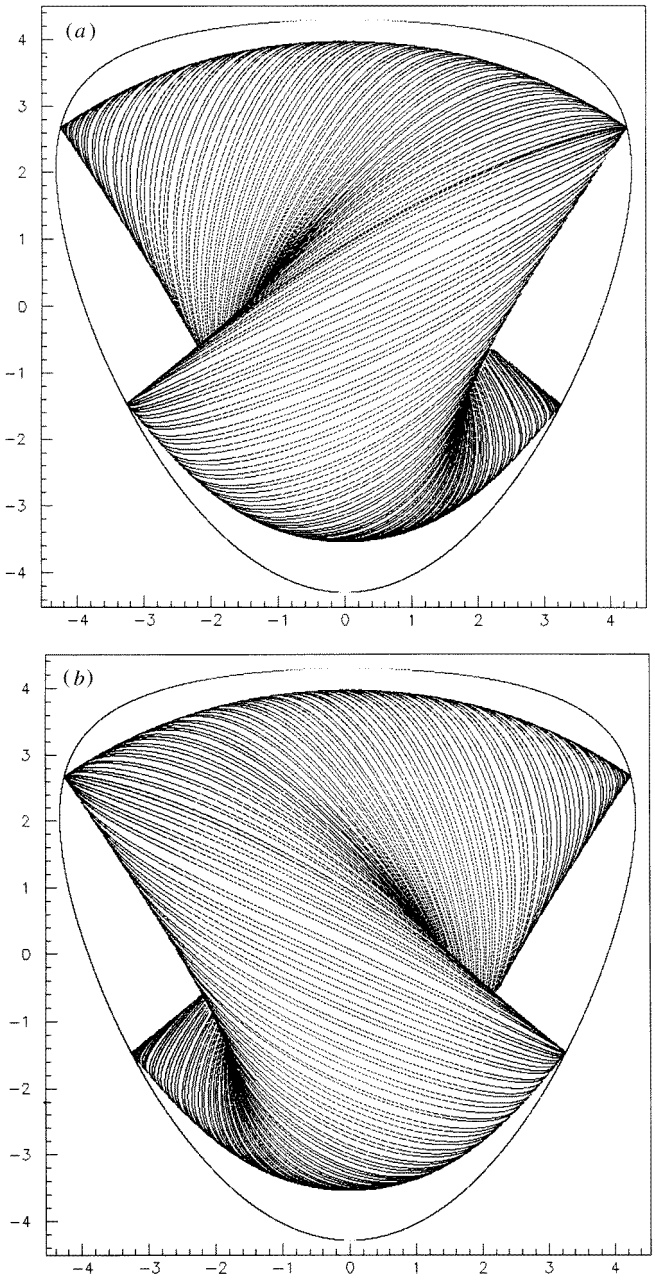

Figure 2. (*a*)–(*d*) The four families of trajectories, extracted from those in figure 1, employed to generate the global solutions for the HJ equation.

the external caustics, and on their respective discontinuity lines belonging to the internal caustics, which signals the local failure of the semiclassical approximation.

Finally, let us observe that the covering procedure described above could also be followed in the previously discussed case of smooth caustics, but in this case it would generate the same results as the Benton's criterion. This latter is instead unavoidable when

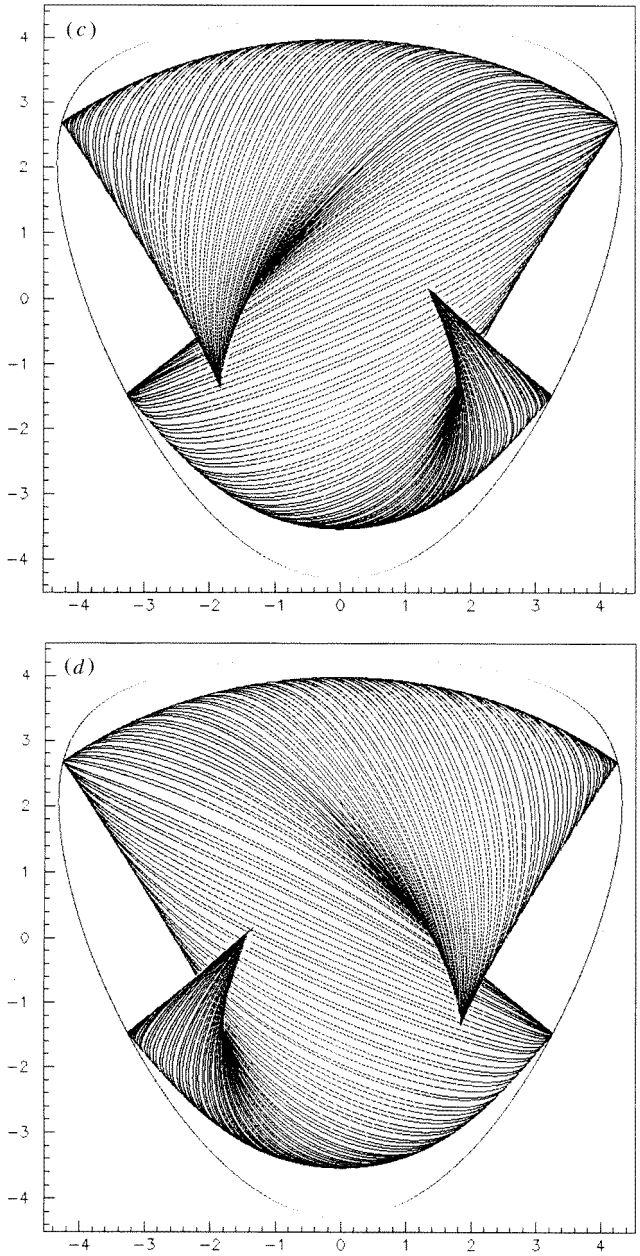

Figure 2. (Continued)

one tries, by means of equation (5), to construct global solutions of Cauchy or Dirichlet problems for the HJ equation in the general situations, when there are no phase space tori.

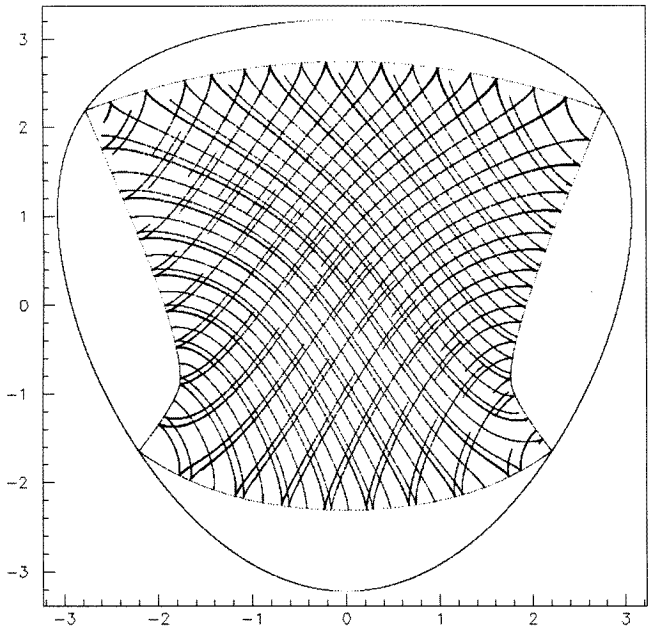

Figure 3. A system of Hamiltonian wavefronts, i.e. the contour lines of the Hamilton characteristic function. The fronts have values between $W = 0$ and $W = 50$, with increments $\Delta W = 1$. The energy is $E = 5.185$.

3. Numerical results

The method described in the previous section has been applied to the construction of some semiclassical wavefunctions for the Barbanis Hamiltonian (3), three of which are presented in this paper. For the same system, semiclassical wavefunctions have been generated by Davis and Heller [12] by a different method. The same parameters' values as in [12] were used, i.e. $\omega_x = 1.1$, $\omega_y = 1.0$, $\lambda = -0.11$, and $\overline{h} = 1$.

The procedure starts by choosing an energy value E. Then a trajectory at that energy is numerically followed in order to generate the caustics, which are obtained by recording the zeroes of the Jacobi equation for the given trajectory [13]. In each caustics' point the momentum $\boldsymbol{p}$ is also recorded; then the procedures exposed in the previous section is applied, by choosing a vertex i and constructing the boundary data $w_i(x_c, y_c)$ by means of equation (4). If the quantization conditions (7) and (8) are satisfied, equation (5) is used, by numerically following a number (some hundreds) of trajectories starting from the caustics, and integrating along them the form $\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}$. In order to facilitate the elimination of the superfluous trajectories, and to represent the solutions, it is convenient to construct Hamiltonian wavefronts, which are the contours of Hamilton's characteristic function W. The wavefronts are orthogonal to the trajectories and their properties and construction are exposed in [14]. Their convenience lies in that a single wavefront shows the behaviour of a whole family of trajectories. Moreover, each intersection of two wavefronts corresponds to two trajectories meeting in the same point with different values of the action W, which makes the elimination of the superfluous trajectories easier. In figure 3, for instance, a system of wavefronts is reported, which refer to a trajectories' family of energy $E = 5.185$. The wavefronts in the figure have action values between $W = 1$ and $W = 50$, with

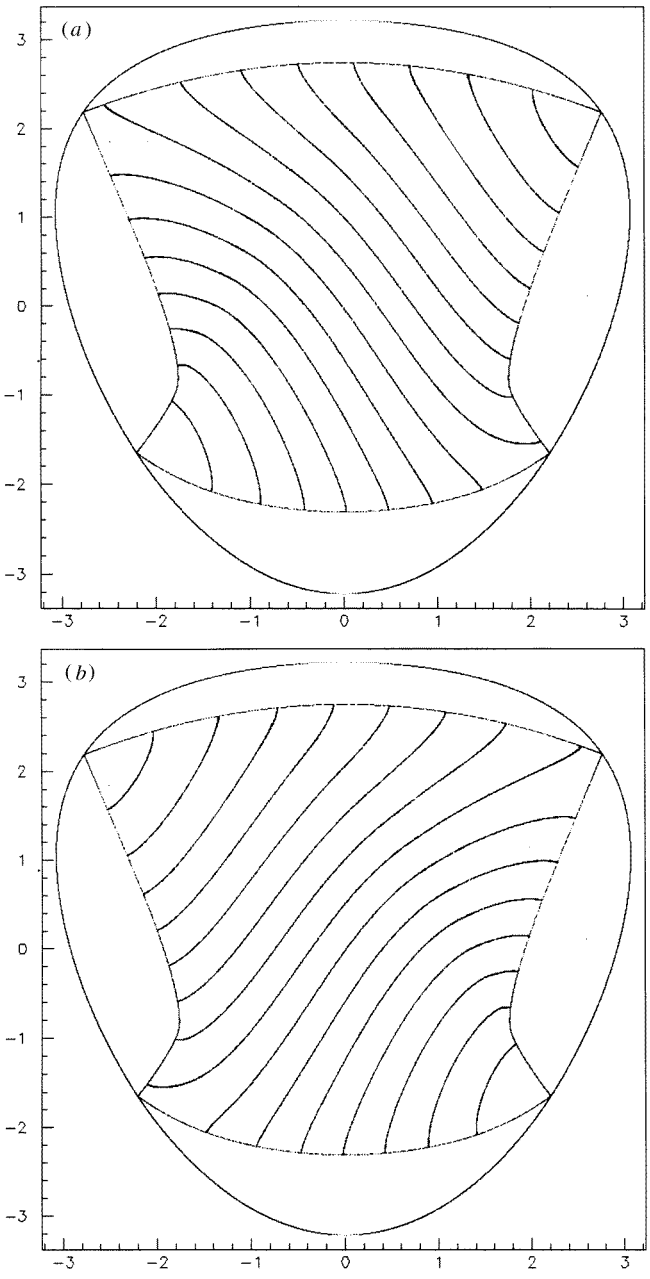

Figure 4. (*a*), (*b*) Wavefronts for two independent solutions W_i, obtained by means of the procedure described in the text. The fronts in figure 4(*a*) refer to the solution generated starting from the lower-left vertex, which therefore has $W = 0$, while the opposite vertex has $W = 15.737$. In figure 4(*b*) the fronts are generated starting from the lower-right vertex.

increments $\Delta W = 1.0$. However, figures 4(*a*) and (*b*) report the wavefronts corresponding to the pair of independent solutions $W_1(\boldsymbol{q})$ and $W_4(\boldsymbol{q})$, obtained in the same case by means of the Benton's elimination procedure. The fronts are smooth curves, which 'start' from

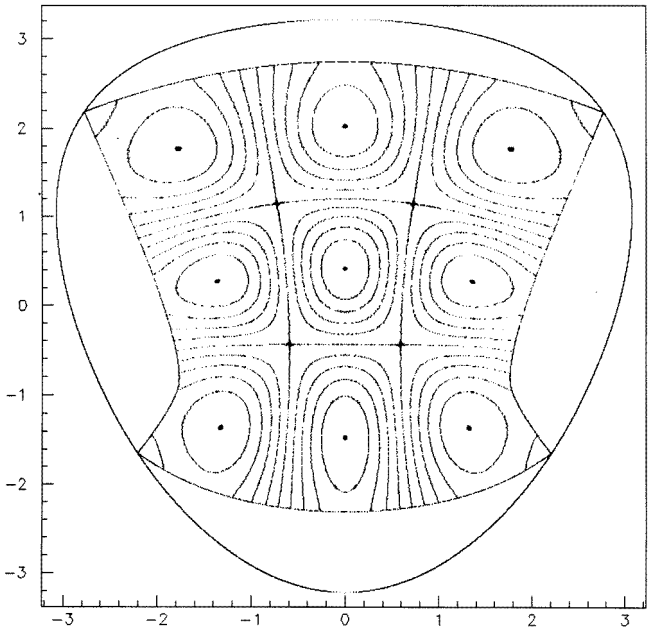

Figure 5. Contour lines for the wavefunction (2, 2), with the energy $E = 5.185$, for the Barbanis Hamiltonian (3). The nodal lines go from a caustic's arc to the opposite one.

the lower-left vertex (figure 4(a)) and from the lower-right vertex (figure 4(b)), which have $W_i = 0$, and 'end' in the opposite vertex, spanning the whole classically allowed region; the figures clearly show that the W_i are continuous and one-value in each point. In figure 5 the contours of the corresponding wavefunction, which, according to equations (7) and (8), has the quantum numbers (2, 2). The nodal lines, which go from a caustic's arc to the opposite one, are clearly seen, together with the alternating system of maxima and minima.

When the energy increases, internal caustics appear, as seen in figure 1; in this case, as discussed in the previous section, it is necessary to relax the Benton's criterion, and the procedure starts by choosing the non-intersecting trajectories' families, covering all the classical region. As seen in the previous section, to the trajectories in figure 1 four semiclassical wavefunctions correspond. In figures 6(a) and (b) the contour lines of two of them are reported; to make the comparison easier, in figure 6(b) the internal caustics are also drawn. The quantum numbers are (4, 4), and the energy $E = 9.211$ compares well with the value $E = 9.215$ ascribed to this state in [12]. As clearly shown by the figures, the wavefunctions differ in the regions bounded by the internal caustics: this is also true for the other two wavefunctions, not reported here. These WKB wavefunctions agree with that generated for the same state by Davis and Heller, as reported in figure 2 of their paper, only in the two-sheeted region of the configuration space; instead, near and inside the internal caustics they correspond to quite different distributions of the probability density. Due to the method used, in which the semiclassical wavefunction is approximated as a linear superposition of Gaussian wavepackets, centred on equally time-spaced positions along the classical trajectory, the wavefunctions obtained in this and similar cases by Davis and Heller can be considered as an average of the various degenerate WKB wavefunctions.

In summary, the results presented in this paper and in the previous one [2] show that the extended WKB method allows the tori quantization of non-separable Hamiltonians, giving

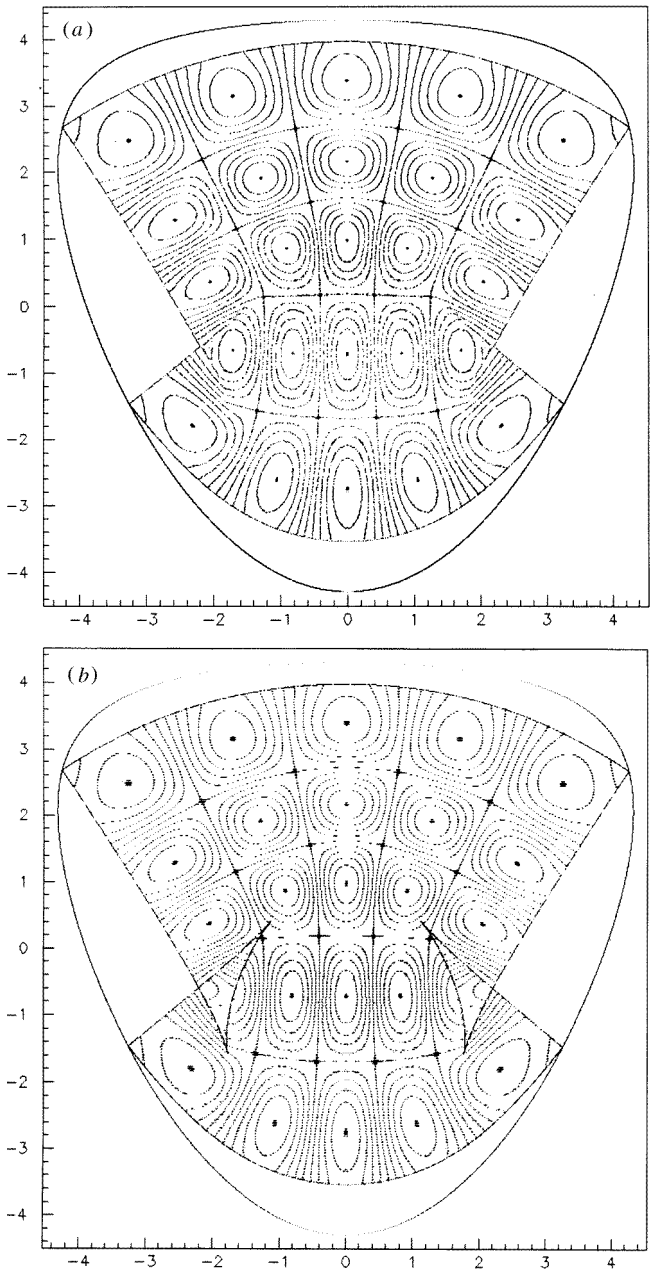

Figure 6. (*a*), (*b*) Contour lines for two degenerate semiclassical wavefunctions, with the quantum numbers (4, 4) and energy $E = 9.211$, for the Barbanis system (3). In figure 6(*b*) the internal caustics, which bound the region where the wavefunctions differ, are also reported.

the energy levels and wavefunctions. The energy levels so computed, fairly agree with those computed by means of other semiclassical approaches [2]. As for the wavefunctions, the method is able to reveal the fine structure and the presence of energy degenerations, which are not seen by means of other approaches.

In conclusion, let us note that a possible future application of the extended WKB method is the investigation of multi-dimensional semiclassical tunnelling, when the integrable but non-separable potentials present multiple wells: the extended EBK quantization rules, which give the energy levels in these cases, have been found by Creagh [15] by means of analytic continuation of Lagrangian manifolds, and by Meyer [16], with an approach based on the use of complex trajectories; the method here presented may be useful to construct the corresponding wavefunctions. Work in this direction is in progress.

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