Third-order equation for harmonic generation: complex canonical transformation and JWKB solution

2004 J. Phys. A: Math. Gen. 37 2611

(http://iopscience.iop.org/0305-4470/37/7/007)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 2611–2624 PII: S0305-4470(04)70173-0

Third-order equation for harmonic generation: complex canonical transformation and JWKB solution

Gabriel Álvarez[1] **and Ramón F Álvarez-Estrada**[2]

[1] Departamento de Física Teórica II, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain
[2] Departamento de Física Teórica I, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain

Received 7 October 2003
Published 4 February 2004
Online at stacks.iop.org/JPhysA/37/2611 (DOI: 10.1088/0305-4470/37/7/007)

Abstract

The quantum description of third harmonic generation can be formulated as an eigenvalue problem for a third-order linear differential equation. We perform a semiclassical study of this third-order equation, generalizing the familiar JWKB theory for the second-order Schrödinger equation, and deriving explicit (albeit approximate) formulas for the eigenvalues within this semiclassical context. A central role in this analysis is played by a nonlinear complex canonical transformation which permits a complete description of the classical motion (generated by a complex polynomial Hamiltonian function) in the complexified position and momentum planes.

PACS numbers: 03.65.Sq, 03.65.Ge, 03.65.−w

1. Introduction

The quantum description of third harmonic generation, an optical process whereby three photons of angular frequency one interact in a nonlinear medium to yield a photon of angular frequency three, can be formulated as an eigenvalue problem for a third-order linear differential equation [1]. Although the calculation of the corresponding eigenvalues and eigenvectors can ultimately be reduced to the diagonalization of a finite matrix [1, 2], explicit expressions of these eigenvalues and eigenvectors are not known, but the existence of the differential equation opens up the possibility of using semiclassical methods to obtain formulas which, albeit approximate, are explicit.

In fact, there is a rigorous theory for the asymptotic solution of high-order differential equations [3–5], but this theory is rather difficult to implement in practice. Specifically, there is not a general and practical method to solve eigenvalue problems by Jeffreys–Wentzel–Kramers–Brillouin (JWKB) techniques for differential equations of order higher than 2, but rather a collection of results applicable to some classes of equations and systems. We mention the results compiled by Fedoryuk [6], the study of boundary value problems for third-order equations by Strelitz [7], the three-level scattering systems solved by Joye and Pfister [8] and Aoki *et al* [9], and the works of Dorey and Tateo [10, 11] and Dorey *et al* [12]. Of special interest for our purposes is the development of connection formulas to track the behaviour of the JWKB solutions through Stokes lines in the complex plane [13], and particularly the observation made by Berk *et al* [14] that new Stokes lines were required for a consistent treatment of equations of order higher than 2. Most recently Aoki *et al* [15–17] have developed a general setting for the complete description of the Stokes geometry of high-order equations via integral representations of the solutions, but again the practical application in cases like ours is not immediate.

In our previous paper on third harmonic generation [1] we bypassed this problem: by separating the two degrees of freedom of the classical real Hamiltonian that describes third harmonic generation, we were able to perform a Bohr–Sommerfeld quantization of the classical orbits. As a result of this study we found a complex canonical transformation that formally related the separated classical and quantum equations through the standard quantization rules. Drawing on these results, in this paper we study in depth this complex canonical transformation, and show that it provides the clues for a JWKB study of the third harmonic quantum equation. In fact, working within this semiclassical framework, we are able to derive the same approximate formulas for the eigenvalues.

There has recently been an interest in the properties of classical Hamiltonian systems under complexification of the canonical variables, usually with the procedure of setting $x = x_1 + \mathrm{i}p_2$ and $p = p_1 + \mathrm{i}x_2$, where (x_1, p_1) and (x_2, p_2) are pairs of standard real canonical variables. Kaushal and Korsch [18] used this complexification to obtain a new class of two-dimensional integrable systems; Kaushal and Singh [19] were able to find new complex invariants; and most recently Kaushal and Parthasarati [20] investigated the ground state of some potentials in the same framework of extended complex phase space. Complex canonical variables are also used to represent normal modes [21], but perhaps the paper whose approach is closest to ours is the study of the complex pendulum by Bender [22], in which the author makes a detailed analysis of the classical paths in the complex coordinate plane of oscillators with Hamiltonians $H = p^2 - (\mathrm{i}x)^N$.

There are two main differences, however, between these earlier complexifications and ours: firstly, our complex canonical transformation is nonlinear, leading from the complicated (real) Hamiltonian to a simpler (complex) polynomial Hamiltonian for which all the semiclassical equations can be solved explicitly; and secondly, this new, polynomial Hamiltonian is not quadratic, but cubic in the new complex momentum (hence the third order of the quantized differential equation), and therefore the complex velocity and momentum are not proportional. We will show in due course the relevance of this fact for the JWKB wavefunction. The organization of the paper is as follows. In section 2 we use the Segal–Bargmann representation to derive the third-order linear differential equation for third harmonic generation. Section 3 reviews the separation of degrees of freedom in the classical Hamiltonian, highlighting the essential features of the corresponding phase map. We stress that sections 2 and 3 not only summarize and clarify (for the reader's benefit) the essentials of [1], but also extend at several points the results therein. In section 4 we study the nonlinear complex canonical transformation which relates the classical and quantum Hamiltonians through the standard quantization rules, paying special attention to the description of the classical motion in the complex coordinate and complex momentum planes. Section 5 is devoted to the semiclassical theory, which we present as closely as possible to the familiar JWKB theory for the second-order Schrödinger equation [23, 24]. Finally, we summarize our results and point out an interesting line for future development in section 6.

2. Quantum theory of third harmonic generation

The Hilbert space for a boson in the Segal–Bargmann representation [25] is the space of entire functions of the form

$$f(z) = \sum_{n=0}^{\infty} \frac{c_n}{\sqrt{n!}} z^n \qquad \left(z \in \mathbf{C}, \sum_{n=0}^{\infty} |c_n|^2 < \infty \right) \tag{1}$$

with the scalar product defined by

$$\langle g, f \rangle = \frac{1}{\pi} \int_{\mathbf{R}\times\mathbf{R}} \mathrm{d}(\mathrm{Re}\, z)\, \mathrm{d}(\mathrm{Im}\, z) \overline{g(z)} f(z)\, \mathrm{e}^{-|z|^2}. \tag{2}$$

In [1, 2] it is shown that the third harmonic generation effective Hamiltonian, usually defined in terms of creation and annihilation operators in Fock space, can be represented by a differential operator acting in the direct product of two copies of the Segal–Bargmann space. More concretely, the third harmonic generation Hamiltonian H is a sum

$$H = H_0 + gH_1 \tag{3}$$

of an unperturbed part H_0 which describes two uncoupled harmonic oscillators of angular frequencies one and three respectively, and a perturbation H_1 whereby three photons of angular frequency one yield a photon of angular frequency three. The strength of this perturbation is given by the coupling constant g.

In the Segal–Bargmann space the action of the unperturbed Hamiltonian is given by the partial differential operator

$$H_0 = z_1 \frac{\partial}{\partial z_1} + \frac{1}{2} + 3\left(z_2 \frac{\partial}{\partial z_2} + \frac{1}{2} \right) \tag{4}$$

with unperturbed eigenvalues and orthonormal eigenfunctions

$$E_0 = n_1 + \frac{1}{2} + 3\left(n_2 + \frac{1}{2} \right) \qquad (n_1, n_2 = 0, 1, 2, \ldots) \tag{5}$$

$$\varphi_{n_1,n_2}(z_1, z_2) = \frac{z_1^{n_1} z_2^{n_2}}{\sqrt{n_1! n_2!}} \qquad (n_1, n_2 = 0, 1, 2, \ldots) \tag{6}$$

and the perturbation Hamiltonian is likewise represented by the partial differential operator

$$H_1 = z_2 \frac{\partial^3}{\partial z_1^3} + z_1^3 \frac{\partial}{\partial z_2}. \tag{7}$$

The key feature of this model from the physical point of view is the energy conservation. Since the unperturbed Hamiltonian and the perturbation commute ($[H_0, H_1] = 0$), the problem can be reduced to the diagonalization of the perturbation H_1 restricted to the finite-dimensional subspaces of constant unperturbed energy E_0. There are three kinds of such subspaces, which depend on a parameter κ (incidentally, only the case $\kappa = 0$ was considered in [1]): if $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x and

$$k = \left\lfloor \frac{n_1}{3} + n_2 \right\rfloor \tag{8}$$

then the eigenfunctions of H_1 are polynomials of the form

$$p_\kappa(z_1, z_2) = z_1^\kappa \sum_{m=0}^{k} c_m z_1^{3(k-m)} z_2^m \qquad (\kappa = 0, 1, 2) \tag{9}$$

with unperturbed energies

$$E_0 = 3k + 2 + \kappa \qquad (\kappa = 0, 1, 2). \tag{10}$$

Equations (6), (7) and (9) show that the actions of the perturbation H_1 within these subspaces are given by $(k+1) \times (k+1)$ selfadjoint matrices $\left[H_1^{(\kappa)}\right]$ whose only nonzero elements are

$$\left[H_1^{(\kappa)}\right]_{i,i+1} = \left[H_1^{(\kappa)}\right]_{i+1,i} = \sqrt{i \prod_{m=1}^{3} (3k - 3i + m + \kappa)} \quad (i = 1, \ldots, k). \tag{11}$$

This explicit tridiagonal matrix representation generalizes for $\kappa \neq 0$ the matrix given in [1], and entails in particular that the eigenvalues are real, simple, and symmetrically distributed around zero [1, 2].

These results can also be derived, with a similar effort, working with the second quantization formalism in Fock space. The main advantage of the Segal–Bargmann representation is that it permits the separation of the two degrees of freedom of the system, arriving at a single ordinary differential equation for the perturbation eigenvalue problem [1, 2]. For our purposes, the most convenient way to separate variables is the following change of independent and dependent variables:

$$z = z_1 z_2^{-1/3} \tag{12}$$

$$p_\kappa(z_1, z_2) = z_2^{k+\kappa/3} Q_\kappa(z) \tag{13}$$

where $Q_\kappa(z)$ is z^κ times a polynomial of degree k in z^3. Substituting equations (12) and (13) into the differential equation $H_1 p_\kappa = E p_\kappa$, or explicitly,

$$\left(z_2 \frac{\partial^3}{\partial z_1^3} + z_1^3 \frac{\partial}{\partial z_2} \right) p_\kappa(z_1, z_2) = E p_\kappa(z_1, z_2) \tag{14}$$

we arrive at a third-order ordinary differential equation for $Q_\kappa(z)$,

$$Q_\kappa^{(3)}(z) - \frac{1}{3} z^4 Q'_\kappa(z) + \left(k + \frac{\kappa}{3}\right) z^3 Q_\kappa(z) = E Q_\kappa(z). \tag{15}$$

Note that the change of variables (12)–(13) has been chosen so that the third-order linear differential equation (15) is in 'normal form', i.e. with the second derivative missing. The condition that $Q_\kappa(z)$ must be z^κ times a polynomial of degree k in z^3 will play a crucial role in section 5.3.

We finish this section with a slight notational simplification. Hereafter we drop the label κ and consider explicitly only the case $\kappa = 0$, i.e. in the rest of the paper we work with the somewhat simpler equation

$$Q^{(3)}(z) - \tfrac{1}{3} z^4 Q'(z) + k z^3 Q(z) = E Q(z). \tag{16}$$

The remaining two cases $\kappa = 1$ and $\kappa = 2$ can be recovered by making the replacements $k \to k + 1/3$ and $k \to k + 2/3$ (respectively) into the final semiclassical expressions for the eigenvalues.

3. Classical theory of third harmonic generation

The classical Hamiltonian function corresponding to the quantum operator defined by equations (3), (4) and (7) is

$$H_c = \frac{1}{2}\left(p_1^2 + x_1^2\right) + \frac{3}{2}\left(p_2^2 + x_2^2\right) + \frac{g}{2}\left(x_1^3 x_2 - p_1^3 p_2 + 3 p_1 x_1^2 p_2 - 3 p_1^2 x_1 x_2\right) \tag{17}$$

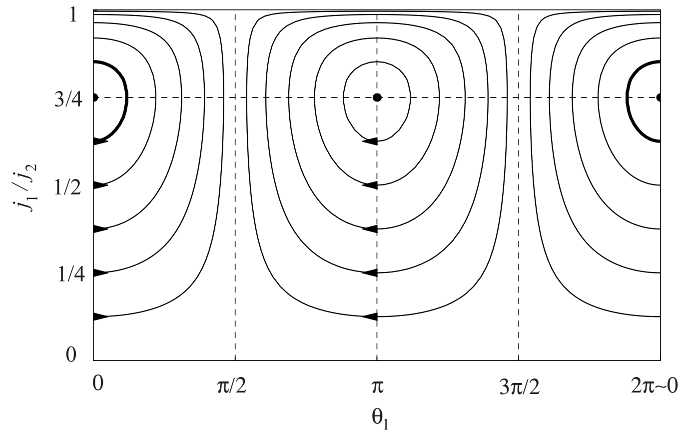

Figure 1. Phase map of the perturbation Hamiltonian $H_{c,1}(\theta_1, j_1)$ for a fixed value of $j_2 = 3 + 2/3$, which corresponds to $\kappa = 0$, $k = 3$ in the quantum case. The vertical dashed lines are separatrices. Trajectories are drawn through the following $(\theta_1, j_1/j_2)$ values: (0, 1/8), (0, 1/4), (0, 3/8), (0, 1/2), (0, 5/8) and (0, 3/4) (constant trajectory marked by a dot), as well as the symmetric trajectories with initial $\theta_1 = \pi$. The thick line highlights the trajectory through (0, 5/8), which is the preimage of the complex trajectory shown in figure 2.

where x_i and p_i are Cartesian coordinates and momenta. In [1] we have shown that in suitable canonical coordinates (θ_1, j_1), (θ_2, j_2), this classical Hamiltonian function is given by

$$H_c = 3j_2 + g6\sqrt{3}j_1^{3/2}(j_2 - j_1)^{1/2}\cos\theta_1 \tag{18}$$

where the canonical coordinate θ_2 is cyclic and therefore the conjugate action j_2 is a constant of the motion, concretely one-third of the unperturbed energy. The nontrivial canonical coordinates are the phase difference between the modes θ_1 and its conjugate momentum j_1, and the perturbation Hamiltonian function is

$$H_{c,1}(\theta_1, j_1) = 6\sqrt{3}j_1^{3/2}(j_2 - j_1)^{1/2}\cos\theta_1. \tag{19}$$

In [1] we also gave a detailed discussion of this Hamiltonian and its corresponding equations of motion, including proofs of the classical counterparts of the properties of the eigenvalues cited in the previous section, but for the purpose of the present paper it will be enough to highlight some features of the phase map for the Hamiltonian (19) that we show in figure 1. (Incidentally, the trajectories in figure 1 of [1] were drawn at equally-spaced values of the perturbation energy; the trajectories in figure 1 of the present paper, as discussed below, are drawn at equally-spaced, easily identifiable values of the action j_1 at $\theta_1 = 0$ and π.)

First note that the periodic angular coordinate θ_1 runs from 0 to 2π, and that the action j_1 runs from 0 to j_2. Therefore, the phase space is topologically a cylinder.

From equation (19) it is easy to see that the perturbation energy is bounded by

$$-\frac{27}{8}j_2^2 \leqslant E \leqslant \frac{27}{8}j_2^2. \tag{20}$$

The trajectories in the θ_1 interval $(\pi/2, 3\pi/2)$ have negative energy, the vertical separatrices at $\theta_1 = \pi/2$ and $\theta_1 = 3\pi/2$ correspond to zero energy, and the symmetric trajectories in the θ_1 interval $(0, \pi/2) \cup (3\pi/2, 2\pi)$ have positive energy.

In figure 1 we have drawn the trajectories through the following (θ_1, j_1) values: $(0, j_2/8)$, $(0, j_2/4)$, $(0, 3j_2/8)$, $(0, j_2/2)$, $(0, 5j_2/8)$ and $(0, 3j_2/4)$ (constant trajectory for which the maximum energy is reached, marked by a dot), as well as the symmetric trajectories with the same initial values of j_1, initial $\theta_1 = \pi$, and, consequently, opposite energies. For concreteness and due to this symmetry of the phase map we will focus on the basin surrounding the constant trajectory $(0, 3j_2/4)$, and use the corresponding innermost oval for our graphical illustrations in the next section, which goes through $(0, 5j_2/8)$.

4. Complex canonical transformation

At this point it is a natural question whether there exists a direct connection between the result of the quantum separation, i.e. the differential equation (16), and the result of the classical separation, i.e. the perturbation Hamiltonian function (19). However, this is indeed the case: in [1] we introduced the following transformation to new classical but complex variables (X, P):

$$X = \mathrm{e}^{\mathrm{i}\theta_1/3}(3j_1)^{1/2}(j_2 - j_1)^{-1/6} \tag{21}$$

$$P = \mathrm{e}^{-\mathrm{i}(\theta_1/3+\pi/2)}(3j_1)^{1/2}(j_2 - j_1)^{1/6} \tag{22}$$

which leads to the same classical Hamiltonian expressed as a complex function

$$H_{c,1} = -\mathrm{i}P^3 - \frac{\mathrm{i}}{3}X^4 P + j_2 X^3. \tag{23}$$

If we write this Hamiltonian function in symmetrized form, substitute the classical unperturbed energy $E_0 = 3j_2$ in terms of the quantum unperturbed energy $E_0 = 3k + 2$, and quantize formally, i.e. if in the expression

$$H_{c,1} = -\mathrm{i}P^3 - \frac{\mathrm{i}}{6}(X^4 P + P X^4) + \left(k + \frac{2}{3}\right) X^3 \tag{24}$$

we apply the usual quantization rules

$$X \to z \tag{25}$$

$$P \to -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z} \tag{26}$$

and act on $Q(z)$ with the resulting operator, we recover the left-hand side of equation (16). As a necessary preparation for the semiclassical study of equation (16), we devote this section to a more detailed study of the transformation defined by equations (21)–(22).

First note that the transformation (21)–(22) is complex canonical, in the sense that

$$\frac{\partial X}{\partial \theta_1}\frac{\partial P}{\partial j_1} - \frac{\partial X}{\partial j_1}\frac{\partial P}{\partial \theta_1} = 1 \tag{27}$$

and that the inverse transformation is given by

$$j_1 = \frac{\mathrm{i}}{3} X P \tag{28}$$

$$\theta_1 = -\frac{\mathrm{i}}{2}\ln\left[\left(\frac{X}{P}\right)^3 \left(\mathrm{i}j_2 + \frac{PX}{3}\right)\right]. \tag{29}$$

(Of course, this inverse transformation is also complex canonical.)

Geometrically, equation (21) maps the (θ_1, j_1) phase space onto the sector $0 \leqslant \arg X \leqslant 2\pi/3$ of the complex X plane (the shaded region in figure 2(c)), where $\arg X = 0$ has to be identified with $\arg X = 2\pi/3$.

Likewise, equation (22) maps the (θ_1, j_1) phase space onto the finite sector $-7\pi/6 \leqslant \arg P \leqslant -\pi/2$, $|P| \leqslant |P_{\max}| = 3(j_2/4)^{2/3}$ of the complex P plane (the shaded region in figure 2(d)), where $\arg P = -7\pi/6$ has to be identified with $\arg P = -\pi/2$.

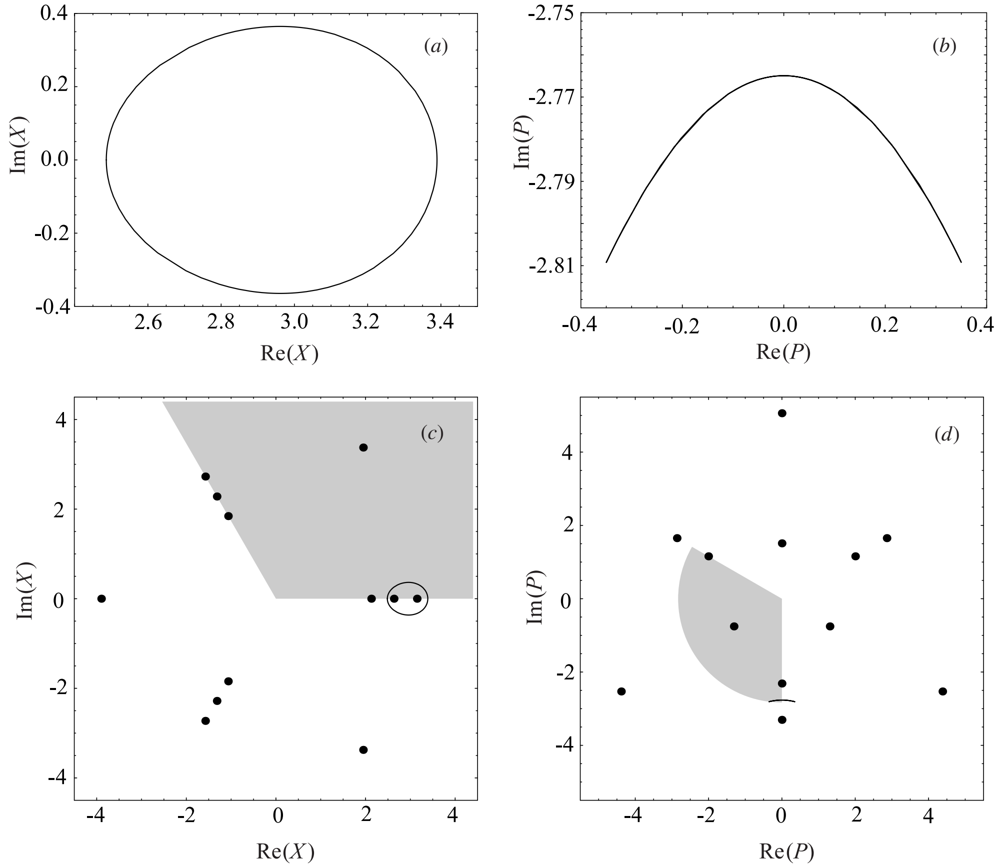

Figure 2. Image of the complex canonical transformation from the real (θ_1, j_1) canonical variables to the complex (X, P) variables defined by equations (21) and (22) respectively. Figures 2(a) and (b) show the images in the complex X and P planes of the trajectory through the point $(\theta_1, j_1) = (0, 5j_2/8)$ in figure 1 (the innermost oval around the constant trajectory). The shaded areas in figures 2(c) and (d) represent the images of the (θ_1, j_1) phase space, where $\arg X = 0$ is identified with $\arg X = 2\pi/3$ and $\arg P = -7\pi/6$ is identified with $\arg P = -\pi/2$. The dots in these two figures mark the turning points at which the first-order semiclassical wavefunction diverges (cf section 5.2, where the turning points are formally defined); the oval in figures 2(a) and (c) traversed in the positive sense is the integration path used in equation (55).

Note that not all pairs of points (X, P) in the respective shaded areas are formed by the images of a point (θ_1, j_1) in the phase space of figure 1 (for example, for j_1 to be real there is a necessary condition that $\arg X + \arg P = -\pi/2$). The complex canonical condition (27), however, ensures that if we start from an initial value $(X(0), P(0))$ which is the image of a point $(\theta_1(0), j_1(0))$, and integrate the complex Hamilton equations derived from the complex Hamiltonian (23),

$$\dot{X}(t) = -3\mathrm{i}P(t)^2 - \frac{\mathrm{i}}{3}X(t)^4 \tag{30}$$

$$\dot{P}(t) = -3j_2X(t)^2 + \frac{4\mathrm{i}}{3}P(t)X(t)^3 \tag{31}$$

then the whole trajectory $(X(t), P(t))$ is the image by equations (21) and (22) of $(\theta_1(t), j_1(t))$ or, conversely, the latter trajectory can be recovered from the former by the inverse transformation (28) and (29). Likewise, the action integrals over both trajectories are equal

$$\oint j_1 \, \mathrm{d}\theta_1 = \oint P \, \mathrm{d}X. \tag{32}$$

Figures 2(*a*) and (*b*) show the images in the complex X and P planes, respectively, of the trajectory through the point $(\theta_1, j_1) = (0, 5j_2/8)$ in figure 1 (the innermost oval around the constant trajectory). The image in the X plane is itself an oval, traversed once clockwise in a period. The image in the P plane is also a closed curve: the arc in the plot is traversed twice in opposite senses. Also note that the ends of the arc are the points most distant from the origin, and precisely at a distance $|P_{\max}|$, (in the case of the figure, where $j_2 = 3 + 2/3$, $|P_{\max}| \approx 2.83$). These same images are also plotted in figures 2(*c*) and (*d*), although in the latter case the scale makes it difficult to see the shape. In both cases the parts of the curves outside the shaded areas have to be understood as folded by periodicity over the identified ray into the other edge of the shaded area. (We have kept them continuous because it is more convenient for the discussion in the next section, where the dots, which mark the turning points, are defined.)

5. Semiclassical theory of third harmonic generation

Our study of the complex canonical transformation in the previous section has prepared us to deal with the semiclassical theory of the quantum third harmonic generation equation (16) derived in section 2. We will follow as closely as possible the lead of the familiar JWKB theory for the second-order Schrödinger equation, according to the following layout: first we will scale equation (16) to put it in suitable form for subsequent calculations; then, in section 5.2, we will discuss the form of the JWKB wavefunction for a third-order equation, drawing attention to the modified definition of turning points; in section 5.3 we will solve the characteristic equation and find the turning points for equation (16); and finally, in section 5.4, we will use these results to set up and evaluate the quantization condition.

5.1. Scaling

Our semiclassical parameter will be $1/k$ or, in other words, the JWKB expansions will be large k expansions, which by equation (8) physically correspond to a large number of photons. Therefore, we scale the coordinate z and the energy E in equation (16) by suitable powers of k so that the derivatives are paired with like powers of k^{-1}. The appropriate scaling is

$$z = k^{1/3} x \tag{33}$$

$$\psi(x) = Q(z) \tag{34}$$

$$E = k^2 \Lambda \tag{35}$$

and the scaled quantum equation is

$$\psi^{(3)}(x) - \frac{k^2}{3} x^4 \psi'(x) + k^3 (x^3 - \Lambda) \psi(x) = 0. \tag{36}$$

We mention that this scaling is the reason to introduce the typographical distinction with the complex X coordinate (which corresponds to the variable z) of section 4. Hereafter, whenever we refer to features in figure 2, it is to be understood that the suitable unscaling has been performed.

5.2. The form of the JWKB wavefunction

The essence of the semiclassical, Liouville–Green, or JWKB approximation [26] is to write the wavefunction in exponential form

$$\psi(x) = \exp\left[\mathrm{i}k\int^x p(s)\,\mathrm{d}s\right] \tag{37}$$

and subsequently expand the integrand as an asymptotic power series in k^{-1}

$$p(x) = p_0(x) + k^{-1}p_1(x) + k^{-2}p_2(x) + \cdots. \tag{38}$$

This expansion is substituted into the differential equation; terms with equal powers of k are collected, and the resulting equations for the $p_i(x)$ are solved recursively.

By substituting the exponential form of the wavefunction (37) into the scaled differential equation for third harmonic generation (36), we find that the unknown function $p(x)$ must satisfy the exact equation

$$k^3\left[x^3 - \Lambda - \frac{\mathrm{i}}{3}x^4 p(x) - \mathrm{i}p(x)^3\right] - 3k^2 p(x)p'(x) + \mathrm{i}kp''(x) = 0. \tag{39}$$

In turn, substitution of the asymptotic expansion (38) into equation (39) shows that the zeroth-order term satisfies the characteristic equation

$$x^3 - \Lambda - \frac{\mathrm{i}}{3}x^4 p_0(x) - \mathrm{i}p_0(x)^3 = 0 \tag{40}$$

and that the remaining terms can be written as explicit functions of $p_0(x)$ and its derivatives. We defer momentarily the solution of this characteristic equation and proceed to the calculation of the next term $p_1(x)$, which can be written in at least two equivalent ways [6]:

$$p_1(x) = \mathrm{i}\frac{p_0(x)p_0'(x)}{p_0(x)^2 + (x^4/9)} \tag{41}$$

$$= \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\left[\ln\sqrt{p_0(x)^2 + (x^4/9)}\right] - \mathrm{i}\frac{2x^3}{x^4 + 9p_0(x)^2}. \tag{42}$$

Note that, in contrast to second-order equations, here the whole term $p_1(x)$ is not a total derivative of a logarithm. Using the last form, which is closer to the well-known expression for second-order equations, we find that the first-order JWKB solution to the differential equation (36) can be written in the form

$$\psi_{\mathrm{JWKB}}(x) = \frac{1}{\sqrt{p_0(x)^2 + (x^4/9)}}\exp\left[\int^x\left(\mathrm{i}kp_0(s) + \frac{2s^3}{s^4 + 9p_0(s)^2}\right)\mathrm{d}s\right] \tag{43}$$

where $p_0(x)$ is a solution of the characteristic equation (40). Pursuing the analogy with the familiar theory for second-order equations, we remark that the JWKB wavefunction (43) diverges at the points where the argument of the square root vanishes,

$$p_0(x)^2 + \frac{x^4}{9} = 0. \tag{44}$$

These points are called the turning points of the JWKB solution, and their physical interpretation is simple: they are the points where the complex velocity vanishes, cf equation (30). Note that in the second-order theory, where the turning points are defined by the condition $p_0(x) = 0$, velocity and momentum are proportional, which is no longer true for the Hamiltonian (23).

5.3. Solutions of the characteristic equation and turning points

We calculate first the turning points which, as we have discussed in the preceding section, are the pairs of values (x, p) that satisfy the characteristic equation (40) and the zero velocity condition (44). That is to say, we have to find the solution of the system of polynomial equations

$$x^3 - \Lambda - \frac{\mathrm{i}}{3}x^4 p - \mathrm{i}p^3 = 0 \tag{45}$$

$$-\frac{\mathrm{i}}{3}x^4 - \mathrm{i}3p^2 = 0. \tag{46}$$

This system can be solved explicitly as a function of the scaled energy Λ, and we find that there exist 12 turning points given by

$$x^3 = \frac{27}{4}\left(-1 \pm \sqrt{1 + \frac{8}{27}\Lambda}\right) \tag{47}$$

$$p = \frac{\mathrm{i}}{3}x^2 \tag{48}$$

and

$$x^3 = \frac{27}{4}\left(1 \pm \sqrt{1 - \frac{8}{27}\Lambda}\right) \tag{49}$$

$$p = -\frac{\mathrm{i}}{3}x^2 \tag{50}$$

where in both cases the three cubic roots of each of the double signs are valid. These points have been marked by dots in the complex X and P planes of figures 2(*c*) and (*d*).

We finally turn to the solution of the characteristic equation (40). This is a cubic equation in p and therefore the three solutions can be written in terms of radicals [27]. Since the asymptotic behaviours of these roots are

$$p \sim \frac{\mathrm{i}x^2}{\sqrt{3}}, \quad -\frac{\mathrm{i}x^2}{\sqrt{3}}, \quad -\frac{3\mathrm{i}}{x} \qquad \text{as} \quad x \to +\infty \tag{51}$$

and, as we pointed in section 2, we are ultimately interested in solutions $\psi(x)$ which are polynomials of degree $3k$ in x, the correct root $p_0(x)$ is identified by

$$p_0(x) \sim -\frac{3\mathrm{i}}{x} \qquad \text{as} \quad x \to +\infty. \tag{52}$$

Consequently, if we denote

$$r(x) = \left[\sqrt{\left(\frac{x^4/3}{3}\right)^3 - \left(\frac{x^3 - \Lambda}{2}\right)^2} - \mathrm{i}\left(\frac{x^3 - \Lambda}{2}\right)\right]^{1/3} \tag{53}$$

where the principal determination of the roots is understood, then

$$p_0(x) = r(x) - \frac{(x^4/9)}{r(x)}. \tag{54}$$

5.4. Quantization condition

As we mentioned in the Introduction, there is not a simple and general method to formulate quantization conditions (or, equivalently, to impose suitable boundary conditions) for JWKB solutions of differential equations of order higher than two. We also mentioned the recent work of Aoki *et al* as particularly promising [15–17], which is well-defined for ordinary differential equations with polynomial coefficients (as is the case of the third harmonic generation equation (36)), although its practical implementation is not immediate.

We follow again the pattern of the usual JWKB theory for second-order equations, and impose the quantization condition for equation (36) in the form

$$\oint \frac{\psi'(x)}{\psi(x)}\,\mathrm{d}x = \mathrm{i}k \oint p(x)\,\mathrm{d}x = 2\pi \mathrm{i} n \qquad (n = 0, \ldots, \lfloor k/2 \rfloor) \tag{55}$$

where the contour integrals are taken along the complex classical trajectory of figure 2(*c*) but traversed in the positive sense (which in this case is opposite to the classical motion).

We will work consistently to order k^{-1}, and therefore replace in equation (55) the wavefunction ψ by the JWKB equation (43). It is elementary to check that the last term in the expression of $p_1(x)$ given in equation (42) can be written exactly as

$$-\mathrm{i}\frac{2x^3}{x^4 + 9p_0(x)^2} = \frac{2}{3}p_0(x) - \frac{2}{3}\Lambda\frac{\partial p_0(x)}{\partial \Lambda} + \frac{\mathrm{i}}{3}\frac{\partial (p_0(x)^4)}{\partial \Lambda} \tag{56}$$

so that working to order k^{-1} and using the notation

$$J(\Lambda) = \frac{1}{2\pi}\oint p_0(x)\,\mathrm{d}x \tag{57}$$

the quantization condition (55) can be written as

$$kJ(\Lambda) + \left[-\frac{1}{2} + \frac{2}{3}J(\Lambda) - \frac{2}{3}\Lambda J'(\Lambda) + \frac{\mathrm{i}}{6\pi}\frac{\partial}{\partial\Lambda}\oint p_0(x)^4\,\mathrm{d}x\right] + O(k^{-1}) = n \tag{58}$$

where the first term in the bracket is the result of the integration of the derivative of the logarithmic term in equation (42), and the prime denotes derivative with respect to Λ. At first sight it seems difficult to solve this condition for Λ as an explicit function of n. To do so we use a result, which can be checked by series expansion in Λ:

$$\frac{\mathrm{i}}{2\pi}\frac{\partial}{\partial\Lambda}\oint p_0(x)^4\,\mathrm{d}x = -2\Lambda J'(\Lambda). \tag{59}$$

Substituting equation (59) into equation (58), the latter can be rewritten as

$$J(\Lambda)\left(1 + \frac{2}{3k}\right) - \frac{4\Lambda}{3k}J'(\Lambda) + O(k^{-2}) = \frac{1}{k}\left(n + \frac{1}{2}\right) \tag{60}$$

or using backwards a Taylor expansion

$$J\left(\Lambda\left(1 + \frac{2}{3k}\right)^{-2}\right) + O(k^{-2}) = \frac{\left(n + \frac{1}{2}\right)}{\left(k + \frac{2}{3}\right)}. \tag{61}$$

Therefore we have reduced the problem to the evaluation of the integral (57), which we do in the form of a power series to facilitate the inversion.

To this aim we return to figure 2(*c*). Note that, again in contrast to the usual JWKB theory for second-order equations, here the relevant turning points do not lie on the trajectory but inside the domain limited by it. These two turning points inside the classical path are given by

$$x_\pm = \frac{3}{2^{2/3}}\left(1 \pm \sqrt{1 - \frac{8}{27}\Lambda}\right)^{1/3} \tag{62}$$

which are branch points of the square root in the definition of $r(x)$ (cf equation (53)). When the scaled energy Λ increases towards its maximum value $27/8$, the turning points coalesce towards $x_+ = x_- = 3 \times 2^{-2/3}$, which corresponds to the constant trajectory (0, 3/4) in figure 1. We take this limit as an expansion centre by introducing a parameter λ through

$$\Lambda = \frac{27}{8}(1 - \lambda). \tag{63}$$

Next, we deform the integration path to the two segments above and below the cut between the turning points, and parameterize the integral (57)

$$J(\lambda) = \frac{1}{\pi} \operatorname{Re}\left[(x_- - x_+)\int_0^1 p_0(x_+(1-s) + x_- s)\,\mathrm{d}s\right]. \tag{64}$$

Then we substitute equation (63) into equations (53), (54) and (62), and these equations in turn into the parameterized expression for the action integral (64), expand the right-hand side as a power series in λ and integrate term by term. Thus we can calculate as many terms as desired of the expansion of the action, the lowest four of which are

$$J(\lambda) = \frac{\sqrt{3}}{4\sqrt{2}}\left(\lambda + \frac{31}{144}\lambda^2 + \frac{6001}{62\,208}\lambda^3 + \frac{2988\,055}{53\,747\,712}\lambda^4 + \cdots\right). \tag{65}$$

And now we reverse this series to obtain $\lambda(J)$, and use equation (63) to find the convergent power series for $\Lambda(J)$, the inverse function of the function $J(\Lambda)$ defined by equation (57):

$$\Lambda(J) = \frac{27}{8}\left(1 - 4\sqrt{\frac{2}{3}}J + \frac{62}{27}J^2 + \frac{235}{729\sqrt{6}}J^3 + \frac{88\,315}{472\,392}J^4 + \cdots\right). \tag{66}$$

Equipped with this result, it is straightforward to solve the implicit quantization condition (61): just make in equation (66) the replacements

$$\Lambda \to \Lambda\left(1 + \frac{2}{3k}\right)^{-2} \tag{67}$$

$$J \to \frac{n + \frac{1}{2}}{k + \frac{2}{3}}. \tag{68}$$

Finally, the relation $E = k^2\Lambda$ between the scaled and unscaled eigenvalues leads us to the explicit semiclassical formula

$$E = \frac{27}{8}\left(k + \frac{2}{3}\right)^2\left(1 - 4\sqrt{\frac{2}{3}}J_n + \frac{62}{27}J_n^2 + \frac{235}{729\sqrt{6}}J_n^3 + \frac{88\,315}{472\,392}J_n^4 + \cdots\right) \tag{69}$$

where

$$J_n = \frac{n + \frac{1}{2}}{k + \frac{2}{3}} \qquad (n = 0, 1, \ldots, \lfloor k/2 \rfloor). \tag{70}$$

As a consistency check, we point out that this result coincides with the series obtained by a Bohr–Sommerfeld quantization of the (θ_1, j_1) orbits in [1], where numerical examples of its accuracy are given.

We would like to stress that the derivation in this section has been done entirely within the semiclassical framework, without any appeal to the correspondence principle, and all features of equation (69) come from a consistent application of the quantization condition (55).

6. Summary

Except for some differential equations whose solutions admit integral representations, there are few third-order differential equations for which a semiclassical treatment can be carried out in full. In our previous work on third harmonic generation we used the Segal–Bargmann representation of quantum mechanics to show that this process can be classified as an eigenvalue problem for a linear third-order differential equation. The key point here is the introduction of a new coordinate $z = z_1 z_2^{-1/3}$, which is a ratio of adequate powers of the Segal–Bargmann variables that describe each mode—so that, in effect, z carries information on the difference between the phases of the oscillators—and permits the separation of the two degrees of freedom. Likewise, the classical Hamiltonian for third harmonic generation can be separated into two one-dimensional problems, and in this case the appropriate coordinates are precisely the phase difference θ_1 and its conjugate momentum. In an attempt to find a direct connection between these quantum and classical descriptions, we also found a nonlinear complex canonical transformation that allowed us to quantize the new complex classical Hamiltonian function with the standard quantization rules and recover the linear third-order differential equation.

In this paper we have made a closer study of this complex canonical transformation, which in turn led us to an explicit semiclassical treatment of the quantum third-order differential equation. The essential feature of the complex canonical transformation is that, for correct initial values of the complexified variables, all the dynamics can be followed in the complex X and P planes with the complexified Hamiltonian, and the inverse (also complex canonical) transformation maps it to the original, real trajectories.

Having at our disposal a description of the classical motion in the complex X plane, we have performed the semiclassical study of the quantum third-order differential equation by following, as closely as possible, the lead furnished by the familiar JWKB theory for the Schrödinger equation. We have discussed the form of the first-order JWKB wavefunction, showing that the zeroth-order term involves the solution of a polynomial equation (the characteristic equation) and that the turning points have to be defined as points of zero complex velocity, not of zero complex momentum (in the Schrödinger equation velocity and momentum are proportional and both definitions are equivalent). Both the polynomial equation for the zeroth-order term $p_0(x)$ and the system of polynomial equations to find the turning points can be solved in closed form, which allowed us to implement the quantization condition by evaluating the action integral along the trajectory in the complex X plane.

As an especially interesting topic for future research we would like to mention the explicit tracking of the JWKB wavefunction across the Stokes graph following the ideas put forward by Berk *et al* [14] and developed by Aoki *et al* [15–17]. More concretely, these authors have developed a formalism valid in general for linear differential equations with polynomial coefficients but, because of the structure of their equations, the practical implementation in concrete cases has been limited to equations where the polynomial coefficients have degree of at most two. We consider an interesting problem to see if their ideas can be recast in a form that can be easily applied to the differential equation for third harmonic generation, where the polynomial coefficients have degrees up to four.

Acknowledgment

We thank the Spanish Ministerio de Ciencia y Tecnología for financial support under projects BFM2002-02646 and FPA2000-0956.

References

[1] Álvarez G and Álvarez-Estrada R F 2001 *J. Phys. A: Math. Gen.* **34** 10045
[2] Álvarez G, Finkel F, González-López A and Rodríguez M A 2002 *J. Phys. A: Math. Gen.* **35** 8705
[3] Guillemin V and Sternberg S 1977 *Geometric Asymptotics* (Providence: American Mathematical Society)
[4] Leray J 1981 *Lagrangian Analysis and Quantum Mechanics. A Mathematical Structure Related to Asymptotic Expansions and the Maslov Index* (Cambridge: MIT Press)
[5] Maslov V P 1994 *The Complex WKB Method for Nonlinear Equations I (Linear Theory)* (Basel: Birkhäuser)
[6] Fedoryuk M V 1993 *Asymptotic Analysis* (New York: Springer-Verlag)
[7] Strelitz S 1999 *Asymptotics for Solutions of Linear Differential Equations Having Turning Points with Applications* (Providence: American Mathematical Society)
[8] Joye A and Pfister C-E 2000 *Asymptotic Analysis* **23** 91
[9] Aoki T, Kawai T and Takei Y 2002 *J. Phys. A: Math. Gen.* **35** 2401
[10] Dorey P and Tateo R 1999 *Nucl. Phys.* B **563** 573
Dorey P and Tateo R 2001 *Nucl. Phys.* B **603** 581 (erratum)
[11] Dorey P and Tateo R 2000 *Nucl. Phys.* B **571** 583
[12] Dorey P, Dunning C and Tateo R 2001 *J. Phys. A: Math. Gen.* **34** 5679
[13] Berk H L and Pfirsch D 1980 *J. Math. Phys.* **21** 2054
[14] Berk H L, Nevins W M and Roberts K V 1982 *J. Math. Phys.* **23** 988
[15] Aoki T, Kawai T and Takei Y 1998 *Asian J. Math.* **2** 625
[16] Aoki T, Kawai T and Takei Y 2000 *Toward the Exact WKB Analysis of Differential Equations, Linear or Nonlinear* ed C J Howls, T Kawai and Y Takei (Kyoto: Kyoto University Press) p 11
[17] Aoki T, Kawai T and Takei Y 2001 *J. Math. Phys.* **42** 3691
[18] Kaushal R S and Korsch H J 2000 *Phys. Lett.* A **276** 47
[19] Kaushal R S and Singh S 2001 *Ann. Phys., NY* **288** 253
[20] Kaushal R S and Parthasarathi 2002 *J. Phys. A: Math. Gen.* **35** 8743
[21] Shapiro V E 2001 *Phys. Lett.* A **290** 288
Shapiro V E 2002 *Phys. Lett.* A **295** 60 (erratum)
[22] Bender C M 1999 *Phys. Rep.* **315** 27
[23] Messiah A 1959 *Mécanique Quantique, Tome 1* (Paris: Dunod)
[24] Fröman N and Fröman P O 1996 *Phase-Integral Method* (New York: Springer)
[25] Hall B C 2000 *Contemporary Mathematics* **20** 1
[26] Fröman N and Fröman P O 2002 *Physical Problems Solved by the Phase-Integral Method* (Cambridge: Cambridge University Press)
[27] Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (New York: Dover)