Semiclassical analysis of a quasi-exactly solvable system: second harmonic generation

Gabriel Alvarez and Ramón F Alvarez-Estrada

Departamento de Física Teórica, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain

Abstract. The usual second harmonic generation effective Hamiltonian is shown to be equivalent to a one-dimensional Schrödinger operator with a sextic polynomial potential. This operator belongs to the class of quasi-exactly solvable models, for which a finite number of eigenvalues and eigenvectors can be determined exactly. A Jeffreys–Wentzel–Kramers–Brillouin analysis provides accurate asymptotic expansions for these eigenvalues in the limit of large unperturbed energies.

1. Introduction

Several nonlinear optical processes of interest can be described by a simple effective Hamiltonian with two degrees of freedom and cubic terms in the creation and destruction operators,

$$H_{\text{eff}} = a_1^\dagger a_1 + 2a_2^\dagger a_2 + g\left(a_2^\dagger a_1^2 + a_1^{\dagger 2} a_2\right). \tag{1}$$

Second harmonic generation, coherent spontaneous emission and down conversion are typical examples [1–6]. Although the dynamical problem generated by equation (1) can be reduced to the diagonalization of a finite-dimensional matrix (see section 3.1), convenient analytic expressions for the eigenvalues and eigenvectors are not known. The exact solution can be written in terms of the algebraic Bethe ansatz [7], but the resulting formulae are too unwieldy for practical calculations, and several approximations have been devised relying on specific features of each particular problem under study [1, 2, 4, 8, 9].

The aim of the present paper is twofold. First we will show that the Hamiltonian (1) is equivalent to a one-dimensional Schrödinger operator with a polynomial potential, a fact that to our knowledge has not been noticed and exploited in previous work. Then we will perform a semiclassical Jeffreys–Wentzel–Kramers–Brillouin (JWKB) analysis of the one-dimensional Schrödinger operator to obtain asymptotic formulae for the eigenvalues valid in the limit of large unperturbed energies. As a side issue, we will also touch briefly upon the problem of classical perturbation theory and quantization of dynamical systems in action variables [10, 11]. The outline of the paper is as follows. In section 2, devoted to the classical dynamics of the system, we use a linear canonical transformation to simultaneously remove the two-to-one resonance in equation (1) (characteristic of second harmonic generation) and to separate the problem into two one-dimensional Hamiltonians. The first one describes the unperturbed harmonic oscillation, while the second is a nonlinear oscillator which has a classical normal form that can be readily calculated. In section 3 we

rewrite the quantum Hamiltonian in the Bargmann representation, study the reduction to a finite-dimensional matrix eigenvalue problem, and prove the equivalence of the perturbation to a one-dimensional Schrödinger operator with a sextic polynomial potential which has coefficients that depend on the unperturbed energy. This double-well potential turns out to be one of the quasi-exactly solvable systems studied by Turbiner and Ushveridze [12, 13]. Section 4 is devoted to the JWKB analysis of the one-dimensional Schrödinger equation and the subsequent semiclassical formulae for the eigenvalues. Terms up to fourth order plus an exponentially small correction due to tunnelling between the two wells are calculated, and the resulting first-order series is compared with the Bohr–Sommerfeld quantization of the classical normal form derived in section 2. The accuracy of the different expansions is illustrated by a numerical example with unperturbed energy in the range of physical interest. The paper ends with a brief summary.

2. Separation of the classical Hamiltonian

Our starting point is the following Hamiltonian written in Cartesian coordinates,

$$H = \frac{1}{2}\left(p_1^2 + x_1^2\right) + p_2^2 + x_2^2 + \frac{g}{\sqrt{2}}\left[\left(x_1^2 - p_1^2\right)x_2 + \left(x_1 p_1 + p_1 x_1\right)p_2\right]. \quad (2)$$

Hereafter H_0 will denote the unperturbed harmonic part, and V the perturbation which has a magnitude that is proportional to the coupling constant g. The following developments are based on the fact that both classically and quantum mechanically the unperturbed Hamiltonian and the perturbation commute:

$$[H_0, V] = 0 \quad (3)$$

where the brackets denote the commutator in the quantum case and the Poisson bracket in the classical case. We begin the classical study by switching to the usual action-angle variables of the harmonic oscillator ($i = 1, 2$),

$$x_i = \sqrt{2\mathcal{J}_i}\cos\vartheta_i \quad (4)$$

$$p_i = \sqrt{2\mathcal{J}_i}\sin\vartheta_i \quad (5)$$

in which the Hamiltonian (2) has the standard form

$$H = \mathcal{J}_1 + 2\mathcal{J}_2 + 2g\mathcal{J}_1\mathcal{J}_2^{1/2}\cos(2\vartheta_1 - \vartheta_2) \quad (6)$$

displaying the second distinctive feature of this system, the two-to-one resonance that makes it a suitable model for second harmonic generation. This resonance can be removed by a linear transformation to new canonical variables (θ_1, j_1) and (θ_2, j_2) with generating function

$$F_2(\vartheta_1, \vartheta_2, j_1, j_2) = (2\vartheta_1 - \vartheta_2)j_1 + \vartheta_2 j_2. \quad (7)$$

The old and new variables are related by

$$\mathcal{J}_1 = 2j_1 \quad (8)$$

$$\mathcal{J}_2 = j_2 - j_1 \quad (9)$$

$$\theta_1 = 2\vartheta_1 - \vartheta_2 \quad (10)$$

$$\theta_2 = \vartheta_2 \quad (11)$$

and the transformed Hamiltonian is

$$H = 2j_2 + 4gj_1\sqrt{j_2 - j_1}\cos\theta_1 \quad (12)$$

where the coordinate θ_2 is cyclic, j_2 is a constant of the motion, and the perturbation energy will be denoted by E:

$$E = 4j_1\sqrt{j_2 - j_1}\cos\theta_1. \tag{13}$$

Note that j_2 is half the unperturbed energy, and for a fixed value of this magnitude the perturbation energy is bounded by

$$|E| \leqslant E_{\max} = \left(\frac{4j_2}{3}\right)^{3/2} \tag{14}$$

in agreement with the result obtained by a different method in [9]. In this allowed energy region the perturbation Hamiltonian describes an oscillation whose phase curves in the (θ_1, j_1) phase plane are ovals with centre $(0, 2j_2/3)$ and vertices $(0, j_1^-)$, $(\theta_{\max}, 2j_2/3)$, $(0, j_1^+)$, and $(-\theta_{\max}, 2j_2/3)$, where $\cos\theta_{\max} = E/E_{\max}$ and the expressions for $j_1^\pm$ will be given below (if $E = \pm E_{\max}$ the oval degenerates to the point $(0, 2j_2/3)$). The phase map is symmetrical around $E = 0$ and for $-E_{\max} \leqslant E \leqslant 0$ (or $0 \leqslant E \leqslant E_{\max}$) it is somewhat similar to the map of the usual pendulum. Our main goal in this section is to calculate the classical normal form of this one-dimensional Hamiltonian for the pair of canonical variables (θ_1, j_1). The strategy will be to obtain first an analytic expression for the period of the oscillation $T(E)$, and then to integrate the equation $\partial E/\partial J_1 = 2\pi/T(E)$ that relates the period to the good action variable J_1. Finally we will have to reverse the resulting relation to obtain the perturbation energy as a function of the action, something we achieve by inversion of an appropriate series expansion. The details are as follows. Eliminating $\cos\theta_1$ between equation (13) and the equation of motion for j_1,

$$\frac{dj_1}{dt} = 4j_1\sqrt{j_2 - j_1}\sin\theta_1 \tag{15}$$

we can write the period of the oscillation in terms of the Gauss hypergeometric function F,

$$T(E) = 2\int_{j_1^-}^{j_1^+} \frac{dj_1}{(16j_1^3 - j_1^2 j_2 + E^2)^{1/2}} \tag{16}$$

$$= \frac{\pi}{2(j_1^- - j_1^0)^{1/2}} F\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{j_1^- - j_1^+}{j_1^- - j_1^0}\right) \tag{17}$$

where $j_1^\pm$ and j_1^0 are the roots of the cubic polynomial in the denominator of equation (16). It is convenient to introduce the small parameter

$$\varepsilon = 1 - \frac{E^2}{E_{\max}^2} \tag{18}$$

in terms of which the roots $j_1^\pm$ and j_1^0 can also be written as combinations of hypergeometric functions,

$$\frac{j_1^0}{j_2} = \frac{1}{3} - \frac{2}{3}F(\frac{1}{3}, -\frac{1}{3}; \frac{1}{2}; \varepsilon) \tag{19}$$

$$\frac{j_1^\pm}{j_2} = \frac{1}{3} + \frac{1}{3}F(\frac{1}{3}, -\frac{1}{3}; \frac{1}{2}; \varepsilon) \pm \frac{2}{3}\sqrt{\frac{1}{3}\varepsilon}F(\frac{1}{6}, \frac{5}{6}; \frac{3}{2}; \varepsilon) \tag{20}$$

and the new action variable J_1 is given by

$$J_1 = \frac{1}{2\pi}\int_0^\varepsilon T(\varepsilon)\frac{\partial E}{\partial\varepsilon}d\varepsilon \tag{21}$$

$$= \frac{j_2}{3\sqrt{3}}\int_0^\varepsilon \left(\frac{j_2}{j_1^- - j_1^0}\right)^{1/2} F\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{j_1^- - j_1^+}{j_1^- - j_1^0}\right)\frac{d\varepsilon}{\sqrt{1-\varepsilon}}. \tag{22}$$

Everything in this expression is ready for direct series expansion of the integrand in powers of ε and subsequent term-by-term integration. However, before proceeding we will make three slight modifications. First we will rename $j_2 = J_2$, since then (J_1, J_2) are good action variables for the full Hamiltonian. Second, from equations (19) and (20) one sees that in equation (22) the actions J_1 and J_2 appear only in the combination

$$J = \frac{3J_1}{4J_2}. \tag{23}$$

Consequently, we will pull out the appropriate factors in equation (22) and obtain an expansion for $J = J(\varepsilon)$. This series, in turn, has to be reversed to obtain $\varepsilon = \varepsilon(J)$, and then substituted into equation (18) to obtain the perturbation energy E as a function of the actions. We will give the result of this lengthy but straightforward calculation in two equivalent forms. First, to compare with the quantum calculations of section 4, we will use

$$\mathcal{E} = \frac{1}{2}\left(1 - \frac{E}{E_{\max}}\right) \tag{24}$$

$$= \frac{1}{2}\left(1 - \sqrt{1 - \varepsilon}\right) \tag{25}$$

which has lowest terms that turn out to be

$$\mathcal{E} = \sqrt{3}J - \frac{5}{6}J^2 - \frac{55}{108\sqrt{3}}J^3 - \frac{3215}{11\,664}J^4 - \frac{92\,513}{139\,968\sqrt{3}}J^5 - \cdots. \tag{26}$$

Second, we will write the first few terms of the full classical Hamiltonian in terms of the good action variables J_1 and J_2:

$$H(J_1, J_2) = 2J_2 + g\left(\frac{4J_2}{3}\right)^{3/2}\left[1 - 2\sqrt{3}\frac{3J_1}{4J_2} + \frac{5}{3}\left(\frac{3J_1}{4J_2}\right)^2 + \frac{55}{54\sqrt{3}}\left(\frac{3J_1}{4J_2}\right)^3 + \cdots\right]. \tag{27}$$

Summing up, we have a straightforward procedure to generate as many terms as desired of these convergent expansions that will be used in section 4.2 to discuss direct Bohr–Sommerfeld quantization.

3. Separation of the quantum Hamiltonian

3.1. The Bargmann representation

In this section we will work with the quantum Hamiltonian written in the Bargmann representation, where the canonical operators x and p are replaced by multiplication and derivation operators with respect to a complex variable z according to the rules

$$\frac{1}{\sqrt{2}}(x + \mathrm{i}p) \rightarrow z \tag{28}$$

$$\frac{1}{\sqrt{2}}(x - \mathrm{i}p) \rightarrow \frac{\mathrm{d}}{\mathrm{d}z} \tag{29}$$

and the normalized harmonic oscillator eigenfunctions are given by

$$f_n(z) = \frac{z^n}{\sqrt{n!}} \qquad n = 0, 1, \ldots. \tag{30}$$

The transformed Hamiltonian is

$$H = z_1\frac{\partial}{\partial z_1} + \frac{1}{2} + 2z_2\frac{\partial}{\partial z_2} + 1 + g\left(z_2\frac{\partial^2}{\partial z_1^2} + z_1^2\frac{\partial}{\partial z_2}\right) \tag{31}$$

and the corresponding unperturbed eigenvalues are

$$E^{(0)}_{n_1 n_2} = n_1 + 2n_2 + \tfrac{3}{2} \qquad n_1, n_2 = 0, 1, \ldots. \tag{32}$$

Incidentally, if one drops the constant terms in equation (31) and recalls the correspondence $z \leftrightarrow a^\dagger$, $d/dz \leftrightarrow a$ between the second quantization formalism and the Bargmann representation, the equivalence between this Hamiltonian and the H_{eff} of equation (1) becomes immediately obvious.

Since H_0 and V commute, the eigenvalues of H are linear functions of the coupling constant g. Furthermore, any non-degenerate eigenvector of H_0 is automatically an eigenvector of the total Hamiltonian, as is the case of the ground state $(n_1, n_2) = (0, 0)$ and the first excited state $(n_1, n_2) = (1, 0)$. On the other hand, a diagonalization of the perturbation V within each degenerate subspace $n_1 + 2n_2 = \text{constant}$ is required to obtain the remaining total eigenvalues and eigenvectors. To simplify the notation a little we will consider explicitly only the case of $n_1 + 2n_2$ even,

$$E^{(0)}_{n_1 n_2} = 2k + \tfrac{3}{2} \tag{33}$$

and point out the trivial modifications for odd $n_1 + 2n_2$ in section 3.4.

The key observation is that the perturbation eigenvectors are homogeneous polynomials in z_1^2 and z_2 of degree k:

$$p(z_1, z_2) = c_1 z_1^{2k} + c_2 z_1^{2k-2} z_2 + \cdots + c_{k+1} z_2^k \tag{34}$$

and the action of the perturbation within this subspace is given by a $(k + 1) \times (k + 1)$ self-adjoint tridiagonal matrix whose non-vanishing elements are

$$V^{(k)}_{i,i+1} = V^{(k)}_{i+1,i} = \sqrt{i(2k - 2i + 2)(2k - 2i + 1)} \qquad i = 1, \ldots, k. \tag{35}$$

Several properties of this matrix representation have been extensively studied, but our analysis will rely only on the elementary fact that for any k the eigenvalues are symmetrically distributed around zero. This property is the quantum analogue of the symmetry of the classical motion around $E = 0$ discussed in section 2.

3.2. Reduction to a one-dimensional Schrödinger operator

Since the diagonalization of the perturbation V mentioned above is equivalent to the solution of the differential equation

$$\left(z_2 \frac{\partial^2}{\partial z_1^2} + z_1^2 \frac{\partial}{\partial z_2} \right) p(z_1, z_2) = E p(z_1, z_2) \tag{36}$$

and the polynomials in equation (34) are homogeneous in z_1^2 and z_2, one can reduce the problem to an ordinary differential equation by the following change of dependent and independent variables:

$$z = z_1^2 / z_2 \tag{37}$$

$$p(z_1, z_2) = z_2^k P(z) \tag{38}$$

where $P(z)$ is again a polynomial of degree k in z. Substitution of these expressions into equation (36) gives the following equation for $P(z)$:

$$P''(z) + P'(z)(2 - z^2) + P(z)(kz - E) = 0 \tag{39}$$

which, in turn, can be put into Schrödinger form with the standard change of variables

$$x = z^{1/2} \tag{40}$$

$$P(z) = \psi(x) e^{x^4/16}. \tag{41}$$

The resulting eigenvalue problem on the real line is

$$-\psi''(x) + [\tfrac{1}{16}x^6 - (k + \tfrac{3}{4})x^2 + E]\psi(x) = 0. \tag{42}$$

3.3. Quasi-exactly solvable systems

The Schrödinger equation (42) has an infinite number of bound states of which, by construction, the $k + 1$ lowest even eigenvalues coincide with the eigenvalues of the matrix $V^{(k)}$ (the only eigenvalues relevant for the original second harmonic generation problem). The corresponding wavefunctions can also be written explicitly:

$$\psi_i(x) = e^{-x^4/16}P_i(x^2) \qquad i = 0, \ldots, k \tag{43}$$

where the coefficients of the polynomials P_i (all of them of degree k) are the coefficients of the corresponding eigenvectors of the matrix $V^{(k)}$. It is interesting to note that higher eigenvectors do not have this simple structure of polynomial times an exponential, and there are no closed formulae for the associated eigenvalues. These potentials have been extensively studied by Turbiner and Ushveridze [12, 13], who paid special attention to the underlying algebraic structure that allows them, among other things, to give the transparent explanation of the phenomenon which we briefly reproduce here. Let us introduce the two operators

$$a_+ = x \tag{44}$$

$$a_- = \frac{1}{4}x^3 + \frac{d}{dx} \tag{45}$$

with commutation relation

$$[a_-, a_+] = 1 \tag{46}$$

and rewrite the Schrödinger Hamiltonian in equation (42) as

$$H_k = \tfrac{1}{2}a_+^2(a_+a_- - 2k) - a_-^2. \tag{47}$$

Consider now the 'vacuum' state $|0\rangle$ defined by the condition

$$a_-|0\rangle = 0 \tag{48}$$

(in coordinate representation it is just a constant times $\exp(-x^4/16)$) as well as the recursively defined states

$$|n\rangle = a_+^n|0\rangle. \tag{49}$$

These states $|n\rangle$ are not eigenstates of the Hamiltonian, but in terms of them its action is particularly simple:

$$H_k|n\rangle = (\tfrac{1}{2}n - k)|n + 2\rangle - n(n - 1)|n - 2\rangle \tag{50}$$

and shows why the states $n = 0, 2, 4, \ldots, 2k$ are decoupled from $n = 2k + 2, \ldots$, since for $n = 2k$ the coefficient of $|n + 2\rangle$ vanishes.

However, it is not the quasi-exactly solvable character of equation (42) what we will exploit in the following section, since the 'quasi-exact solvability' means that to calculate these lowest eigenvalues and eigenvectors one has to solve precisely the matrix equation we are trying to study. Instead, we will rescale the Schrödinger equation (42) and perform a JWKB semiclassical analysis in the limit of large k.

3.4. Modifications for odd $n_1 + 2n_2$

In this subsection we will succinctly point out the modifications to handle the case of unperturbed eigenvalues of the form

$$E_{n_1 n_2}^{(0)} = 2k + 1 + \tfrac{3}{2}. \tag{51}$$

The eigenvectors in the Bargmann representation now have the structure

$$p(z_1, z_2) = c_1 z_1^{2k+1} + c_2 z_1^{2k-1} z_2 + \cdots + c_{k+1} z_1 z_2^k \tag{52}$$

and the action of the perturbation within this subspace is again given by a $(k+1) \times (k+1)$ self-adjoint tridiagonal matrix which has non-vanishing elements

$$V_{i,i+1}^{(k)} = V_{i+1,i}^{(k)} = \sqrt{i(2k - 2i + 3)(2k - 2i + 2)} \qquad i = 1, \ldots, k. \tag{53}$$

The appropriate change of variables is

$$z = z_1^2 / z_2 \tag{54}$$

$$p(z_1, z_2) = z_1 z_2^k P(z) \tag{55}$$

where $P(z)$ is again a polynomial of degree k in z. This transformation reduces equation (36) to

$$4z P''(z) + P'(z)(6 - z^2) + P(z)(kz - E) = 0 \tag{56}$$

which, in turn, can be put into Schrödinger form with the substitution

$$x = z^{1/2} \tag{57}$$

$$P(z) = \psi(x) x^{-1} e^{x^4/16}. \tag{58}$$

The resulting Schrödinger equation on the real line is

$$-\psi''(x) + [\tfrac{1}{16} x^6 - (k + \tfrac{5}{4}) x^2 + E] \psi(x) = 0 \tag{59}$$

from which it follows that the case of odd $n_1 + 2n_2 = 2k + 1$ can be recovered from the even $n_1 + 2n_2 = 2k$ by formally replacing everywhere $k \to k + \tfrac{1}{2}$.

4. Semiclassical analysis of the eigenvalues

4.1. The JWKB expansion

Our goal in this section is to obtain asymptotic formulae for the eigenvalues valid in the limit of large unperturbed energies, i.e. of large k. A zeroth-order implicit equation for these eigenvalues was obtained in [9] via Einstein–Brillouin–Keller quantization of the two-dimensional Hamiltonian (2). Our approach, a JWKB analysis of the one-dimensional equation (42), allows us to obtain systematically *explicit* convergent expansions for the zeroth-order as well as higher-order corrections to the energy and other magnitudes of physical interest (e.g. the density of states). With this aim, we rescale the Schrödinger equation (42) replacing x by $2h^{-1/4}x$, where

$$h = (\tfrac{4}{3} k + 1)^{-1} \tag{60}$$

will play the role usually assumed by $\hbar$. The resulting equation is

$$-h^2 \psi''(x) + [v(x) - 8\mathcal{E}] \psi(x) = 0 \tag{61}$$

with the potential

$$v(x) = 16x^6 - 12x^2 + 4 \tag{62}$$

and the spectral parameter $\mathcal{E}$ given by

$$\mathcal{E} = \tfrac{1}{2}\left(1 - h^{3/2}E\right). \tag{63}$$

We write the wavefunction in exponential form

$$\psi = \exp\left(\frac{1}{h}\int S(x)\,\mathrm{d}x\right) \tag{64}$$

so that $S(x)$ must be a solution of the Riccati equation

$$S(x)^2 + hS'(x) = v(x) - 8\mathcal{E}. \tag{65}$$

Expansion of $S(x)$ as a power series in h,

$$S(x) = \sum_{N=0}^{\infty} h^N S_N(x) \tag{66}$$

reduces the solution of the Riccati equation to a recursive evaluation of the S_N. In particular one obtains

$$S_0 = \sqrt{v(x) - 8\mathcal{E}} \tag{67}$$

$$S_1 = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\ln S_0 \tag{68}$$

$$S_2 = -\frac{1}{2}S_0^{-1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}S_0^{-1/2} \tag{69}$$

$$S_3 = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(S_0^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}S_0^{-1/2}\right) \tag{70}$$

$$S_4 = -\frac{1}{8}\left(S_0^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2}S_0^{-1/2}\right)^2 - \frac{1}{4}\frac{\mathrm{d}}{\mathrm{d}x}\left[S_0^{-1}\frac{\mathrm{d}}{\mathrm{d}x}\left(S_0^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}S_0^{-1/2}\right)\right] \tag{71}$$

where we have tried to isolate total derivatives of single-valued functions which will not contribute to the quantization condition. This condition is given by Dunham's formula [16],

$$\frac{1}{2\pi\mathrm{i}}\oint S(x)\,\mathrm{d}x = nh \qquad n = 0, 1, \ldots, [(k-1)/2] \tag{72}$$

where the path of integration is a loop enclosing the classical turning points, the square brackets denote integer part, and the quantum number n has been restricted to the physically relevant states with $E \geqslant 0$ (or $0 < \mathcal{E} \leqslant \tfrac{1}{2}$). Furthermore, in our case the potential $v(x)$ defined in equation (62) is a double well and, for the lowest eigenvalues, there are four classical turning points. Since we are interested in the limit of large k, we will first neglect tunnelling and defer an estimate of the exponentially small correction to section 4.4.

The classical turning points are the roots of a cubic polynomial in x^2, and will be denoted by $\pm\sqrt{a}$, $\pm\sqrt{b}$, and $\pm\sqrt{c}$, where a, b and c can again be conveniently written in terms of Gauss hypergeometric functions:

$$a = -F(\tfrac{1}{3} - \tfrac{1}{3}; \tfrac{1}{2}; \mathcal{E}) \tag{73}$$

$$b = -\frac{a}{2} - \sqrt{\frac{\mathcal{E}}{3}}F(\tfrac{1}{6}, \tfrac{5}{6}; \tfrac{3}{2}; \mathcal{E}) \tag{74}$$

$$c = -\frac{a}{2} + \sqrt{\frac{\mathcal{E}}{3}}F(\tfrac{1}{6}, \tfrac{5}{6}; \tfrac{3}{2}; \mathcal{E}). \tag{75}$$

The two turning points in the right well are $+\sqrt{b}$ and $+\sqrt{c}$. To lowest order in h, the Riccati equation is equivalent to a classical Hamilton–Jacobi equation, and the classical

action can be evaluated in terms of a hypergeometric function of two variables (or Appell function) F_1 [17, 18],

$$J = \frac{1}{2\pi i} \oint S_0(x) \, dx \tag{76}$$

$$= \tfrac{1}{4}(c - b)^2 (1 - a/b)^{1/2} F_1 \left(\tfrac{3}{2}, -\tfrac{1}{2}, \tfrac{1}{2}; 3; \frac{b-c}{b-a}, \frac{b-c}{b} \right) \tag{77}$$

where the path of integration has been deformed to the segment between the classical turning points. Equation (77) can be readily expanded in a convergent power series in $\mathcal{E}$, which has first terms

$$J\sqrt{3} = \mathcal{E} + \frac{5}{18}\mathcal{E}^2 + \frac{205}{972}\mathcal{E}^3 + \frac{22\,715}{104\,976}\mathcal{E}^4 + \frac{983\,213}{3\,779\,136}\mathcal{E}^5 \cdots \tag{78}$$

and inversion of this series yields

$$\mathcal{E} = \sqrt{3}J - \frac{5}{6}J^2 - \frac{55}{108\sqrt{3}}J^3 - \frac{3215}{11\,664}J^4 - \frac{92\,513}{139\,968\sqrt{3}}J^5 - \cdots. \tag{79}$$

Note that this equation is precisely the classical normal form (26) obtained in section 2, and, to this order in h, quantization amounts to the substitution $J = nh$. Its radius of convergence can be determined by an argument given initially by Turchetti [19] in a related context. It is the value of the classical action J corresponding to the separatrix (in our case $E = 0$ or $\mathcal{E} = \tfrac{1}{2}$). In this case the integration in equation (76) is elementary and the radius of convergence turns out to be $\tfrac{3}{8}$.

Since S_1 is proportional to the logarithmic derivative of S_0, the next term in equation (72) is simply

$$\frac{h}{2\pi i} \oint S_1(x) \, dx = -\frac{h}{2} \tag{80}$$

and to this order, quantization is equivalent to the substitution $J = (n + \tfrac{1}{2})h$ in the classical series. Note that all the bound states with $E > 0$ (i.e. $n = 0, 1, \ldots, [k/2 - 1]$) fall within the radius of convergence of equation (26), since $(k/2)/(4k/3 + 1) < \tfrac{3}{8}$. Although at this point there are contributions from orders zero and one, the resulting semiclassical series (i.e. the classical series with J replaced by $(n + \tfrac{1}{2})h$) will be denoted by $\mathcal{E}_0(J)$.

We will finish this subsection by giving the first-order approximation to another magnitude of practical interest: the density of states $\rho(E)$. It can be readily calculated by differentiating the quantization condition (76) with respect to the energy, with the result

$$\rho(E) = \frac{\partial n}{\partial \mathcal{E}} \frac{\partial \mathcal{E}}{\partial E} = -\frac{h^{1/2}}{4c^{1/2}(b-a)^{1/2}} F \left(\tfrac{1}{2}, \tfrac{1}{2}; 1; \frac{a(b-c)}{c(b-a)} \right) \tag{81}$$

where it is understood that in the right-hand side the spectral parameter $\mathcal{E}$ has been expressed in terms of E with equation (63). Numerical calculations have shown that in the range of physical interest, equation (81) gives a very accurate approximation to the density of states. On the other hand, although it is straightforward to expand equation (81) as a power series in $\mathcal{E}$:

$$\rho(E) = -\frac{h^{1/2}}{4\sqrt{3}} \left(2 + \frac{10}{9}\mathcal{E} + \frac{205}{162}\mathcal{E}^2 + \frac{22\,715}{13\,122}\mathcal{E}^3 + \frac{4\,916\,065}{1\,889\,568}\mathcal{E}^4 + \cdots \right) \tag{82}$$

many terms of this series are required to reproduce accurately the characteristic dip of the density of states at $E = 0$.

4.2. Direct quantization in action variables and the classical dynamics revisited

Since in section 2 we have been able to write the classical Hamiltonian in terms of good action variables, it is interesting to compare a direct Bohr–Sommerfeld quantization of this Hamiltonian (see [10, 11, 15]) with the JWKB result obtained in the previous subsection. In the classical Hamiltonian (27) the action J_2 is half the unperturbed energy, i.e. one should quantize (including the Maslov index)

$$J_2 \rightarrow \tfrac{1}{2}\left(2k + \tfrac{3}{2}\right) \tag{83}$$

while J_1 can be quantized with the usual rule

$$J_1 \rightarrow n + \tfrac{1}{2}. \tag{84}$$

With these replacements,

$$J = \frac{3J_1}{4J_2} \rightarrow \frac{n + \tfrac{1}{2}}{4k/3 + 1} \tag{85}$$

in agreement with the first-order JWKB result.

Although we have arrived at the one-dimensional Schrödinger equation (42) mainly guided by the homogeneity of the polynomials in the Bargmann representation, the correspondence between classical and quantum series hints at the possibility of looking for a canonical transformation from (θ_1, j_1) to new variables (x, p) in which equation (13) would be the exact classical analogue of the Schrödinger equation (42). In fact, if one traces back the transformations in equations (28), (29), (37), and (40), their classical analogue is

$$x = \frac{(2j_1)^{1/2}}{(j_2 - j_1)^{1/4}} e^{i\theta_1/2} \tag{86}$$

and the corresponding conjugate momentum turns out to be

$$p = \frac{(2j_1)^{1/2}}{i(j_2 - j_1)^{3/4}} \left[(j_2 - j_1)e^{-i\theta_1/2} - \frac{j_1}{2}e^{i3\theta_1/2} \right]. \tag{87}$$

One can easily check that this is a complex canonical transformation,

$$[x, p] = \frac{\partial x}{\partial \theta_1} \frac{\partial p}{\partial j_1} - \frac{\partial x}{\partial j_1} \frac{\partial p}{\partial \theta_1} = 1 \tag{88}$$

and that in these new variables (x, p), the classical perturbation Hamiltonian of equation (13) is precisely

$$p^2 + \frac{x^6}{16} - j_2 x^2 + E = 0 \tag{89}$$

that is to say, the formal classical analogue of equation (42).

4.3. Higher-order quantum corrections

The general method to evaluate higher-order terms can be summarized as follows. For odd $N \geqslant 3$, the S_N are total derivatives of single-valued functions, and do not give a contribution to the quantization condition. For even $N \geqslant 2$, repeated integration by parts can be used to reduce the integrals to equivalent expressions that can be calculated by shrinking the path to the segment between the classical turning points [20]. The next two orders are

$$\oint S_2(x)\,dx = \frac{1}{32} \oint \frac{v'(x)^2}{(v(x) - 8\mathcal{E})^{5/2}}\,dx \tag{90}$$

$$= \frac{1}{192} \frac{d}{d\mathcal{E}} \oint \frac{v''(x)}{(v(x) - 8\mathcal{E})^{1/2}}\,dx \tag{91}$$

and

$$\oint S_4(x)\,dx = \frac{35}{2048}\oint \frac{v'(x)^4}{(v(x)-8\mathcal{E})^{11/2}}\,dx - \frac{1}{128}\oint \frac{v''(x)^2}{(v(x)-8\mathcal{E})^{7/2}}\,dx \tag{92}$$

$$= \frac{1}{1\,474\,560}\frac{d^3}{d\mathcal{E}^3}\oint \frac{5v'(x)v'''(x)-7v''(x)^2}{(v(x)-8\mathcal{E})^{1/2}}\,dx. \tag{93}$$

The integrals which appear in these formulae can now be evaluated, shrinking the path to the interval between the two branch points, and turn out to be particular instances of

$$I_p(\mathcal{E}) = \int_{\sqrt{b}}^{\sqrt{c}} \frac{x^{2p}}{(v(x)-8\mathcal{E})^{1/2}}\,dx \tag{94}$$

$$= \frac{i\pi b^{p-1/2}}{8(b-a)^{1/2}} F_1\left(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}-p;1;\frac{b-c}{b-a},\frac{b-c}{b}\right). \tag{95}$$

The last step is to expand the spectral parameter $\mathcal{E}$ as a power series in h. Since only even powers of h are non-zero in the left-hand side of equation (72) (except the first which gets absorbed in the definition of J), only even powers of h occur in the expansion:

$$\mathcal{E} = \mathcal{E}_0(J) + h^2\mathcal{E}_2(J) + h^4\mathcal{E}_4(J) + \cdots. \tag{96}$$

The result of collecting equal powers of h in the quantization condition is that the $\mathcal{E}_N$ with $N > 0$ are given explicitly in terms of hypergeometric functions and their derivatives evaluated at $\mathcal{E}_0(J)$. Only the classical series $\mathcal{E}_0(J)$ is given as the solution of an implicit equation. Moreover, all the substitutions of power series are carried out inside their radii of convergence, the final radius of convergence being determined by the above-mentioned argument for $\mathcal{E}_0(J)$. That is to say, one can generate as many terms as desired of the convergent (with radius of convergence $|J| < \frac{3}{8}$) series expansions for each of the quantum corrections

$$\mathcal{E}_{2N}(J) = \sum_{i=0}^{\infty} c_{2N}^{(i)} J^i. \tag{97}$$

By way of example, table 1 shows the exact values of the first coefficients for $\mathcal{E}_0$, $\mathcal{E}_2$ and $\mathcal{E}_4$.

4.4. Tunnelling correction

As we mentioned in section 4.1, the potential (62) is a double well, and up to this point we have neglected tunnelling between the two wells. The main consequence of this assumption is that the asymptotic formulae for the eigenvalues that we have derived so far lose accuracy as the eigenvalues get closer to the top of the barrier between the two wells ($E = 0$). The next degree of approximation is to realize that in fact there are two independent, degenerate JWKB solutions—one in each well—that give rise to two linear combinations, even and odd, separated in energy by an exponentially small quantity. These exponentially small corrections to the JWKB eigenvalues have been extensively studied [21–23] but for our practical purposes we will use the simplest formula:

$$\Delta\mathcal{E} \approx -2h\left[\int_{\sqrt{b}}^{\sqrt{c}} \frac{dx}{(8\mathcal{E}_{\text{JWKB}}-v(x))^{1/2}}\right]^{-1} \exp\left[-\frac{1}{h}\int_{-\sqrt{b}}^{\sqrt{b}} (v(x)-8\mathcal{E}_{\text{JWKB}})^{1/2}\,dx\right] \tag{98}$$

where the subindex in $\mathcal{E}_{\text{JWKB}}$ means that the integrals have to be evaluated for the values of the parameter $\mathcal{E}$ given by the JWKB expansions, and the negative sign of the correction

Table 1. Lowest coefficients of the JWKB series $\mathcal{E}_{2N}(J) = \sum_{i=0}^{\infty} c_{2N}^{(i)} J^i$ for $N = 0$, 1, and 2.

i	$-108^{i/2}c_0^{(i)}$	$-108^{i/2}c_2^{(i)}$	$-108^{i/2}c_4^{(i)}$
0	0	$\dfrac{5}{144}$	$\dfrac{13\,207}{14\,929\,920}$
1	-18	$\dfrac{25}{72}$	$\dfrac{41\,177}{622\,080}$
2	90	$\dfrac{2185}{216}$	$\dfrac{2\,918\,699}{1\,866\,240}$
3	330	$\dfrac{140\,845}{432}$	$\dfrac{44\,245\,349}{746\,496}$
4	3215	$\dfrac{78\,925}{8}$	$\dfrac{396\,904\,321}{186\,624}$
5	$\dfrac{92\,513}{2}$	$\dfrac{2\,210\,924\,345}{7776}$	$\dfrac{4\,943\,621\,500\,633}{67\,184\,640}$
6	$\dfrac{2\,398\,025}{3}$	$\dfrac{20\,700\,155\,315}{2592}$	$\dfrac{500\,275\,357\,652\,683}{201\,553\,920}$
7	$\dfrac{90\,965\,185}{6}$	$\dfrac{20\,694\,525\,533\,215}{93\,312}$	$\dfrac{13\,245\,692\,055\,818\,959}{161\,243\,136}$
8	$\dfrac{21\,881\,438\,645}{72}$	$\dfrac{1\,287\,784\,640\,196\,175}{209\,952}$	$\dfrac{1\,942\,747\,684\,044\,029\,369}{725\,594\,112}$
9	$\dfrac{16\,413\,482\,959\,885}{2592}$	$\dfrac{569\,337\,606\,784\,188\,275}{3\,359\,232}$	$\dfrac{500\,108\,510\,351\,164\,506\,071}{5\,804\,752\,896}$

reflects the even nature of the eigenstates in which we are interested. Once more the integrations can be explicitly done in terms of hypergeometric functions, and the result is

$$\Delta\mathcal{E} \approx -\frac{2hc^{1/2}(b-a)^{1/2}}{\pi F\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{a(b-c)}{c(b-a)}\right)} \exp\left[-\frac{2\pi}{h}b(-ac)^{1/2}F_1\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}; 2; \frac{b}{a}, \frac{b}{c}\right)\right]. \tag{99}$$

Note that series expansions are not required to calculate $\Delta\mathcal{E}$: one just uses the raw JWKB eigenvalues and evaluates the functions. We will briefly study the effect of this exponentially small correction for unperturbed energies in the region of physical interest in the next subsection.

4.5. Double-series structure of $\mathcal{E}$: a numerical example

The spectral parameter $\mathcal{E}$ is in fact given by a double series in $(n + \frac{1}{2})$ and h:

$$\mathcal{E} = \sum_{N=0}^{\infty} \sum_{i=0}^{\infty} c_{2N}^{(i)} h^{2N+i} (n + \tfrac{1}{2})^i. \tag{100}$$

Equation (96) is the result of summing first in the index i in equation (100), i.e. evaluating first the convergent series of equation (97). From the practical point of view, however, it may seem more natural to use an approach closer to perturbation theory, and reorder the

Table 2. Accuracy of three asymptotic approximations to the eigenvalues of $V^{(k)}$

n	To order $k^{-3/2}$	From table 1	Table 1 plus $\Delta\mathcal{E}$	Exact
		$k = 12$		
0	63.069 266 469	63.070 866 350	63.070 866 350	63.070 868 400
1	49.594 861 695	49.627 768 140	49.627 768 141	49.627 777 367
2	36.928 909 005	37.087 108 671	37.087 108 921	37.087 146 105
3	25.071 408 399	25.539 187 061	25.539 230 148	25.539 659 444
4	14.022 359 875	15.119 299 303	15.123 270 989	15.127 712 933
5	3.781 763 435	6.049 470 261	6.231 155 370	6.210 552 602
6	−5.650 380 921	−1.280 559 236		0.000 000 000
		$k = 24$		
0	179.705 314 047	179.705 891 773	179.705 891 773	179.705 891 963
1	160.385 824 158	160.397 377 037	160.397 377 037	160.397 377 687
9	26.719 223 762	30.670 108 831	30.670 360 644	30.709 145 625
10	12.622 063 551	18.319 486 591	18.330 845 882	18.458 201 845
11	−0.894 837 806	7 160 597 489	7.489 282 348	7.767 963 489
12	−13.831 480 310	−2.606 449 488		0.000 000 000
		$k = 50$		
0	542.435 604 220	542.435 798 541	542.435 798 541	542.435 798 558
1	514.345 210 971	514.349 045 051	514.349 045 051	514.349 045 098
⋮	⋮	⋮	⋮	⋮
20	57.619 624 608	71.535 164 368	71.535 165 149	71.737 519 406
21	37.633 640 345	54.223 358 421	54.223 392 331	54.588 829 649
22	18.052 876 530	37.737 542 726	37.738 751 327	38.397 485 449
23	−1.122 666 835	22.139 367 300	22.173 881 976	23.358 654 705
24	−19.892 989 751	7.500 313 286	8.242 933 808	10.043 303 431
25	−38.258 092 217	−6 096 700 732		0.000 000 000

double series by increasing powers of $1/k$:

$$\mathcal{E} = \sum_{M=1}^{\infty} \mathcal{E}^{(M)} h^M \tag{101}$$

where

$$\mathcal{E}^{(M)} = \sum_{N=0}^{[M/2]} c_{2N}^{(M-2N)} (n + \tfrac{1}{2})^{M-2N}. \tag{102}$$

This double-series structure is typical of the transition between classical and quantum mechanics, and illustrates the relation between JWKB expansions and Rayleigh–Schrödinger perturbation theory (see [24]). Since a concrete example helps to fix the pattern, let us remove the intermediate variables and write the asymptotic behaviour of the eigenvalues of the perturbation energy E to order $O(k^{-3/2})$ as a function of the unperturbed energy $E^{(0)} = 2k + \frac{3}{2}$. The result is

$$E_{k,n} \approx \left(\frac{4k}{3} + 1\right)^{3/2} \left\{ 1 - 2\sqrt{3} \frac{n + \tfrac{1}{2}}{4k/3 + 1} + \frac{5}{3(4k/3 + 1)^2} [(n + \tfrac{1}{2})^2 + \tfrac{1}{24}] \right\}. \tag{103}$$

Since all the asymptotic approximations we have derived are valid in the limit of large k, it is still necessary to study their accuracy for unperturbed energies in the range of

physical interest. We have performed an extensive numerical analysis, of which table 2 is a representative example. It shows (some of) the non-negative perturbation eigenvalues for $k = 12$, 24 and 50 (typical test cases studied previously in the literature [1]) calculated by four different procedures. The second column contains the values given by equation (103), the third column has been calculated with all the coefficients in table 1, the fourth column equals the third column plus the tunnelling correction of equation (99), and the last column shows the exact eigenvalues calculated by numerical diagonalization of the corresponding matrices $V^{(k)}$. From this and similar calculations the following trends can be inferred. Even for relatively moderate values of k the highest eigenvalues ($n = 0, 1, \ldots$) are accurately approximated by the simplest asymptotic formulae. The accuracy gradually decreases as we consider eigenvalues closer to $E = 0$, to the point that equation (103) incorrectly reports the last three eigenvalues of $V^{(50)}$ as negative—the effect is more obvious for large values of k, when many states pile up close to the top of the barrier. The main factor to restore this lost accuracy are the higher-order terms and, in particular, the higher-order terms of $\mathcal{E}_0(J)$. The exponentially small correction $\Delta\mathcal{E}$ is only significant for eigenvalues very close to $E = 0$ (for example, the next to last in the fourth column of table 2); furthermore, this correction can be used only when the JWKB is sufficiently accurate so as to give a positive approximate eigenvalue—hence the missing values in this column. Although the approximation breaks down for $E = 0$, this does not raise a problem, since it is known to be an exact eigenvalue whenever k is even.

5. Summary

We have carried out a JWKB semiclassical analysis of a system of two quantum oscillators with cubic coupling in the creation and destruction operators, which provides the usual model for second harmonic generation in nonlinear optics. An essential feature of this model is that the unperturbed (harmonic) part and the perturbation commute, opening up the possibility of explicit separation of the Hamiltonian into two one-dimensional problems. We have been able to perform this separation both classically and quantum mechanically and, in both cases, the perturbation is equivalent to a highly nonlinear one-dimensional oscillator. Specifically, the main results of our analysis are as follows.

(i) There is a linear canonical transformation which simultaneously removes the two-to-one resonance and separates the classical Hamiltonian.

(ii) A method has been given to generate as many terms as desired of the classical normal form of the Hamiltonian.

(iii) Working in the Bargmann representation, the quantum version of the model has been shown to be equivalent to a one-dimensional Schrödinger operator with a sextic quasi-exactly solvable polynomial potential.

(iv) We have performed a JWKB analysis of this one-dimensional Schrödinger equation which provides a procedure to generate as many terms as desired of the convergent series for the quantum corrections (numerical values are given for the first ten coefficients up to fourth order).

(v) The Bohr–Sommerfeld quantization rules applied to the classical normal form give a convergent series which coincides with the first order JWKB result. Furthermore, the classical perturbation Hamiltonian is equivalent, via a complex canonical transformation, to the classical analogue of the one-dimensional Schrödinger operator mentioned in item (iii).

(vi) We have briefly discussed the accuracy of the asymptotic formulae for the eigenvalues and their breakdown for eigenvalues close to zero, due to the coalescence of classical turning points.

As a final remark, we would like to point out the interest of performing a similar semiclassical study of the eigenfunctions and time evolution of this system. Of particular relevance are the results in [3], where the aperiodicity of the time evolution is related to the non-uniform spacing of the eigenvalues (for k fixed) as a function of n, i.e. to the terms beyond the first and second order in our asymptotic expansions.

Acknowledgment

References

[1] Walls D F and Barakat B 1970 *Phys. Rev.* A **1** 446
[2] Bonifacio R and Preparata G 1970 *Phys. Rev.* A **2** 336
[3] Walls D F and Tindall C T 1972 *J. Phys. A: Math. Gen.* **5** 534
[4] Kumar S and Metha C L 1980 *Phys. Rev.* A **21** 1573
[5] Drobný G and Jex I 1992 *Phys. Rev.* A **46** 499
[6] Drobný G, Jex I and Buzek V 1993 *Phys. Rev.* A **48** 569
[7] Jurco B 1989 *J. Math. Phys.* **30** 1739
[8] Mostowski J and Rzazewski K 1978 *Phys. Lett.* **66A** 275
[9] Alvarez-Estrada R F, Gómez Nicola A, Sánchez-Soto L L, Luis A and Tanaś R 1995 *J. Phys. A: Math. Gen.* **28** 3439
[10] Graffi S and Paul T 1987 *Commun. Math. Phys.* **108** 25
[11] Graffi S 1993 *Le Radici della Quantizzazione* (Pavia: Università degli Studi di Pavia)
[12] Turbiner A V and Ushveridze A G 1987 *Phys. Lett.* **126A** 181
[13] Ushveridze A G 1993 *Quasi-Exactly Solvable Models in Quantum Mechanics* (Bristol: IOP)
[14] Jensen R V 1984 *Phys. Rev.* A **30** 386
[15] Degli Esposti M, Graffi S and Herczynski J 1991 *Ann. Phys.* **208** 364
[16] Dunham J L 1932 *Phys. Rev.* **41** 713
[17] Gradshteyn I S and Ryzhik I M 1979 *Table of Integrals, Series, and Products* (New York: Academic)
[18] Slater L J 1966 *Generalized Hypergeometric Functions* (London: Cambridge University Press)
[19] Turchetti G 1984 *Nuovo Cimento* B **82** 203
[20] Krieger J B, Lewis M L and Rosenzweig C 1967 *J. Chem. Phys.* **47** 2942
[21] Coleman S 1977 The uses of instantons *Proc. Int. School of Physics (Erice)*
[22] Harrell E M 1980 *Commun. Math. Phys.* **75** 239
[23] Simon B 1984 *Ann. Math.* **120** 89
[24] Alvarez G, Graffi S and Silverstone H J 1988 *Phys. Rev.* A **38** 1687