Semiclassical energy quantization of anharmonic potential motion-complex trajectory contributions versus higher-order corrections

Semiclassical energy quantization of anharmonic potential motion—complex trajectory contributions versus higher-order corrections

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Abstract. In the present investigation we assess the relevance of both classically forbidden phenomena and higher-order asymptotic contributions for the semiclassical energy quantization of a particle in the anharmonic oscillator potential $V(x) = x^2/2 + \lambda x^4$. We propose an iterative method (iq) for obtaining higher-order semiclassical corrections, which is similar to the WKB and phase-integral methods in the lowest order, but in higher orders the approximation differs significantly. A 'primitive' Bohr–Sommerfeld energy quantization is compared with a more complete semiclassical quantization, taking into account both complex trajectory contributions and higher-order (quantal) corrections.

1. Introduction

A successful semiclassical quantization method for nonlinear classical systems has to reflect mechanisms of nonlinear classical phenomena as well as classically forbidden phenomena. This is evident from semiclassical research over the last couple of decades. It is also clear that semiclassical quantization methods are parts of asymptotic solutions of a singular perturbation problem. In the present investigation we assess the relevance of both classically forbidden phenomena and higher-order asymptotic contributions for the semiclassical energy quantization of a particle in the anharmonic oscillator potential $V(x) = x^2/2 + \lambda x^4$.

A problem of some concern for nonlinear classical systems is that primitive semiclassical methods (leading to quantization conditions equivalent to a leading-order Bohr–Sommerfeld one) cannot predict the individual energy levels in the sense that the ratio of the average absolute error of the semiclassical eigenvalues and the local mean level spacing may increase indefinitely in some cases; see [1]. The present investigation may give quantitative estimates of contributions left out by such primitive semiclassical methods.

Recent research on higher-order contributions [2] suggests that numerous ways of obtaining them remain to be explored. The present authors have undertaken a thorough theoretical and numerical investigation of various new iterative methods that will be presented elsewhere. One iterative method is presented in [2], and in this article we briefly outline how another iterative method can be developed.

The underlying second-order ordinary differential (time-independent Schrödinger) equation is of the general form

$$\psi'' + R(z)\psi = 0 \tag{1.1}$$

where the assumed slowly varying coefficient $R(z)$ is an analytic function of the variable z. The derivative ψ'' represents the second-order derivative with respect to z. Equation (1.1) is quite general, since all homogeneous second-order ordinary differential equations can be reduced to that form. Numerous applications of (1.1) can be found in quantum and classical mechanics, and several methods have been developed to solve it. In the present paper we propose an iterative method which is similar to the WKB and phase-integral methods [3–5] in the lowest order of approximation, but the higher-order approximations contain important differences.

In section 2 we derive the so-called q-equation, equivalent to the Schrödinger equation (1.1), by an amplitude-phase decomposition of the wavefunction. Section 2 also introduces the iterative solutions of the q-equation in terms of an unspecified base function and a sequence of correction factors corresponding to the contributions from each order of iteration. The first two correction factors are expressed in terms of higher-order phase-integral quantities. The q-iteration method is used in section 3 to determine some low-lying energy levels of the reduced anharmonic oscillator potential $V(x) = x^2/2 + \lambda x^4$, with $\lambda = 0.1$, 1 and 1000. The importance of complex classical turning points and higher-order corrections in the quantization condition is discussed by comparing the 'primitive' (real classical motion and no higher-order contributions) quantization results with more general higher-order semiclassical quantization results and with numerical quantum ones. Conclusions are in section 4.

2. Higher-order contributions

In this section we propose an iterative asymptotic approximation method which is similar to the phase-integral (or symmetric WKB) method for solving second-order ordinary differential equations; see [5]. In their lowest order of approximation the phase-integral method and its iterative version are identical. Most aspects of the connection problem relating the linear combinations of the fundamental approximants across isolated transition regions of simple (complex) classical turning points can be taken over from the so-called F-matrix method. Some limitations of applying the iterative approximation in combination with already existing, approximate phase-integral formulae are pointed out at the end of the sections. A more detailed theoretical outline using formal expansion parameters, and giving a critical justification of the iterative technique used in section 2.2, is given in a paper by Dammert and Thylwe [6].

2.1. Phase-integral q-equation

The iteration procedure is based on a non-linear equation for the exact frequency (or wavenumber) function q of the solutions. This function is defined and its equation, the q-equation, is derived below.

The starting point is a phase-amplitude decomposition of the solution to (1.1). This idea is easy to adopt for regions of z-values where the solutions are oscillatory, and can then be generalized to other regions by analytic continuation. Hence, two fundamental

solutions of (1.1) are now constructed in the form

$$\psi^{\pm} = A(z) \exp\left(\pm i \int_{z_0}^{z} q(z') \, dz'\right) \tag{2.1}$$

where $A(z)$ and $q(z)$ are still to be determined. Once they have been determined, the general solution of (1.1) can be expressed as a linear combination of ψ^{+} and ψ^{-}. In order for the Wronskian of the two independent solutions (2.1) to be a constant W, we find

$$W = \psi^{+}\psi'^{-} - \psi^{-}\psi'^{+} = -2iA^2(z)q(z). \tag{2.2}$$

From (2.2) follows that $A(z)$ is determined by $q(z)$ and we can equally well define our fundamental solutions in the more specific form

$$\psi^{\pm} = q^{-1/2}(z) \exp\left(\pm i \int_{z_0}^{z} q(z') \, dz'\right). \tag{2.3}$$

By inserting (2.3) into the differential equation (1.1) we obtain a nonlinear equation for $q(z)$, the q-equation

$$R(z) - q^2(z) + q^{1/2}(z) \frac{d^2}{dz^2} q^{-1/2}(z) = 0. \tag{2.4}$$

In the (symmetrical) phase-integral approximation one now expands (in a certain way) the function $q(z)$ as a power series in a formal expansion parameter and equates in (2.4) the terms of each order. The resulting sequence of equations can then be solved successively. This technique, which is reviewed in [2] (section 2), corresponds to an outer expansion in the language of boundary layer theory, and it is thereby assumed that the function $R(z)$ is not too small. The boundary layers represent the regions of the complex-z plane near the zeros, or transition points, of $R(z)$. Here we shall proceed differently by solving (2.4) using a direct iterative technique.

2.2. Iterative solution

First we introduce a so-called base function $Q(z)$, which is approximately equal to $R^{1/2}(z)$ except, possibly, at certain points in the complex-z plane. By inserting $q = Qg$ in (2.4) above and dividing by Q^2 one obtains (see also [2])

$$g^2 = 1 + \varepsilon(Q) + g^{1/2} \frac{d^2}{d\zeta^2} g^{-1/2} \tag{2.5}$$

where

$$\varepsilon(Q) = \frac{R - Q^2}{Q^2} + Q^{-3/2} \frac{d^2}{dz^2} Q^{-1/2} \tag{2.6}$$

and

$$d\zeta = Q \, dz. \tag{2.7}$$

The nonlinear equation (2.5) for g is exact. To the lowest order of approximation for

g we take

$$G_0 = \pm 1. \tag{2.8}$$

By neglecting only the last term in the right member of (2.5), we find the first-order approximate solution G_1 in terms of the unspecified base function:

$$G_1 = \pm \sqrt{1 + \varepsilon(Q)}. \tag{2.9}$$

To continue the iterative procedure we subsequently introduce the improved base function $Q_1 = Q G_1$, which we use to insert a new $q = Q_1 g$ into the q-equation (2.4) and dividing it by Q_1^2. The resulting equation for the new multiplicative correction function g is

$$g^2 = 1 + \varepsilon(Q_1) + g^{1/2} \frac{\mathrm{d}^2}{\mathrm{d}\zeta_1^2} g^{-1/2} \tag{2.10}$$

with

$$\mathrm{d}\zeta_1 = Q_1 \, \mathrm{d}z \tag{2.11}$$

in complete analogy to (2.5). The second correction factor is, in the same spirit as before, given as

$$G_2 = \pm \sqrt{1 + \varepsilon(Q_1)} \tag{2.12}$$

and so on. Obviously, after N iterations one finds the following approximate result:

$$G_N = \pm \sqrt{1 + \varepsilon(Q_{N-1})} \tag{2.13}$$

so that the Nth-order iteration expression for q becomes

$$q = Q_N = Q_0 G_1 G_2 \ldots G_N \tag{2.14}$$
$$= \pm Q_0 \sqrt{[(1 + \varepsilon(Q_0))(1 + \varepsilon(Q_1)) \ldots (1 + \varepsilon(Q_{N-1}))]}.$$

The expression for $\varepsilon(Q_n)$, in the $(n+1)$th iteration step, is obtained in analogy to (2.6). Using equation (6) in [2], one finds

$$\varepsilon(Q_n) = \frac{1 + \varepsilon(Q_{n-1}) - G_n^2}{G_n^2} + G_n^{-3/2} \frac{\mathrm{d}^2}{\mathrm{d}\zeta_{n-1}^2} G_n^{-1/2}$$
$$= G_n^{-3/2} \frac{\mathrm{d}^2}{\mathrm{d}\zeta_{n-1}^2} G_n^{-1/2}. \tag{2.15}$$

Equation (2.15) can be used to calculate $\varepsilon(Q_n)$ only for $n \geqslant 1$. $\varepsilon(Q_0)$ ($= \varepsilon(Q)$) is calculated separately from (2.6). In (2.15), we have used the notation $\mathrm{d}\zeta_n = Q_n \, \mathrm{d}z$ with $\mathrm{d}\zeta_0 = Q_0 \, \mathrm{d}z$, as a special case.

2.3. Relation to phase-integral quantities

We now wish to express the iterative correction factors of section 2.2 in terms of the phase integral quantities ε_n, given by

$$\varepsilon_n \equiv \frac{\mathrm{d}^n \varepsilon_0}{\mathrm{d}\zeta^n} = \left(\frac{\mathrm{d}}{Q \, \mathrm{d}z} \right)^n \varepsilon_0 \tag{2.16}$$

with

$$\varepsilon_0 \equiv \varepsilon(Q).$$

This correspondence is more of computational importance, since some elaborated routines for the phase-integral quantities ε_n already exist. To begin with, we already consider G_1 to be explicitly expressed in terms of the phase-integral quantity ε_0, i.e.

$$G_1 = \pm\sqrt{1+\varepsilon_0}. \tag{2.17}$$

To proceed one more step, from (2.12) we see that G_2 is related to $\varepsilon(Q_1)$, but $\varepsilon(Q_1)$, in turn, is related to G_1 according to (2.15), i.e.

$$\varepsilon(Q_1) = G_1^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta^2}G_1^{-1/2}. \tag{2.18}$$

Performing the differentiation in (2.18) together with (2.17), we find

$$\varepsilon(Q_1) = \tfrac{1}{16}(1+\varepsilon_0)^{-3}[5\varepsilon_1^2 - 4(1+\varepsilon_0)\varepsilon_2]. \tag{2.19}$$

Now the expression for G_2 is clear for the computational purposes of the present investigation.

2.4. On F-matrix theory

The F-matrix theory for Stokes's constants and connection formulae described in the book by Fröman and Fröman can be taken over directly. For example, connections across isolated turning points, with rigorous error bounds, can be found. It is important to emphasize, however, that existing uniform, comparison-equation techniques in higher approximations *cannot* be used in its present form. Such uniform methods are important in, for example, barrier penetration problems *close* to the top of the potential barrier.

In the application to energy quantization in the quartic oscillator potential of the next section, the positions of real and complex classical turning points, as well as the patterns of Stokes's and anti-Stokes's lines, are similar to those of a double-well problem. As long as the energy is far above the top of the local barrier in a double-well problem there is only a slight perturbation in the analytic behaviour of the wavefunctions if the barrier is inverted. Semiclassically, this means that one does not encounter the case where the barrier turning points coalesce. Hence, no comparison equation technique is necessary and the F-matrix method in [4] (see chapter 6) applies.

3. Energy quantization in an anharmonic potential

This particular application is, from a technical point of view, considered as an extrapolation of a double-well oscillator problem for energies far above the little barrier in the middle of a symmetric well. The anharmonic potential, which has no barrier, is given the reduced form

$$V(z) = \tfrac{1}{2}z^2 + \lambda z^4 \qquad \lambda > 0. \tag{3.1}$$

The Schrödinger equation in reduced units ($\hbar = 1$ and $m = 1$) can be written as

$$-\tfrac{1}{2}\psi_n'' + V(z)\psi_n = E_n\psi_n. \tag{3.2}$$

The coefficient $R(z)$ introduced in (1.1) is thus given by

$$R(z) = 2E - z^2 - 2\lambda z^4. \tag{3.3}$$

We use as the so-called base function $Q(z) = R^{1/2}(z)$, with real and imaginary classical turning points

$$z_R^{\pm} = \pm \left(\frac{1}{4\lambda} (\sqrt{1 + 16\lambda E} - 1) \right) \tag{3.4}$$

and

$$z_I^{\pm} = \pm i \left(\frac{1}{4\lambda} (\sqrt{1 + 16\lambda E} + 1) \right). \tag{3.5}$$

The primitive semiclassical quantization condition, without higher-order corrections and contributions from complex turning points, is in this case the Bohr–Sommerfeld formula

$$\int_{z_R^-}^{z_R^+} Q(z) \, dz = (n + \tfrac{1}{2})\pi \tag{3.6}$$

where the integration is performed along the real axis (see figure 1) between the two real turning points.
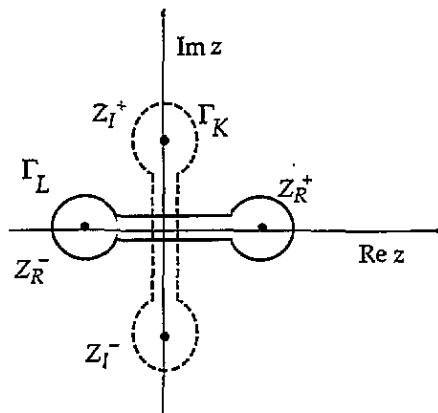

Figure 1. Illustration of complex contours of integration used in the quantization condition (3.7). In leading-order calculations the contours can be replaced by straight lines connecting the relevant turning points.

To incorporate the two complex turning points in the present problem, we argue that it is a valid procedure to use a symmetric double-well quantization condition with neglection of correction phases typically present for energies close to the top of the barrier, which does not exist here. Hence, from [7], assuming the correction phase is zero, we get the quantization formula

$$\tfrac{1}{2} \oint_{\Gamma_L} q \, dz = (n + \tfrac{1}{2})\pi + (-1)^n \sin^{-1} \left(\frac{e^K}{\sqrt{1 + e^{2K}}} \right) \tag{3.7}$$

where

$$K = \tfrac{1}{2} \oint_{\Gamma_K} q \, dz < 0 \qquad (3.8)$$

is the action corresponding to a classically forbidden trajectory with the same energy. The contours of integration, circumventing the real and complex turning points, are illustrated in figure 1.

In the numerical computations we consider only low-lying energy levels since the semiclassical results are less accurate for them. We have chosen the states $n = 0$, 4 and 8 to illustrate the rapid progess of the semiclassical accuracy. In table 1, one column shows the energy levels obtained by the 'primitive' Bohr–Sommerfeld condition (3.6), another shows energy levels from the iterated-q version (ιq version) of the semiclassical condition (3.7) for the three leading iteration orders. For the ground state, the second-order ιq approximation occasionally failed to satisfy the quantization condition within 20 Newton–Raphson iterations to the desired accuracy of 10^{-13}. Therefore this order of ιq approximation is systematically left out for the ground state. Zeroth-order ιq results are compared separately with the 'primitive' Bohr–Sommerfeld results to understand the importance of including complex trajectories without implementing higher-order contributions. A third column in table 1 contains energy levels obtained by higher-order standard phase-integral approximations (see [2], equations $(14a)$–$(14e)$ and (17)) using the condition (3.7). With this column it is possible to judge the efficiency of the ιq approximation to incorporate higher-order contributions. For completeness, numerical quantum results, reported by Hioe and Montroll [8] and occasionally corrected by the present authors, are included in the table.

The ground state $n = 0$ is generally the most difficult one to approximate semiclassically. However, for the exceptional case $\lambda = 0$ the ground state and all other levels are exactly obtained by the 'primitive' Bohr Sommerfeld formula. The quantization condition (3.7) also reduces to a Bohr–Sommerfeld formula and higher-order corrections vanish. As λ is increased only slightly, say up to $\lambda = 0.1$, semiclassical approximations, with and without complex-trajectory contributions, are accurate to within 7%. With higher-order corrections the errors become smaller by at least an order of magnitude. For weak anharmonicity, the influence of complex trajectories is thus much less important than higher-order contributions.

Already for $\lambda = 1$ the turning points of the complex trajectories come closer to real values, and a modification in the quantization conditions shows a significant improvement, of the same order of magnitude as the higher-order corrections. The ground-state relative error, corresponding to the 'primitive' Bohr–Sommerfeld formula, is approximately 12%, but only 6% if the complex trajectory contributions are included in the quantization formula. Again, with a first correction of higher order the relative error decreases well below 1%.

The importance of complex trajectories is more pronounced for large values of λ, like $\lambda = 1000$ in table 1. The 'primitive' semiclassical quantization yields a relative error in the ground state of approximately 18%. If complex trajectories are taken into account, the relative error stays around 6%. Further improvements are accounted for by higher-order corrections in the quantization formula. The situation for the ground-state accuracy is not expected to change significantly if λ is increased towards infinity. The best result we can get for the ground state $n = 0$ of an almost quartic oscillator is a relative error of about 1%. In all cases we have analysed, the errors of neglecting

Table 1. The table shows the energy levels from the 'primitive' Bohr–Sommerfeld (PBS) quantization using (3.6), and from the iterated-q (Iq) and phase-integral approximations (PIA) using quantization condition (3.7). The anharmonic oscillator potential is $V(z) = \frac{1}{2}z^2 + \lambda z^4$, $\hbar = 1$, $m = 1$. Numerical quantum results are also included for comparison.

Level	Iteration	E^{Iq}	Order	E^{PIA}	E^{PBS}
$\lambda = 0.1$					
	0	0.534	1	0.534	0.533
0	1	0.559 380	3	0.558 198	
	2	—	5	0.559 324	
			7	0.559 468	
			9	0.559 444	
			11	0.558 989	
		Numerical	0.559 146		
	0	6.212	1	6.212	6.212
4	1	6.220 301 418	3	6.220 302 455	
	2	6.220 300 898	5	6.220 301 466	
			7	6.220 300 916	
			9	6.220 300 898 638	
			11	6.220 300 899 682	
		Numerical	6.220 301		
	0	13.377	1	13.377	13.377
8	1	13.382 474 847	3	13.382 476	
	2	13 382 474 807 43	5	13.382 474 851	
			7	13.382 474 807 593	
			9	13.382 474 807 427	
			11	13.382 474 807 444	
		Numerical	13,382 475		
$\lambda = 1$					
	0	0.750	1	0.750	0.704
0	1	0.806 753	3	0.811	
	2	—	5	0.806 896	
			7	0.785	
			9	0.720	
			11	0.920	
		Numerical	0.803 771		
	0	10.946	1	10.946	10.946
4	1	10.963 585	3	10.963 634	
	2	10.963 583 073 91	5	10.963 585 540	
			7	10.963 582 972	
			9	10.963 583 069 258	
			11	10.963 583 096 750	
		Numerical	10.963 583		
	0	24.983	1	24.983	24.983
8	1	24.994 936 527	3	24.994 946	
	2	24.994 936 409 40	5	24.994 936 542	
			7	24.994 936 407 385	
			9	24.994 936 409 382	
			11	24.994 936 409 504	
		Numerical	24.994 936		

Table 1. (continued)

Level	Iteration	E^{Iq}	Order	E^{PIA}	E^{PBS}
$\lambda = 1000$					
	0	6.293	1	6.293	5.480
0	1	6.631 658	3	6.800	
	2	—	5	6.647 542	
			7	6.312	
			9	7.530	
			11	8.959	
		Numerical	6.694 221		
	0	102.338	1	102.338	102.338
4	1	102.516 177	3	102.516 859	
	2	102.516 156 942 60	5	102.516 179	
			7	102.516 154.554	
			9	102.516 156 889	
			11	102.516 157 216	
		Numerical	102.516 157		
	0	238.895	1	238.895	238.895
8	1	239.011 578 681	3	239.011 704	
	2	239.011 577 549 52	5	239.011 578 826	
			7	239.011 577 515	
			9	239.011 577 549 301	
			11	239.011 577 550 633	
		Numerical	239.011 578		

complex trajectories and higher corrections add together, yielding a too low ground-state energy.

The estimated absolute ground-state error divided by the local level spacing (predictability error) for each approximation is presented in table 2. Note that the leading-order semiclassical (Iq and phase-integral approximations) results, containing complex-trajectory contributions, have been given a separate column (CWKB) in the table.

When we turn to higher quantum numbers the influence of complex trajectories rapidly becomes insignificant. However, the higher-order corrections become more consistent and lead to *extremely* accurate results for the energy levels. The Iq approximation is very effective already with the first-order iteration formula.

Table 2. Predictability errors for the ground-state level, i.e. $|(E_0^a - E_0^{num})/(E_1^{num} - E_0^{num})|$, for three cases of the anharmonicity parameter λ, with a indicating the type of approximation: PBS ('primitive' Bohr–Sommerfeld), CWKB (first-order complex WKB), Iq optimal result, and PIA (phase-integral approximation) optimal result.

λ	PBS	CWKB	Iq	PIA
0.1	0.02	0.02	$2e\text{-}4$	$2e\text{-}4$
1	0.05	0.03	$2e\text{-}3$	$3e\text{-}3$
1000	0.07	0.02	$4e\text{-}3$	$3e\text{-}3$

4. Conclusions

For separable dynamical quantum systems which reduce to one-dimensional, uncoupled quantizations, there is a fair understanding of the asymptotics of semiclassical approximations and the singular classical limit that we would like to influence our work on more general systems. The details of real and *complex* classical turning points and other transition points like potential poles of various orders turn out to be of importance for the accuracy. In this paper we demonstrate that if one is interested in details of low-lying quantum levels near the classical limit, one has to be prepared to include not only complex turning points, but also higher-order terms in the semiclassical quantization conditions. Typically, a 'primitive' Bohr–Sommerfeld quantization yields gradually more accurate energy levels as the quantum number increases. However, one can predict cases where complex turning points become important at quite high quantum numbers (multi-well potentials), or else real, physical boundary points for the wavefunction may come too close to the important turning points in the quantization [1].

We also like to point out that higher-order semiclassical contributions can be efficiently included by the iterative method presented in this paper. Formal aspects and questions concerning optimal orders (relevant for asymptotic expansions) of this and similar iteration methods will be published separately [6].

Acknowledgment

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