Accuracy of the Semi–Classical Approximation: the Pullen Edmonds Hamiltonian[1]

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Abstract

A test on the numerical accuracy of the semiclassical approximation as a function of the principal quantum number has been performed for the Pullen–Edmonds model, a two–dimensional, non–integrable, scaling invariant perturbation of the resonant harmonic oscillator. A perturbative interpretation is obtained of the recently observed phenomenon of the accuracy decrease on the approximation of individual energy levels at the increase of the principal quantum number. Moreover, the accuracy provided by the semiclassical approximation formula is on the average the same as that provided by quantum perturbation theory.

Recently, there has been considerable renewed interest in the various aspects of the Semi–Classical Approximation (SCA), a powerful motivation behind that being the problem of the so–called quantum chaos (see for example references [1,2,3,4,5]). An important aspect is represented by the quantum energy levels, and in this connection one recent work [6] shows that the predictions of individual levels by SCA (by this we mean the Bohr–Sommerfeld formula, or one of its generalizations to the non–integrable case, such as EBK; see e.g. [3,4]), worsen as the quantum number increases, contrary to the naive expectation. We argue that this result can be interpreted as follows: if $\hbar$, no matter how small, is kept fixed, the SCA on the individual levels has the meaning of a perturbation theory (PT) in $\hbar$. Therefore the accuracy of the approximation decreases for higher levels (to get good agreement it is necessary, as is well known, to implement the classical limit $\hbar \to 0$, $n \to \infty$, $n\hbar = I$ classical action; see e.g. [7]).

The aim of this paper is to clarify this point, from the theoretical standpoint and from the computational one as well, considering a scaling invariant potential, which makes ordinary quantum PT strictly equivalent to a power expansion in $\hbar$. We do actually observe that, for $\hbar$ fixed, the perturbation strength has to be decreased to keep the accuracy at a constant value as the quantum number increases; however we also observe that the algorithm provided by the appropriate SCA is always comparable to the algorithm provided by ordinary quantum PT. A very good agreement between the "exact" eigenvalues, obtained by numerical diagonalization of the Schroedinger operator, and the semi–classical ones, is indeed observed in presence of high unperturbed degeneracy.

The most significant examples to carry out this comparison are represented by non–separable two dimensional systems exhibiting both regular and irregular spectrum [8], i.e. in particular, non–uniform behaviour of the level spacing, and among these the simplest one is the Pullen–Edmonds model [9]. Its quantum hamiltonian is:

$$H = -\frac{\hbar^2}{2}(\frac{\partial^2}{\partial q_1^2} - \frac{\partial^2}{\partial q_2^2}) + \frac{1}{2}(q_1^2 + q_2^2) + \chi q_1^2 q_2^2, \tag{1}$$

where m has been put equal to 1. For $\chi = 0$ (1) reduces to a resonant two–dimensional harmonic oscillator of levels $(n_1 + n_2 + 1)\hbar = m_1\hbar$, $m_1 = 1, 2, ...,$ of multiplicity m_1.

The scaling transformation $q_1 \to \sqrt{\hbar}q_1$, $q_2 \to \sqrt{\hbar}q_2$ yields the unitary equivalent operator:

$$\tilde{H} = -\hbar[\frac{1}{2}(\frac{\partial^2}{\partial q_1^2} - \frac{\partial^2}{\partial q_2^2}) + \frac{1}{2}(q_1^2 + q_2^2) + \chi\hbar q_1^2 q_2^2]. \tag{2}$$

The coupling constant has become $\chi\hbar$, which clearly shows equivalence between expansions in powers of χ or of $\hbar$ (an analogous result holds for any other polynomial perturbation). Moreover, the symmetry of the potential enables us to split the hamiltonian matrix, computed on the harmonic oscillator basis, into submatrices reducing the computer storage required. The matrix elements of (1) can be written:

$$\begin{aligned} &< n_1^{'} n_2^{'}|H|n_1 n_2 >= \hbar(n_1 + n_2 + 1)\delta_{n_1^{'} n_1}\delta_{n_2 n_2} + \chi\frac{\hbar^2}{4}[\sqrt{n_1(n_1 - 1)}\delta_{n_1^{'} n_1 - 2} + \\ &+\sqrt{(n_1 + 1)(n_1 + 2)}\delta_{n_1^{'} n_1 + 2} + (2n_1 + 1)\delta_{n_1^{'} n_1}] \times \\ &\times[\sqrt{n_2(n_2 - 1)}\delta_{n_2^{'} n_2 - 2} + \sqrt{(n_2 + 1)(n_2 + 2)}\delta_{n_2^{'} n_2 + 2} + (2n_2 + 1)\delta_{n_2^{'} n_2}] \end{aligned} \tag{3}$$

and each submatrix can be labelled by the parity of the occupation numbers n_1, n_2. We restrict from now on to the invariant subspace spanned by m_1

even, i.e. n_1 and n_2 of opposite parity. The eigenvalues of H in this subspace have constant multiplicity 2 [9]. Therefore the level $m_1\hbar = 2s\hbar$ splits into s levels for $\chi > 0$.

The appropriate SCA is here provided by the Bohr–Sommerfeld quantization of the resonant (or secular) canonical perturbation theory [10], also known, in this particular case, as the Birkoff–Gustafson normal form [11,12], which we now construct at first order. Starting from the classical Pullen–Edmonds hamiltonian:

$$H_{cl} = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + \chi q_1^2 q_2^2, \tag{4}$$

we introduce the standard action–angle variables (I, θ) by the canonical transformation:

$$\begin{cases} q_i &= \sqrt{2I_i}\cos\theta_i \\ p_i &= \sqrt{2I_i}\sin\theta_i. \end{cases} \quad i = 1, 2. \tag{5}$$

Then (4) becomes:

$$H_{cl} = I_1 + I_2 + 4\chi I_1^2 I_2^2 \cos^2\theta_1 \cos^2\theta_2. \tag{6}$$

The second canonical transformation into the well known "slow" and "fast" variables:

$$\begin{cases} A_1 &= I_1 + I_2 \\ A_2 &= I_1 - I_2 \end{cases} \qquad \begin{cases} \theta_1 &= \phi_1 + \phi_2 \\ \theta_2 &= \phi_1 - \phi_2, \end{cases} \tag{7}$$

eliminates the dependence on the "slow action" A_2 in the unperturbed part, so that the hamiltonian becomes:

$$H_{cl} = A_1 + \chi(A_1^2 - A_2^2)\cos^2(\phi_1 + \phi_2)\cos^2(\phi_1 - \phi_2). \tag{8}$$

We now eliminate the dependence on the angles up to order χ^2 by resonant (or secular) canonical perturbation theory [10]. To eliminate the dependence on the "fast angle" ϕ_1 it is enough to average the perturbation on this variable. This yields:

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi_1 \cos^2(\phi_1+\phi_2)\cos^2(\phi_1-\phi_2) = \frac{1}{8}(2+\cos 4\phi_2), \tag{9}$$

and thus:

$$\bar{H}_{cl} = A_1 + \frac{\chi}{8}(A_1^2 - A_2^2)(2+\cos 4\phi_2). \tag{10}$$

The dependence of ϕ_2 on the perturbation part can now eliminated by a further canonical transformation. The Hamilton–Jacobi equation for the perturbation part is in fact:

$$[A_1^2 - (\frac{\partial S}{\partial \phi_2})^2](2+\cos 4\phi_2) = K, \tag{11}$$

$$\frac{\partial S}{\partial \phi_2} = \pm\sqrt{\frac{A_1^2(2+\cos 4\phi_2) - K}{2+\cos 4\phi_2}}, \tag{12}$$

and thus the Hamiltonian (9) becomes:

$$\bar{H}_{cl} = B_1 + \frac{\chi}{8}K(B_1, B_2), \tag{13}$$

where:

$$B_1 = A_1, \quad B_2 = \frac{1}{2\pi}\oint d\phi_2 \frac{\partial S}{\partial \phi_2}. \tag{14}$$

It appears from the structure of equation (12) that the motions generated by the perturbation part of our system have the following qualitative behaviour:

$$\begin{array}{cc} 0 < K < B_1^2 & \textit{rotational motion} \\ K = B_1^2 & \textit{separatrix} \\ B_1^2 < K < 3B_1^2 & \textit{librational motion.} \end{array} \tag{15}$$

The appearance of a separatrix (which is not immediately obvious in the (p, q) coordinates) accounts as is well known (see e.g. [3]) for the stochastic layers originating near it. This corresponds to local irregular behaviour of the quantum spectrum; one of its manifestations is (see D. Delande in [4]) the local shrinking of the level spacing and the tendency to avoided crossing. The shrinking of the level spacing is best accounted by the SCA, as we will discuss below.

On the separatrix we have:

$$B_1^2(2 + \cos 4\phi_2) = K, \tag{16}$$

while in general:

$$B_2 = \pm\frac{2}{\pi}\int_a^b dx\sqrt{\frac{B_1^2(2+\cos 4x) - K}{2+\cos 4x}}, \tag{17}$$

where:

$$\begin{array}{cc} a = 0, \;\; b = \frac{\pi}{2} & \textit{rotational motion} \\ a = \phi_-(K, B_1), \;\; b = \phi_+(K, B_1) & \textit{librational motion} \end{array} \tag{18}$$

with:

$$\phi_\pm(K, B_1) = \pm\frac{1}{4}\arccos(\frac{K}{B_1^2} - 2). \tag{19}$$

Now the approximate hamiltonian (13) depends only on the actions so that a semiclassical quantization formula for the (m_1 even part) of spectrum of the operator (1) can be obtained by a straightforward application of the Bohr–Sommerfeld quantization rules [10]. Set therefore:

$$\left\{ \begin{array}{rcl} I_1 & = & (n_1 + 1/2)\hbar \\ I_2 & = & (n_2 + 1/2)\hbar, \end{array} \right. \tag{20}$$

whence, from (6):

$$\begin{cases} A_1 &= (n_1+n_2+1)\hbar \\ A_2 &= (n_1-n_2)\hbar. \end{cases} \tag{21}$$

Set:

$$\begin{cases} A_1 &= m_1\hbar \\ A_2 &= m_2\hbar, \end{cases} \tag{22}$$

by comparison of (19) and (20) we obtain:

$$\begin{cases} m_1 &= n_1+n_2+1 \\ m_2 &= n_1-n_2, \end{cases} \tag{23}$$

where $m_1 = 2, 4, ...$ and $m_2 = \pm(m_1-1), \pm(m_1-3), \pm(m_1-5), ...$.

Finally:

$$B_1 = m_1\hbar, \quad B_2 = m_2\hbar; \tag{24}$$

then the semiclassical approximation to the quantum spectrum is:

$$E_{m_1,m_2} = m_1\hbar + \frac{\chi}{8}K(m_1\hbar, m_2\hbar), \tag{25}$$

where K is implicitly defined by the relation:

$$m_2\hbar = \pm\frac{2}{\pi}\int_a^b dx\sqrt{\frac{(m_1\hbar)^2(2+\cos 4x)-K}{2+\cos 4x}}, \tag{26}$$

and:

$$\begin{array}{cc} a=0, \quad b=\frac{\pi}{2} & 0<K<(m_1\hbar)^2 \\ a=\phi_-(K,B_1), \quad b=\phi_+(K,B_1) & (m_1\hbar)^2<K<3(m_1\hbar)^2. \end{array} \tag{27}$$

Remark that for $|m_2| < [\alpha m_1]$ we obtain the quantization of the rotational motions, while for $|m_2| > [\alpha m_1]$ ($[x]$=integer part of x) we have the quantization of the librational ones. Here, by (17):

$$\alpha = \frac{2}{\pi}\int_0^{\frac{\pi}{2}} dx\sqrt{\frac{1+\cos 4x}{2+\cos 4x}} \simeq 0.602. \tag{28}$$

Moreover, it immediate to see that for m_1 fixed the function K, and hence the semiclassical energy E_{m_1,m_2}, is a decreasing function of the secondary quantum number m_2. It is furthermore proved in [13] that (25) coincides with the exact quantum spectrum up to terms of order $\hbar$ and χ^2. The numerical computations (see Fig. 4 below) show that at order 1 in χ the corrections of order $\hbar$ affect at most the eight decimal figure.

The "exact" levels have been computed, and compared with the semiclassical ones as well as with the levels computed by degenerate first order quantum perturbation theory [14], for $m_1 = 1, ..., 60$ at $\hbar = 0.1$ and for different values of χ (given the degeneracy, this is equivalent to compute 1800 different levels). The results obtained for $m_1 = 30$, $\hbar = 0.1$, $\chi = 10^{-3}$ and $m_1 = 60$, $\hbar = 0.1$, $\chi = 10^{-5}$ are shown in Figure 1 and Figure 2, respectively. The local shrinking of the spacing, reproduced by both methods, can be immediately noticed; remark that the corresponding semiclassical levels are those near the separatrix (by (28), $m_2 \sim 18$ and $m_2 \sim 36$, respectively).

In Figure 3 the function:

$$\Delta = |E^{Ex} - E^{Sc}| \tag{29}$$

vs m_1 is plotted for $m_1\chi = 1$; this shows that, if the coupling constant is decreased in inverse proportion to the principal quantum number the accuracy of SCA not only remains constant but actually improves, as anticipated because the scaling invariance makes the limit $m_1 \to \infty$, $\chi \to 0$, $m_1\chi \to const$ equivalent to the classical limit $m_1 \to \infty$, $\hbar \to 0$, $m_1\hbar \to const$.

In Figure 4 the accuracies obtained thorough semiclassical and quantum first order perturbation theories are compared for $m_1 = 60$, $\chi = 10^{-5}$, $\hbar =$

0.1, and in Fig. 5 the difference between the two perturbation theories is plotted (remark that the energy decreases as m_2 increases). As can be seen the agreement with the "exact" levels is very good and the accuracy is on the average the same. Remark however that, as it should be expected (the Bohr–Sommerfeld rules take no account of tunneling [15]), the lowest accuracy of the SCA is reached near $m_2 = 36$ which corresponds to the levels near the separatrix: for those levels the quantum PT is therefore better than SCA.

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Figure Captions

Figure 1: Comparison between the "exact" levels (a), the semi–classical ones (b), and the levels obtained by first order perturbation theory (c), for $\chi = 10^{-3}$, $\hbar = 0.1$, $m_1 = 30$.

Figure 2: Comparison between the "exact" levels (a), the semi–classical ones (b), and the levels obtained by first order perturbation theory (c), for $m_1 = 60$, $\chi = 10^{-5}$.

Figure 3: The difference Δ between the "exact" levels and the semi–classical ones *vs* m_1, with $m_2 = m_1 - 1$ and $m_1\hbar = 1$.

Figure 4: (a) The difference between the "exact" levels and the semi–classical ones; (b) the difference between the "exact" levels and the first order quantum PT ones; ($m_1 = 60$, $\hbar = 0.1$, $\chi = 10^{-5}$).

Figure 5: The difference between the semi–classical levels and the first order quantum PT ones; ($m_1 = 60$, $\hbar = 0.1$, $\chi = 10^{-5}$).

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