High-Precision Numerical Determination of Eigenvalues for a Double-Well Potential Related to the Zinn-Justin Conjecture

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A numerical method of high precision is used to calculate the energy eigenvalues and eigenfunctions for a symmetric double-well potential. The method is based on enclosing the system within two infinite walls with a large but finite separation and developing a power series solution for the Schrödinger equation. The obtained numerical results are compared with those obtained on the basis of the Zinn-Justin conjecture and found to be in an excellent agreement.

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1 Introduction

Quantum mechanical tunneling through finite barriers is a well established phenomenon in theory and application. The symmetric double well potential is one of the many examples exhibiting this phenomenon. In this case, the energy splitting generated by tunneling can be estimated with the help of the well-known semi-classical WKB approximation and instanton techniques (see for example [1]). However, to calculate this splitting accurately, one needs an effective method of high precision.

In a series of papers, Zinn-Justin [2] developed a conjecture (to be termed 'the Zinn-Justin conjecture') to determine the energy levels of a quantum Hamiltonian H, in cases where the potential has degenerate minima. This conjecture takes the form of the generalized Bohr-Sommerfeld quantization formulae. It has been applied, among other potentials, to the case of the symmetric double well. In this case the Hamiltonian is

$$H = -\frac{g}{2}\frac{\partial^2}{\partial q^2} + \frac{1}{g}V(q), \qquad \text{where} \qquad V(q) = \frac{1}{2}q^2(1-q)^2. \tag{1}$$

It is obvious that this Hamltonian is invariant under the transformation ($q \to 1-q$). The energy eigenvalues for this potential can be obtained by finding a solution to the Zinn-Justin conjecture equation:

$$\frac{1}{\sqrt{2\,\pi}}\Gamma\left(\frac{1}{2} - D(E,g)\right)\left(-\frac{2}{g}\right)^{D(E,g)} \exp\left[-A(E,g)/2\right] = \pm i. \tag{2}$$

The function $D(E, g)$ has a perturbative expansion in powers of g, of which the first few terms are

$$D(E, g) = E + g\left(3E^2 + \frac{1}{4}\right) + g^2\left(35E^3 + \frac{25}{4}E\right) + O(g^3). \tag{3}$$

The other function $A(E, g)$ receives contributions from the instanton expansion in the path integral and its first few terms are

$$A(E, g) = \frac{1}{3g} + g\left(17E^2 + \frac{19}{12}\right) + g^2\left(227E^3 + \frac{187}{4}E\right) + O(g^3). \tag{4}$$

The energy $E_{N,\pm}$ can be extracted from equation (2) by expanding in powers of g and in the two quantities

$$\lambda(g) = \ln\left(-\frac{2}{g}\right) \quad \text{and} \quad \xi(g) = \frac{\exp\left[-1/(6g)\right]}{\sqrt{\pi\, g}}. \tag{5}$$

The complete semi-classical expansion of $E_{N,\pm}$ has the form [4]

$$E_{\pm,N}(g) = \sum_{l=0}^{\infty} E^{(0)}_{N,l} g^l + \sum_{n=1}^{\infty}\left(\frac{2}{g}\right)^{Nn}\left((\mp)\frac{e^{-1/6g}}{\sqrt{\pi g}}\right)^n \sum_{k=0}^{n-1}\left(\ln\left(-2/g\right)\right)^k \sum_{l=0}^{\infty}\epsilon^{(N,\pm)}_{nkl} g^l. \tag{6}$$

The coefficients ϵ relevant to the numerical calculation have been explicitly calculated in [3]. The number N is the unperturbed quantum number which corresponds to

$$E_{\pm,N}(g) = N + 1/2 + O(g). \tag{7}$$

A detailed exposition of the above equations can be found in [4].

In [3], numerical calculations have been carried out and led to the energy eigenvalues for the ground and the first excited states respectively, for $g = 0.001$,

$$\begin{aligned} E_{0,+}(0.001) \;&=\; 0.49899\;54548\;62109\;17168\;91308\;39481\;92163\;68209\;47240\;20809 \\ &\quad\; 66532\;93278\;69722\;01391\;\underline{15135\;28505\;38294\;45798\;45759\;95999} \\ &\quad\; \underline{06739\;55175\;84722\;67802\;81306\;96906\;01325\;25943\;77289\;94365} \\ &\quad\; \underline{88255\;24440\;17437\;12789\;27978\;99793}, \end{aligned} \tag{8}$$

$$\begin{aligned} E_{0,-}(0.001) \;&=\; 0.49899\;54548\;62109\;17168\;91308\;39481\;92163\;68209\;47240\;20809 \\ &\quad\; 66532\;93278\;69722\;01391\;\underline{29839\;92959\;55803\;70812\;27749\;92448} \\ &\quad\; \underline{48259\;36743\;64757\;68328\;84835\;35511\;34663\;06309\;82331\;51885} \\ &\quad\; \underline{23308\;08622\;84780\;52722\;10103\;67282}. \end{aligned} \tag{9}$$

The above numerical results have been obtained by lattice extrapolation using a modified Richardson algorithm [3].

This tiny difference encourages us to seek for an independent but simple and direct method, which allows us to obtain the energy eigenvalues for the potential in equation (1) and compare them with the above numerical results. In addition, the present method allows us to obtain an accurate description for the corresponding wavefunctions. This method has been previously applied to various potential functions with and without degenerate minima, leading to results with high accuracy [5].

The method, as will be described in the next two sections, is based on power series solution of the Schrödinger equation in a finite range. It has appeared from time to time in the literature [6, 7, 8], but has not been developed to its maximum efficiency. We shall show that, by using the computer algebra systems (for example Mathemtica) which can deal with exact numbers, the accuracy of the method can be substantially improved.

In the following section, for illustrative purpose, we explain our method by applying it to the well-known exactly solvable harmonic oscillator potential and then extend it to the symmetric double well.

2 Calculations and Results

In this section we, first, consider the well-known exactly solvable harmonic oscillator. In this case, the Schrödinger equation reads ($\hbar = 1, m = 1$)

$$\left[-\frac{1}{2} \frac{d^2}{d\,q^2} + E - V(q) \right] \Psi(q) = 0, \tag{10}$$

where

$$V(q) = \frac{1}{2}\, q^2. \tag{11}$$

The exact energy eigenvalues and the corresponding eigenfunctions are

$$\begin{aligned} E_N &= \left(N + \frac{1}{2} \right), \qquad N = 0, 1, 2, \cdots, \\ \Psi_N(q) &= 2^{-\frac{N}{2}}\, (N!)^{-\frac{1}{2}}\, \pi^{-\frac{1}{4}}\, \exp\left(-\frac{q^2}{2} \right) H_N(q), \end{aligned} \tag{12}$$

where $H_N(q)$ are the Hermite polynomials.

For the harmonic oscillator confined between two infinite walls at $q = \pm\, L$, we develop a power series solution in the form

$$\Psi(q) = \sum_{i=0}^{\infty} a_i\, q^i. \tag{13}$$

Substituting in equation (10), one gets the following recursion relation:

$$a_i = \frac{a_{i-4} - 2\,E\,a_{i-2}}{i\,(i-1)}, \quad i \neq 0, 1 \quad \text{and} \quad a_i = 0 \quad \text{when} \quad i < 0. \tag{14}$$

The symmetry of the potential implies that we have two types of solutions: the even solutions obtained by imposing (ignoring normalization) $a_0 = 1, a_1 = 0$ and the odd ones by imposing $a_0 = 0, a_1 = 1$. The energy eigenvalues are then obtained from the condition $\Psi(E, L) = 0$ for both cases.

For numerical calculations, we approximate the power series in equation (13) with a truncated one having a finite number of terms $\Psi_I(E, q)$, where I is the number of non-vanishing terms. The boundary condition for a specific value of L corresponds to $\Psi_I(E, L) = 0$. To get the zeros of $\Psi_I(E, L)$ with respect to E, we first plot a graph for $\Psi_I(L, E)$ as a function of E to locate where $\Psi_I(L, E)$ changes sign. We then can use two nearby points containing one single root as the initial iteration for the 'bisection method' to find the zeros. In doing this we have used Mathematica package version 3 and also have relied extensively on its ability to manipulate exact numbers. The stability of the numerical results to a certain degree of accuracy is checked, for a particular L, by increasing I till the obtained value of E stays fixed.

In table 1 we present the calculated energies for the ground and the first three excited states for the bounded harmonic oscillator as compared to the exact results of the unbounded one.

I	L	N	E_N	$E_N^{\text{exact}} = (N+\frac{1}{2})$
250	8	0	0.5000000000000000000000000	$\frac{1}{2}$
		1	1.500000000000000000000000	$\frac{3}{2}$
		2	2.50000000000000000000000	$\frac{5}{2}$
		3	3.5000000000000000000000	$\frac{7}{2}$

Table 1: The calculated first four energy levels for the bounded harmonic oscillator compared to the unbounded one. $(2L)$ is the width of the well and I refers to the number of the non-vanishing terms in the truncated series of the wavefunction.

The present method, as can be seen from table 1, reproduces for a large value of L, the exact ones even for a moderate number of non-vanishing terms in the truncated series of the wavefunction. Moreover, one can get an accurate description for the wavefunctions shown in figure 1 which can not be distinguished from the exact ones when drawn within the same interval $|q| \leq L = 8$.

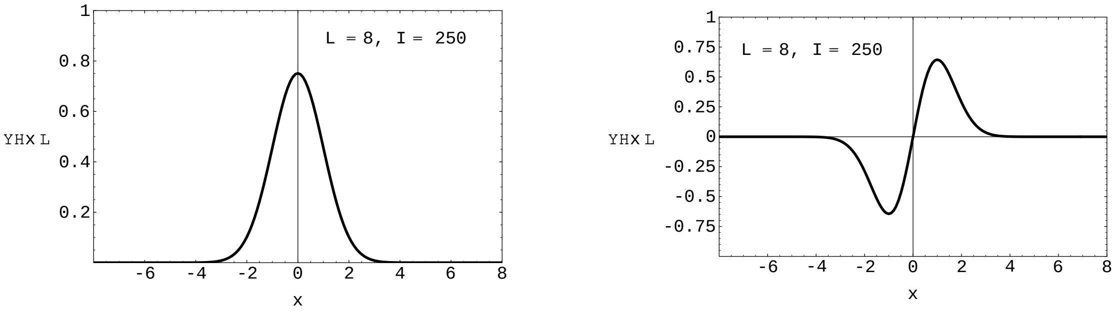

Figure 1: The normalized ground (left) and first excited (right) state wavefunctions for the bounded harmonic oscillator for $L = 8$.

Now we apply the above-explained method to the double well potential in equation (1). For our convenience, we use the substitution $q \to q + \frac{1}{2}$, so the potential in equation (1) now takes the form

$$V(q) = \frac{1}{2}\,(q+1/2)^2\,(q-1/2)^2\,. \tag{15}$$

This form of the potential has now inversion symmetry $(q \to -q)$ which is suitable for our calculation. It should be evident that rewriting the potential in this form doesn't affect the eigenvalues of the Hamiltonian in equation (1). As explained above, for this potential we again use the power series expansion of the wavefunction in the finite range. The Schrödinger equation, for the potential $V(q)$ in equation (15), is

$$\left[\frac{g}{2}\frac{d^2}{d\,q^2} + E - \frac{1}{g}V(q)\right]\Psi(q) = 0, \qquad -L < q < L. \tag{16}$$

In substituting the power series expansion,

$$\Psi(q) = \sum_i a_i\, q^i, \tag{17}$$

in equation (16), one gets the following recurrence formula for the expansion coefficients, a_i:

$$a_i = \left(\frac{2}{g}\right) \frac{\frac{1}{2g}\left[a_{i-6} - \frac{1}{2}a_{i-4} + \frac{1}{16}a_{i-2}\right] - Ea_{i-2}}{i(i-1)}, \quad i \neq 0, 1 \;\text{ and }\; a_i = 0 \text{ when } i < 0. \tag{18}$$

For $L = 3$, the obtained eigenvalues are

$$\begin{aligned} E_{0,+}(0.001) \;=\; & 0.49899\ 54548\ 62109\ 17168\ 91308\ 39481\ 92163\ 68209\ 47240\ 20809 \\ & 66532\ 93278\ 69722\ 01391\ \underline{15135\ 28505\ 38294\ 45798\ 45759\ 95999} \\ & \underline{06739\ 55175\ 84722\ 67802\ 81306\ 96906\ 01325\ 25943\ 77289\ 94365} \\ & \underline{88255\ 24440\ 17437\ 12789\ 27978\ 99793\ 98922\ 00536\ 06978\ 04138} \\ & \underline{65255\ 73028\ 37723\ 50241\ 67171}, \end{aligned} \tag{19}$$

$$\begin{aligned} E_{0,-}(0.001) \;=\; & 0.49899\ 54548\ 62109\ 17168\ 91308\ 39481\ 92163\ 68209\ 47240\ 20809 \\ & 66532\ 93278\ 69722\ 01391\ \underline{29839\ 92959\ 55803\ 70812\ 27749\ 92448} \\ & \underline{48259\ 36743\ 64757\ 68328\ 84835\ 35511\ 34663\ 06309\ 82331\ 51885} \\ & \underline{23308\ 08622\ 84780\ 52722\ 10103\ 67282\ 72047\ 61340\ 01672\ 24803} \\ & \underline{65523\ 52410\ 13798\ 16304\ 58360}. \end{aligned} \tag{20}$$

These values agree with the ones obtained from the numerical calculations based on the Zinn-Justin conjecture. In figure 2 we present the ground and the first excited state wavefunctions for the bounded double-well potential for $g = 1/1000$, $I = 4600$ and $L = 1$.

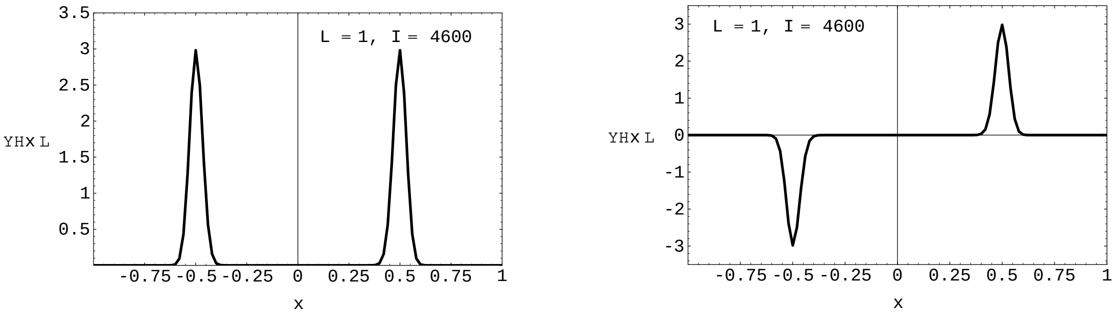

Figure 2: The normalized ground (left) and first excited (right) state wavefunctions for the bounded double-well potential with $g = 1/1000$.

3 Discussion

It is important to note the following generic remarks. First, a reason for the capability of the present method is that for a bound state, the wavefunction is spatially localized which means that the probability density ($|\Psi|^2$) has appreciable values in a finite region of space behind which the probability density tends rapidly to zero. Thus, to a good approximation, it is, therefore, reasonable to consider the corresponding problem in a finite interval, with a suitable width, bounded by two infinite walls. The criteria for a suitable value of L can be quantitatively given by the condition $E << V(L)$. Second, from the WKB approximation, it can be made plausible that the zeros of $\Psi(E, L)$ provide upper bounds for the energy eigenvalues while the zeros of the derivative–with respect to q– $\Psi'(E', L)$ provide the lower ones; the same finding can be proved in a rigorous way as shown in [9]. Thus, by matching the digits of the two zeros, one can get an accurate energy eigenvalue up to the number of coincident digits. As an example for the ground state of the bounded harmonic oscillator, with $L = 8$ and $I = 250$, one gets

$$\begin{aligned} E &= 0.50000000000000000000000000143627070547557659037565 98\\ &\quad 26757972824824621785332078167891514939744867648,\\ E' &= 0.49999999999999999999999999854055435732786820927446 52\\ &\quad 58622103903146216005437303539479001558808137418. \end{aligned} \tag{21}$$

The corresponding wavefunctions and their slopes are

$$\begin{aligned} \Psi(E,8) &= 4.8 \times 10^{-49} \quad , \quad \Psi'(E',8) = 8.1 \times 10^{-48},\\ \Psi(E',8) &= 2.6 \times 10^{-14} \quad , \quad \Psi'(E,8) = -2 \times 10^{-13}. \end{aligned} \tag{22}$$

After matching the digits of the two numbers in equation (21), one gets the ground-state energy accurate up to 25 digits as shown in table 1. The remaining eigenvalues are obtained by the same procedure. However, one should pay attention that this accuracy is expected to be less than the accuracy of the bisection method. In this method, the accuracy estimation is $\varepsilon = (c - a)/2^n$ where n, here, is the number of iteration, and c and a are two points enclosing only one root. In our case, we have taken for the ground state $n = 200$, $c = \frac{6}{10}$ and $a = 4/10$, giving $\varepsilon = 1.2 \times 10^{-61}$. Finally according to the WKB approximation, the wavefunction behaves for large q in the inaccessible region as

$$\Psi_{WKB}(q) \;\propto\; \frac{1}{(V(q) - E)^{\frac{1}{4}}} \exp\left(- \int_{q_t}^{q} \sqrt{(V(q') - E)}\, dq' \right), \tag{23}$$

where q_t is a turning point just left to the inaccessible region. The value of $\Psi_{WKB}(q = 8)$ is 6.5×10^{-14}, while for the truncated series solution of equation (13) it has the value 4.8×10^{-49} as given in equation (22). The reason for this huge difference is that the series solution is valid and convergent as long as q is finite [10]. In addition to this, the energy eigenvalues as extracted from the zeros of $\Psi(E, L)$ (for suitable L) result in a delicate cancellation between terms of opposite signs in the power series solution.

One may suspect that using a series solution in the form

$$\Psi(x) = \exp\left(-b\, x^2\right) \sum_j a_j\, x^j, \tag{24}$$

may help improving the rate of convergence for the obtained eigenvalues. In contrast, one needs more terms in the series expansion to achieve the same level of accuracy obtained by the series solution of the form given in equation (13). The reason behind this stems from the fact that any finite truncation for the series in the form given in equation (24) always decays, due to the exponential factor, as q becomes large making the determination of the energy eigenvalues less reliable, especially when the parameter b is large. As an example, when $b = \frac{1}{2}$ we can achieve the same accuracy reported in table 1 with the same number of non-vanishing terms in the truncated series, while for $b = 8$ we need 600 non-vanishing terms to achieve the same accuracy. Thus, the best thing which can be done is to work with the parameter b having zero value. However, it should be kept in mind that both series in equation (13) and equation (24) are equivalent but only in the infinite sum limit.

We also study the effect of the parameter b in the case of the double-well potential given by

$$V(x) = -10\, x^2 + x^4, \qquad \left(\text{in units} \quad \hbar = 1, m = \frac{1}{2}\right). \tag{25}$$

As an example, when we work with the precision 100 digits, then we find for $b = 0$, $I = 750$ and $L = 8$, that the ground state energy has the value (accurate up to 69 digits)

$$\begin{aligned} E_0 &= -20.63357\ 67029\ 47799\ 14995\ 85548\ 37431 \\ &\quad 50876\ 53159\ 46057\ 73551\ 39057\ 10311\ 42892\ 92. \end{aligned} \tag{26}$$

To achieve the same accurate energy determination for $b = 10$, we find that it is possible to use 500 terms which is not considerably less than the case of $b = 0$. However, this comes with the high cost of working with precision 300 digits. Working with such a high precision renders the calculation slow. At intermediate values of b like $2, 3$ and 4, we can use less terms but with high precision as shown in table 2. According to our numerical investigations for the case of the double well, in the finite range, the choice $b = 0$ is the best compromise between the number of terms used and the degree of precision to get a more efficient calculation.

b	0	$\frac{1}{2}$	1	2	3	4	5	10
I	750	750	750	500	500	500	500	500
Precision	100	100	150	150	200	200	200	300

Table 2: Precision versus I and the parameter b

It is important to point out that in dealing with low accuracy results (like nine digits), one cannot decide which is better, to work with or without the parameter b. Furthermore, employing the method in a non-efficient way may lead to wrong conclusions as in [8], where it is emphasized that setting a non-vanishing value for the parameter b greatly reduces the number of terms used. To clarify these points, we obtain for the potential given by equation (25) the four first energy levels ($E_0 = -20.6335767$, $E_1 = -20.6334568$, $E_3 = -12.3795437$, $E_4 = -12.3756738$) accurate up to 10 digits as presented in [8]; our results (using $L = 4.2$) are summarized in table 3. It is evident from table 3 that one can not say it is a big advantage to use 90 terms (for $b = 2$) rather than 125 terms (for $b = 0$). However, numerical studies clearly indicate that the situation becomes worse when b increases (for $b = 10$ we need 200 terms). Another clear example is the pure quartic potential ($V(x) = x^4$) for which we get, for $b = 0$, $L = 3.5$, and $I = 75$, low-energy eigenvalues (the first five) determined accurately up to nine digits while obtaining the same results for the choice $b = 3$ and $I = 50$. Furthermore, the tenth eigenvalue is determined accurately up to 9 digits, for $L = 3.9$, using $I = 75$ for $b = 3$, while $I = 125$ for $b = 0$. These findings are in contradiction with what has been claimed in [8], where it was mentioned that one should use about 2000 terms in the power series to determine the energy for the choice $b = 0$. Similar findings occur for the potential $V(x) = x^2 + x^8$. In such a situation for $L = 2.5$, we can use 125 terms in the power series solution for $b = 0$ and 75 terms for $b = 5$, while getting the same accurate results up to nine digits.

b	0	$\frac{1}{2}$	1	2	3	4	5	10
I	125	100	90	90	90	90	90	200

Table 3: The parameter b versus I (number of non-vanishing terms)

The problem in the calculations found in [6, 8] comes from evaluating every term in the power series to a certain precision, and then summing the series which leads to an error accumulation, resulting in low-accuracy results despite using a large number of terms. In our approach, we sum all terms in the power series exactly, and then only in determining the roots (energy) from the condition $\Psi_I(E, L) = 0$, do we resort to numerical calculation with a certain precision. Although the ability of the computer algebra system to deal with exact numbers was available from the early 1980s, it has not been used since then in such calculations.

4 Conclusion

In this paper we have presented an independent simple method leading to eigenvalues which agree well with the recently obtained numerical results based on the Zinn-Justin conjecture for the symmetric double-well potential. We have also included results with more significant digits than reported. It has been applied to some other potentials to illustrate its capability, and its precision has been compared with other calculations based on introducing an exponentially decaying factor ($e^{-b\,x^2}$). Several subtle points related to its precision have also been discussed and clarified. The method we opted also enables us to get an accurate numerical determination of the corresponding wavefunctions.

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