

Very-high-precision normalized eigenfunctions for a class of Schrödinger type equations

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Abstract—We demonstrate that it is possible to compute wave function normalization constants for a class of Schrödinger type equations by an algorithm which scales linearly (in the number of eigenfunction evaluations) with the desired precision P in decimals.

Keywords—Eigenvalue problems; Bound states; Trapezoidal rule; Poisson resummation

I. INTRODUCTION

IN a recent paper[1] it was demonstrated that it is possible to solve some eigenvalue problems of the Schrödinger type to almost arbitrary high precision. The cases presented explicitly were (i) the ground state eigenenergy of the anharmonic oscillator,

$$-\psi'' + x^4 \psi = \varepsilon \psi, \quad (1)$$

which was found to an accuracy of more than 1 000 000 decimal digits, (ii) the eigenstate number 50 000 of the same equation where the eigenenergy was found to an accuracy of more than 50 000 decimal digits, and (iii) the lowest even and odd parity states of the double-well potential,

$$-s^2 \psi''_{\pm} + (x^2 - 1)^2 \psi_{\pm} = \varepsilon_{\pm} \psi_{\pm}, \quad (2)$$

where the two eigenenergies were found to an accuracy of more than 30 000 decimal digits for the case $s = 1/50\,000$.

In the latter case the two eigenenergies are degenerate to almost 29 000 decimals, with the difference directly computable by the WKB method. The 10th order WKB expansion given in [2] provide an accuracy of about 48 decimals for the difference, all of which agrees with the difference between the two numerical calculated eigenenergies.

Also the eigenenergies of the highly excited states of equation (1) can be calculated by the WKB method. The 12th order WKB expansion given in [3] provide an accuracy of about 67 decimals, all of which agrees with the numerical result.

It is certainly difficult to find physical systems where one need to know eigenenergies to tens of thousands of decimals or more. However, if one need to compute the wavefunction very accurately to very high values of x (to f.i. evaluate matrix elements) the value depends extremely sensitively on the eigenvalue parameter. Thus, in our opinion, algorithms for very-high-precision evaluation of eigenvalues may be useful in combination with routines for very-high-precision evaluation of matrix elements and normalization integrals.

In this paper we demonstrate that the latter can be achieved very simply, with the number of eigenfunction evaluations growing only linearly with the desired precision P in decimal digits. Each eigenfunction evaluation will in turn require a number of high-precision multiplications which grows linearly with P , and each such multiplication require a

CPU time which scales asymptotically between $P^{1.6}$ and $P \log P \log \log P$ (depending on which high-precision multiplication algorithm is used). Thus, the total time to evaluate one normalization integral to P decimals precision can be expected to increase somewhat faster than P^3 . However, since the eigenfunction evaluations are independent they can be run in parallel.

The rest of this paper is organized as follows. In section II we make some general remarks on numerical integration rules. We base our analysis on the Euler-Maclaurin summation formula and the Poisson resummation formula. Our conclusion is that the trapezoidal rule is not only the simplest one but also the best one. For integrals over finite intervals some there are endpoint corrections which should be considered separately; these corrections vanish for our normalization integrals. In section III we consider some simple example cases similar to our wavefunction normalization integrals. For an infinite (in principle) integration range and a fixed number M of integration steps one must strive for a balance between the error $\varepsilon(h)$ due to using a finite stepsize h , and the error $\varepsilon(x_{\max})$ due to covering only a finite integration range. These errors can be estimated by respectively analysing the Fourier transform $\hat{f}(p)$ of the integrand $f(x)$ as $|p| \rightarrow \infty$ (by the method of steepest descent), and the asymptotic behaviour of $f(x)$ as $|x| \rightarrow \infty$. It appears that both analyses can be extended to wavefunction normalization integrals by use of the WKB approximation. This extension is done in section IV.

II. REMARKS ON INTEGRATION FORMULAE

There is no scarcity of numerical integration formulae in the literature[4]. Standard choices are rules for $I\{f\} \equiv \int_a^b dx f(x)$ which reproduces integrals of polynomials below a certain order exactly,

$$\begin{aligned} I\{f\} &\approx \frac{1}{2} (f_0 + f_1) h \equiv T(h), \\ I\{f\} &\approx \frac{1}{3} (f_0 + 4f_1 + f_2) h \equiv S(h), \\ I\{f\} &\approx \frac{3}{8} (f_0 + 3f_1 + 3f_2 + f_3) h \equiv S_{3/8}(h), \\ I\{f\} &\approx \frac{2}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) h \equiv B(h), \end{aligned} \quad (3)$$

with $h = (b - a)/M$ and $f_m = f(a + mh)$ when there is $M + 1$ terms in the integration rule. These are known respectively as the trapezoidal, Simpson's, Simpson's $\frac{3}{8}$, and Boole's rule. They are automatically exact for polynomials which are antisymmetric about the midpoint $\bar{x} = (b - a)/2$. The M independent coefficients are chosen to give exact results for all symmetric (about \bar{x}) polynomials of order below $2M$. However, as M increases the weight coefficients develop in a suspicious way. To integrate functions over large intervals to very high precision it seems dubious to extend the procedure above.

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A. Extended Simpson's rule

An alternative way to handle integration over large intervals is to divide them into many smaller ones, and apply one of the rules above to each of the subintervals. We denote this by a bar over the rule, $T(h) \rightarrow \bar{T}(h)$ etc. A rather common choice is to extend Simpson's rule, leading to the formula

$$\int_a^b dx f(x) \approx \bar{S}(h) \equiv \frac{1}{3} (f_0 + 4f_1 + 2f_2 + \dots + 2f_{M-2} + 4f_{M-1} + f_M) h, \quad (4)$$

which looks curious to any member of an equal society. What is wrong with half of the points? Are they of the wrong gender? Which mysterious force of numerical error analysis leads to this spontaneous breakdown of translation invariance?

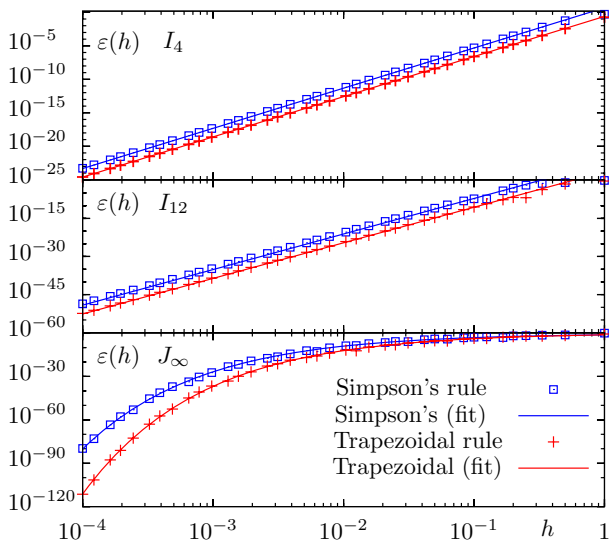


Fig. 1 Comparison of accuracy of the extended trapezoidal and Simpson's rules for some integrands with very smooth boundary behaviour.

In our opinion only $\bar{T}(h)$ is a logically sensible procedure. We claim that this is also the best procedure. To support and exemplify this claim we have evaluated the integrals below:

$$I_n = \int_0^1 dx (1 - x^2)^n, \quad (5)$$

$$J_\infty = \int_0^1 dx \left[1 - \tanh \left(\frac{2x - 1}{1 - (2x - 1)^2} \right) \right], \quad (6)$$

by the $\bar{T}(h)$ and $\bar{S}(h) = \frac{4}{3}\bar{T}(h) - \frac{1}{3}\bar{T}(2h)$ rules. The relative errors of the two methods as function of discretization length h are shown in figure 1. The result is as expected that \bar{S} behave as well as \bar{T} with twice the discretization length h .

B. Euler-Maclaurin summation formula

The examples in figure 1 are untypical in the sense that the integrands are very smooth at the endpoints (which is typical for the normalization integrals we are primarily interested in). One may use the Euler-Maclaurin summation formula to see which quantity is actually computed by the various integration

rules

$$\left[\frac{1}{2}f_0 + \sum_{m=1}^{M-1} f_m + \frac{1}{2}f_M \right] h = \int_a^b dx f(x) + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \Delta^{(2k-1)} + \dots = \int_a^b dx f(x) + \frac{\Delta^{(1)}}{12} - \frac{\Delta^{(3)}}{720} + \frac{\Delta^{(5)}}{30240} - \frac{\Delta^{(7)}}{1209600} + \dots, \quad (7)$$

where $\Delta^{(k)} = [f^{(k)}(b) - f^{(k)}(a)] h^{k+1}$, and the ellipsis in the first line denote "non-perturbative" terms depending on how $f(x)$ varies in the full integration range. With $\bar{S}(h) = \frac{4}{3}\bar{T}(h) - \frac{1}{3}\bar{T}(2h)$ one finds the corresponding quantity for the extended Simpson's rule:

$$\bar{S}\{f\} = \int_a^b dx f(x) + \frac{1}{3} \sum_{k=1}^{\infty} (4 - 2^{2k}) \frac{B_{2k}}{(2k)!} \Delta^{(2k-1)} + \dots \quad (8)$$

I.e., the $\Delta^{(1)}$ -coefficient has been eliminated at the cost of increasing all the remaining coefficients¹.

A natural way to eliminate the $\Delta^{(1)}$ -coefficient would be to calculate f' explicitly at the endpoints, or use a numerical approximations like

$$f'(x) = \frac{f(x + \delta) - f(x - \delta)}{2\delta} - \frac{1}{6} f^{(3)}(x) \delta^3 + \dots,$$

$$f'(x) = -\frac{3f(x) - 4f(x + \delta) + f(x + 2\delta)}{2\delta} + \frac{1}{3} f^{(3)}(x) \delta^3 + \dots,$$

$$f'(x) = \frac{3f(x) - 4f(x - \delta) + f(x - 2\delta)}{2\delta} + \frac{1}{3} f^{(3)}(x) \delta^3 + \dots,$$

for sufficiently small δ . One should take δ somewhat smaller than h . The modified trapezoidal rule described in [5] is generally worse than the extended Simpson's rule because of an inaccurate approximation of f' . However, there are few reasons to use the same discretization length for computing derivatives at the endpoints as for computing the bulk contribution to the integral. To avoid introduction of significant new errors it is sufficient to choose $\delta < h/2$ in the first formula. By choosing $\delta = h/\sqrt{20}$ in the last two one also eliminates the $\Delta^{(3)}$ -term in equation (7).

C. Poisson resummation formula

There exist expressions for the "non-perturbative" terms in equation (7), but we find the Poisson resummation formula more clarifying: Assume $f(x)$ is an entire, integrable function, with Fourier transform

$$\tilde{f}(p) = \int_{-\infty}^{\infty} dx f(x) e^{ipx}. \quad (9)$$

Then one version of the Poisson resummation formula reads

$$\sum_{m=-\infty}^{\infty} h f(mh) = \sum_{k=-\infty}^{\infty} \tilde{f}\left(\frac{2\pi k}{h}\right). \quad (10)$$

This can be used to estimate the accuracy of the numerical integration formula

$$\int_{-\infty}^{\infty} dx f(x) = \sum_{m=-\infty}^{\infty} h f(mh) - \sum_{k \neq 0} \tilde{f}\left(\frac{2\pi k}{h}\right). \quad (11)$$

When $f(x)$ is an entire function its Fourier transform $\tilde{f}(p)$ will vanish faster than any inverse power of p as $p \rightarrow \infty$. This means that the numerical approximation to the (infinite range)

¹Note that the error terms given for the "extended" rules in reference [4] are in disagreement with our results.

integral of an entire function will converge *very fast* towards the exact value as $h \rightarrow 0$.

Integrals of $f(x)$ over a finite range $[a, b]$ can be viewed as integrals of $g(x) \equiv \theta(b-x)\theta(x-a)f(x)$ over an infinite range. But $g(x)$ will usually be discontinuous, with a Fourier transform $\tilde{g}(p)$ which vanishes only algebraically as $p \rightarrow \infty$. The “perturbative” endpoint corrections of the Euler-Maclaurin formula can be used to account for these algebraic terms in a systematic way. But there is no point in making endpoint corrections beyond the error in the bulk contribution, the latter being of magnitude $\tilde{f}(\frac{2\pi}{h}) + \tilde{f}(-\frac{2\pi}{h})$.

III. EXAMPLE INTEGRALS

In this section we will analyze the behaviour of some simple cases which are similar to typical ground state normalization integrals.

A. e^{-x^2}

Consider first the ground state of the harmonic oscillator, $f(x) = e^{-x^2}$, in which case

$$\tilde{f}(p) = \sqrt{\pi} e^{-p^2/4}. \quad (12)$$

Hence we have

$$\int_{-\infty}^{\infty} dx e^{-x^2} = \sum_{m=-\infty}^{\infty} h e^{-(mh)^2} - \sqrt{4\pi} e^{-\pi^2/h^2} - \dots \quad (13)$$

In practise we must approximate the infinite sum by a finite one,

$$\int_{-\infty}^{\infty} dx e^{-x^2} = h + 2h \sum_{m=1}^M e^{-(mh)^2} + 2he^{-(M+1)^2 h^2} + \dots - \sqrt{4\pi} e^{-\pi^2/h^2} - \dots$$

If we make h too small the first correction term (on the second line above) becomes too large. If we make h too large the second correction term becomes too large. I.e., the optimal choice of h occurs approximately when $e^{-(M+1)^2 h^2} = e^{-\pi^2/h^2}$,

$$h = \sqrt{\frac{\pi}{M+1}}. \quad (14)$$

This leads to an expected error of order

$$\varepsilon(M) = e^{-\pi(M+1)}. \quad (15)$$

I.e., to evaluate this integral numerically to P decimals accuracy one must choose

$$M+1 \geq \frac{\log 10}{\pi} P \approx 0.73 P. \quad (16)$$

B. $e^{-x^{2n}}$

In more generality consider $f(x) = e^{-x^{2n}}$ with n a positive integer. In this case the integral is

$$K_n \equiv \int_{-\infty}^{\infty} dx e^{-x^{2n}} = \frac{1}{n} \Gamma\left(\frac{1}{2n}\right). \quad (17)$$

We use the saddle point method to estimate its Fourier transform

$$\tilde{f}(p) = \int_{-\infty}^{\infty} dx e^{-x^{2n} + ipx} \equiv \int_{-\infty}^{\infty} dx e^{\phi(x,p)}. \quad (18)$$

The saddle point equation becomes

$$\phi'(x_s, p) = -2nx_s^{2n-1} + ip = 0, \quad (19)$$

with $2n - 1$ solutions

$$x_s = e^{i\pi(4k+1)/(4n-2)} \left(\frac{p}{2n}\right)^{1/(2n-1)}, \quad k = 0, 1, \dots, 2n-2. \quad (20)$$

The two most relevant saddle points² occur for $k = 0$ and $n - 1$, at which the real part of the exponent $\phi(x, p)$ is (when $p = 2\pi/h$)

$$\begin{aligned} \text{Re } \phi(x_s, p) &= -(2n-1) \sin\left(\frac{\pi}{4n-2}\right) \left(\frac{\pi}{nh}\right)^{2n/(2n-1)} \\ &\equiv a_n h^{-2n/(2n-1)}. \end{aligned} \quad (21)$$

I.e., the leading error due to a finite stepsize h is of magnitude $e^{\text{Re } \phi(x_s, p)} = e^{-a_n h^{-2n/(2n-1)}}$ (apart from a prefactor of less importance). On the other hand, including only the M first terms of the sum leads to an error of magnitude $e^{-[(M+1)h]^{2n}}$. For a given M we should choose h to balance these errors, i.e.

$$h = b_n (M+1)^{-(1-1/2n)}, \quad (22)$$

with $b_n = \left(\frac{\pi}{n}\right)^{1/2n} \left[(2n-1) \sin\left(\frac{\pi}{4n-2}\right)\right]^{(2n-1)/4n^2}$. This leads to an error of magnitude

$$\varepsilon(M) = e^{-c_n(M+1)}, \quad (23)$$

with $c_n = \frac{\pi}{n} \left[(2n-1) \sin\left(\frac{\pi}{4n-2}\right)\right]^{1-1/2n}$. I.e., to evaluate the integral numerically to P decimals accuracy one must choose

$$M+1 \geq \frac{\log 10}{c_n} P \approx (0.12 + 0.467n) P. \quad (24)$$

where the numerical approximation is very good for $n \geq 2$.

C. $e^{-(x^2-a^2)^2}$

Finally consider $f(x) = e^{-(x^2-a^2)^2}$. In this case

$$\begin{aligned} I(a) &= \int_{-\infty}^{\infty} dx e^{-(x^2-a^2)^2} \\ &= a e^{-\frac{1}{2}a^4} \left[\frac{1}{\sqrt{2}} K_{\frac{1}{4}}\left(\frac{1}{2}a^4\right) + \pi I_{\frac{1}{4}}\left(\frac{1}{2}a^4\right) \right] \\ &\rightarrow \begin{cases} 2^{-1} \Gamma(1/4) & \text{as } a \rightarrow 0, \\ \sqrt{\pi}/a & \text{as } a \rightarrow \infty. \end{cases} \end{aligned} \quad (25)$$

The saddle point approximation to the Fourier transform

$$\tilde{f}(p) = \int_{-\infty}^{\infty} dx e^{-(x^2-a^2)^2 + ipx} \equiv \int_{-\infty}^{\infty} dx e^{\phi(x,p)}, \quad (26)$$

leads to the saddle point equation

$$\phi'(x_s, p) = -x_s^3 + a^2 x_s + i \frac{p}{4} = 0. \quad (27)$$

We introduce

$$x_s = y + \frac{a^2}{3y}, \quad (28)$$

which leads to a quadratic equation for y^3 ,

$$y^3 - i \frac{p}{4} + \frac{a^6}{27y^3}. \quad (29)$$

²The deformation of the integration path so that it passes through these saddle points is an interesting exercise[6]

It is convenient to rewrite p so that $(p/8) = (a/\sqrt{3})^3 \sinh 3\eta$. (4/3) $a^4 \sinh^2 \eta \cosh 2\eta$,
Then the solutions for equation (29) becomes

$$y^3 = i \left(\frac{p}{8} \pm \sqrt{\frac{p^2}{64} + \frac{a^6}{27}} \right) = \left(\frac{a}{\sqrt{3}} e^{\pm(\eta+i\pi/6)} \right)^3. \quad (30)$$

I.e.,

$$y = \frac{a}{\sqrt{3}} e^{\pm(\eta+i\pi/6)}, \quad \frac{a^2}{3y} = \frac{a}{\sqrt{3}} e^{\mp(\eta+i\pi/6)},$$

which in both cases of \pm leads to the solution

$$x_s = \frac{2a}{\sqrt{3}} \cosh(\eta + i\pi/6). \quad (31)$$

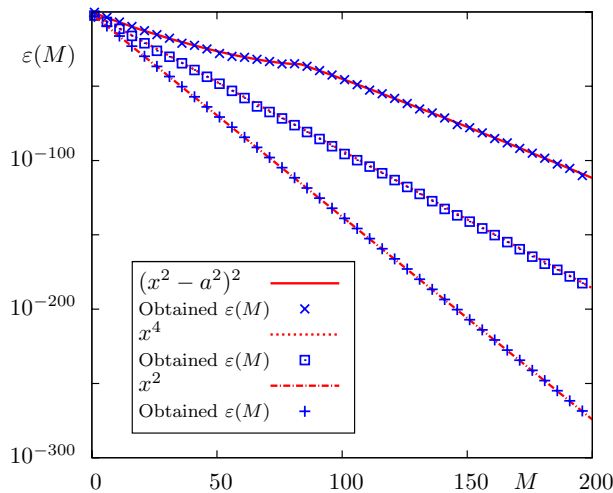


Fig. 2 Predicted (lines) and obtained (points) precision as function of M , for the three example integrals discussed in the text. In order from top to bottom: $\int dx e^{-(x^2-a^2)^2}$, $\int dx e^{-x^4}$, $\int dx e^{-x^2}$. The number of function evaluations in each case is $M + 1$. As can be seen, the obtained precision agrees well with the theoretical estimate.

There are two more ways to take the cube root. One of them leads to an equally relevant saddle point,

$$x_s = \frac{2a}{\sqrt{3}} \cosh(\eta + i5\pi/6), \quad (32)$$

while the last one is irrelevant. The real part of the exponent at the relevant saddle points is

$$\text{Re } \phi(x_s, \eta) = -\frac{4}{3} a^4 \sinh^2 \eta \cosh 2\eta. \quad (33)$$

This provides an error estimate in parametric form: If we choose a finite stepsize

$$h = \frac{\sqrt{27} \pi}{4 a^3 \sinh 3\eta}, \quad (34)$$

the corresponding error will be of magnitude

$$\varepsilon(h) \approx e^{-\frac{4}{3} a^4 \sinh^2 \eta \cosh 2\eta}. \quad (35)$$

The error caused by summing over only a finite range of x -values, $0 \leq x_{\min} \leq x \leq x_{\max}$, should be chosen to be of the same magnitude as $\varepsilon(h)$. I.e., with $s \equiv$

$$x_{\max} = a (1 + \sqrt{s})^{1/2}, \quad (36)$$

$$x_{\min} = \begin{cases} 0 & \text{if } s \geq 1, \\ a (1 - \sqrt{s})^{1/2} & \text{otherwise.} \end{cases} \quad (37)$$

I.e., we must use $M = (x_{\max} - x_{\min})/h$ evaluation steps in the numerical integration.

IV. WAVEFUNCTION NORMALIZATION INTEGRALS

Our investigation of the example integrals gives us confidence that we can obtain a fairly good *a priori* estimate of the obtainable precision $\varepsilon(M)$ at a given number M of discretization steps, at least asymptotically for large M . For this we need to (i) estimate the behaviour of the Fourier transform, $\tilde{\psi}^2(p)$, of the integrand at large $p = 2\pi/h$ (to find the obtainable accuracy $\varepsilon(h)$ at a given stepsize h), and (ii) estimate how the integrand decays away from its maxima (to find the required x -range of summation for the same accuracy).

Both quantities can be obtained to reasonable accuracy by use of the WKB approximation.

A. WKB estimates of wavefunctions for x^{2n} potentials

For large x an estimate of solutions to the eigenvalue problems

$$-\psi'' + (x^{2n} - E) \psi = 0, \quad (38)$$

can be written in the form³

$$\psi(x) = \exp\left(-\int_{x_0}^x dt \sqrt{t^{2n} - E}\right) \approx C \exp\left(-\frac{1}{n+1} x \sqrt{x^{2n} - E}\right),$$

where $x_0^{2n} = E$, and

$$\begin{aligned} C &= \exp\left\{\frac{n}{n+1} \int_{x_0}^{\infty} dt \frac{E}{\sqrt{t^{2n} - E}}\right\} \\ &= \exp\left\{\frac{B(\frac{1}{2}, \frac{n-1}{2n})}{2(n+1)} E^{(n+1)/2n}\right\} \\ &= \exp\left\{\frac{\pi}{2} \tan\left(\frac{\pi}{2n}\right) \left(N + \frac{1}{2}\right)\right\}, \end{aligned} \quad (39)$$

with $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ the Beta function. We have evaluated the WKB integral using partial integration, and let $x \rightarrow \infty$ in the remainder. Further, in the last equality we have assumed $E \equiv E_N$ to be eigenvalue number N , and evaluated it by the WKB approximation.

We use this approximation to estimate the Fourier transform,

$$\tilde{\psi}^2(p) \equiv \int dx \psi(x)^2 e^{ipx}, \quad (40)$$

by the saddle point method. The saddle point equation can be written

$$x_s^{2n} = E - (p/2)^2, \quad (41)$$

giving

$$\begin{aligned} \left| \tilde{\psi}^2(p) \right| &\approx C^2 \exp\left(\frac{-n}{n+1} \text{Re}(ipx_s)\right) \\ &= C^2 \exp\left\{-\frac{n}{n+1} \sin\left(\frac{\pi}{2n}\right) p [(p/2)^2 - E]^{1/2n}\right\}. \end{aligned} \quad (42)$$

³We ignore the algebraic prefactor $(x^{2n} - E)^{-1/4}$.

Thus, to compute the normalization integral to P decimals precision one must choose $p = 2\pi/h$ so that the right hand side of (42) becomes equal to 10^{-P} (or smaller). The value of h is best found numerically. But note that one at least must have $(p/2)^2 > E$, or

$$h^{-1} > \pi^{-1} E^{1/2}.$$

For large x the normalization integrand behaves like

$$\begin{aligned} \psi(x)^2 &\approx \exp\left(-2 \int_0^x dt \sqrt{t^{2n} - E}\right) \\ &\approx C^2 \exp\left(-\frac{2}{n+1} x \sqrt{x^{2n} - E}\right). \end{aligned} \quad (43)$$

Thus, to compute the normalization integral to P decimals precision one should integrate to a value $x = x_{\max}$ for which the right hand side of (43) becomes less than 10^{-P} . The value of x_{\max} is best found numerically. But note that one at least must have $x_{\max}^{2n} > E$, or

$$x_{\max} > E^{1/2n}.$$

This provides a lower limit on the number of integration steps,

$$M + 1 = \frac{x_{\max}}{h} > \frac{1}{\pi} E^{(n+1)/2n} \approx \frac{N + \frac{1}{2}}{\int_{-1}^1 du \sqrt{1 - u^{2n}}}. \quad (44)$$

Here we have assumed $E \equiv E_N$ to be eigenvalue number N , and used the WKB approximation to estimate its value. Since N is the number of nodes in the eigenfunction, the inequality (44) quite reasonably says that the number of evaluation points must be larger than the number of oscillations.

B. Ground state wavefunction of x^4 potential

Specializing the results of the previous section to the ground state of the x^4 -potential, and approximating E_0 by zero, one finds from equation (42) that

$$\left|\widetilde{\psi^2}(p)\right| \approx e^{-p^{3/2}/3}, \quad (45)$$

and from equation (43) that

$$\psi(x)^2 \approx e^{-2x^3/3}. \quad (46)$$

From this one deduces that the optimal choices for $h = 2\pi/p$ and $x_{\max} = Mh$ are so that

$$e^{-\frac{1}{3}(2\pi/h)^{3/2}} \approx e^{-\frac{2}{3}(M+1)^3 h^3}.$$

I.e.,

$$h = 2^{1/9} \pi^{1/3} (M+1)^{-2/3} \approx 1.58 (M+1)^{-2/3}. \quad (47)$$

The corresponding estimated error becomes

$$\varepsilon(M) = e^{-\frac{1}{3} 2^{4/3} \pi (M+1)} \approx e^{-2.64 (M+1)}. \quad (48)$$

I.e., if one wants to compute the normalization integral to P decimals precision one has to choose

$$M + 1 = \frac{3 \ln 10}{2^{4/3} \pi} P \approx 0.87 P. \quad (49)$$

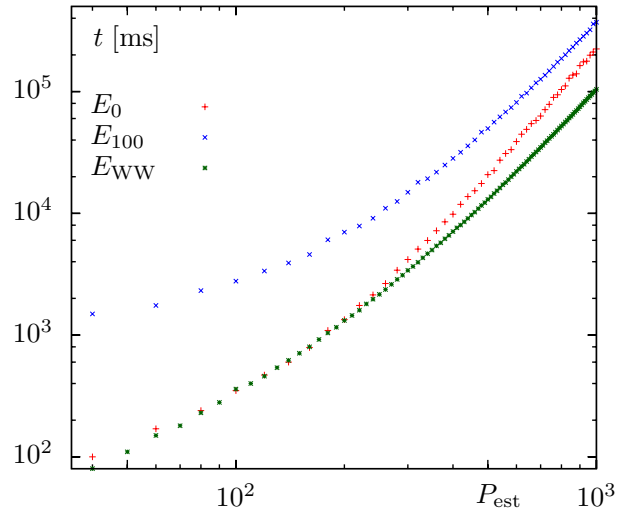


Fig. 3 This figure displays the computer time (measured in milliseconds) required to compute some normalization integrals to P decimals estimated precision. The cases considered are (i) the ground state wavefunction of the x^4 -potential (E_0), (ii) the 100th excited state wavefunction of the x^4 -potential (E_{100}), and (iii) the ground state wavefunction of the $(x^2 - 1)^2$ -potential (E_{WW}) with $s = 1/100$.

C. Excited state wavefunctions of x^4 potential

The main effect of having highly excited states E_N lies in the extra factors C^2 in the error estimates, with C found in equation (39). Clearly C becomes large for large N . To account for this factor we must replace 10^{-P} by $C^{-2} 10^{-P}$ in the error analysis. I.e., make the replacement

$$P \log 10 \rightarrow P \log 10 + \pi \tan\left(\frac{\pi}{2n}\right) \left(N + \frac{1}{2}\right) \quad (50)$$

in the expressions like (49). There are also E -dependent corrections to the remaining factors, but they are best treated numerically.

D. Ground state wavefunction of $(x^2 - 1)^2$ potential

We next consider the lowest even parity eigenstate of

$$-s^2 \psi'' + (x^2 - 1)^2 \psi = \varepsilon \psi, \quad (51)$$

with s is small and positive. By WKB analysis one finds that the solution behaves like

$$\psi(x) \sim e^{-(x-1)^2(x+2)/3s}, \quad (52)$$

(up to an algebraic prefactor) in the region of interest ($\text{Re} x > 0$, $|(x-1)^2(x+2)/3s| \gg 1$). We again estimate Fourier transform of $\psi(x)^2$ by the saddle point method, assuming the relevant saddle point to be in a region where the approximation (52) is valid. The saddle point equation,

$$\phi'(x, p) = -\frac{d}{dx} \left[\frac{2}{3s} (x-1)^2(x+2) - ipx \right] = 0, \quad (53)$$

has a solution consistent with this assumption,

$$x_s = (1 + i \frac{ps}{2})^{1/2}. \quad (54)$$

The corresponding exponent is

$$\phi(x_s, p) = \frac{4}{3s} \left[(1 + ips/2)^{3/2} - 1 \right] \approx -\frac{1}{3s} (1-i)(ps)^{3/2}, \quad (55)$$

where the last equality is valid for $ps \gg 1$. To evaluate the integral to P decimals precision one must choose $p = 2\pi/h$ so that $\phi(x_s, p) = -P \log 10$ (or smaller). For very large P one may use the last approximation in equation (55) to find

$$h \approx \frac{2\pi}{(3 \log 10)^{2/3}} s^{1/3} P^{-2/3} \approx 1.73 s^{1/3} P^{-2/3}, \quad (56)$$

otherwise it is simplest to determine h numerically. Further, to evaluate the integral to P decimals precision one must add contributions from the (positive) x -range where

$$\psi(x)^2 \approx e^{-2(x-1)^2(x+2)/3s} > 10^{-P}. \quad (57)$$

I.e., we must take x_{\max} to be the largest solution to the equation $(x-1)^2(x+2) = (3/2) \log 10 sP$. For very large P the solution becomes

$$x_{\max} \approx \left(\frac{3}{2} \log 10\right)^{1/3} s^{1/3} P^{1/3} \approx 1.51 s^{1/3} P^{1/3}. \quad (58)$$

Hence the number of required function evaluations again grow asymptotically for large P like

$$M + 1 = \frac{x_{\max}}{h} \approx 0.87 P, \quad (59)$$

cf. equation (49).

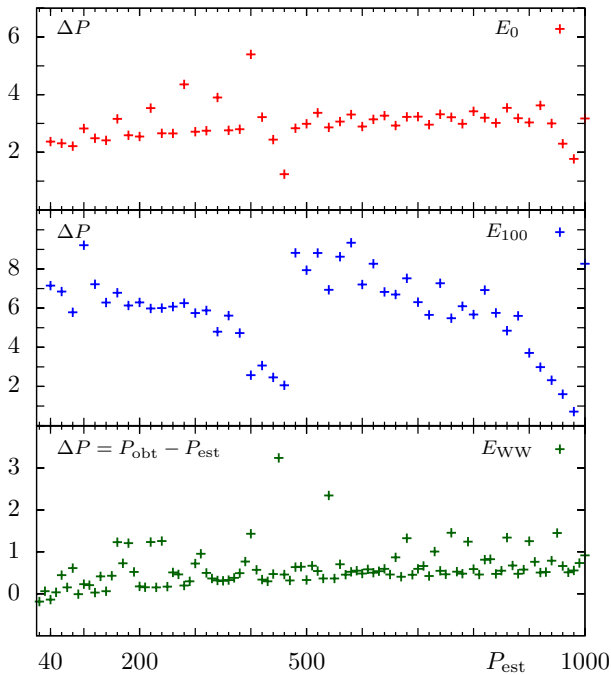


Fig. 4 These figures display the difference between the actually obtained precision P_{obt} and the estimated one P_{est} , for some normalization integrals, with precisions measured in decimal digits. The cases considered are (i) the ground state wavefunction of the x^4 -potential (E_0), (ii) the 100th excited state wavefunction of the x^4 -potential (E_{100}), and (iii) the ground state wavefunction of the $(x^2 - 1)^2$ -potential (E_{ww}) with $s = 1/100$.

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REFERENCES

- [1] A. Mushtaq, A. Noreen, K. Olaussen, and I. Øverbø, *Very-high-precision solutions of a class of Schrödinger type equations*, Computer Physics Communications, (in press) doi:10.1016/j.cpc.2010.12.046 (2011)
- [2] J. Zinn-Justin, *Expansion around instantons in quantum mechanics*, J. Math Phys. **22**, 511 (1981)
- [3] C.M. Bender, K. Olaussen and P.S. Wang, *Numerological analysis of the WKB approximation in large order*, Physical Review **D16**, 1740 (1977)
- [4] A collection is given in M. Abramowitz and I.A. Stegun, *Handbook of mathematical functions*, sect. 25.4, Dover Publications, (1970).
- [5] Ibid, equation. 25.4.4
- [6] Ø. Tafjord, Master thesis, Institutt for fysikk, NTH 1994.
- [7] B. Haible and R.B. Kreckel, *CLN – Class Library for Numbers*, <http://www.ginac.de/CLN/>