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2016 Eur. J. Phys. 37 035402

(http://iopscience.iop.org/0143-0807/37/3/035402)

IOP Publishing European Journal of Physics
Eur. J. Phys. **37** (2016) 035402 (7pp) doi:10.1088/0143-0807/37/3/035402

On the numerical solution of the one-dimensional Schrödinger equation

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Received 8 December 2015, revised 9 February 2016
Accepted for publication 15 March 2016
Published 8 April 2016

Abstract

We discuss two sources of error in the numerical calculation of eigenvalues and eigenfunctions of the one-dimensional Schrödinger equation. By means of suitable examples we analyse the effect of both a finite mesh size and the use of approximate boundary conditions.

Keywords: Schrödinger equation, numerical integration, extrapolation, numerical errors

1. Introduction

In a recent paper Hugdal and Berg [1] discussed the advantages of introducing a numerical solution of the Schrödinger equation in an undergraduate course on quantum mechanics. One of the goals is to illustrate the occurrence of allowed energy levels which is one of the main differences between classical and quantum mechanics. After discussing the shortcomings of exactly solvable models, like the particle in a box or the harmonic oscillator, the authors outline a simple shooting method for the calculation of eigenvalues and eigenfunctions.

It is worth mentioning that the numerical solution of the Schrödinger equation in undergraduate courses was discussed by several authors in the past [2–9] and recently we have resorted to one of the available shooting methods for the discussion of the Wronskians that enable us to take into account the asymptotic behaviour of the eigenfunctions [10, 11].

There are two sources of error in the application of a shooting method: the first one is due to a finite mesh size and the second one is the use of approximate boundary conditions. Since one calculates the wavefunction at mesh points $x_j = jh$, $j = 0, 1, \ldots, N$ the error is expected to depend on the magnitude of h. The smaller the value of h the more accurate the eigenvalue and eigenfunction. In addition to it, when the physical problem requires the wavefunction to be square-integrable in $-\infty < x < \infty$ one solves the problem on a finite interval $a < x < b$ with the boundary conditions $\psi(a) = \psi(b) = 0$. In this case the accuracy of the results increases as $b - a$ increases. A rigorous analysis of these two sources of error is typically

beyond the scope of an undergraduate course on quantum mechanics [12]. However, it is possible to attempt a simple approach to them that is suitable for students with some elementary knowledge of mathematics. The aim of this paper is to carry out such an approach.

In section 2 we outline the simplest shooting method proposed by Hugdal and Berg [1] and discuss the error due to a finite mesh size. In section 3 we show how to reduce that error by means of extrapolation. To illustrate the resulting algorithm in section 4 we resort to an exactly solvable problem (treated in detail in the appendix). Section 5 is devoted to the effect of choosing approximate boundary conditions which is commonly necessary for practical reasons. The main ideas of those sections are tested in section 6 by means of a non-trivial example. Finally, in section 7 we summarise the main results and draw conclusions.

2. Simplest algorithm for numerical integration

A prototypical example of the simplest models that a student faces in a quantum mechanics course is given by the dimensionless Schrödinger equation

$$\psi''(x) + [E - V(x)]\psi(x) = 0, \tag{1}$$

where E is the mechanical energy and $V(x)$ the potential-energy function. The wavefunction $\psi(x)$ should satisfy some given boundary conditions which, for concreteness, we assume to be

$$\psi(a) = \psi(b) = 0. \tag{2}$$

It is well known that such boundary conditions force the occurrence of allowed energy levels $E_0 < E_1 < \ldots$ in direct contradiction to the continuum interval met in classical mechanics.

In order to solve equation (1) numerically by means of a shooting method we substitute the central difference [12]

$$\delta_h\psi(x) = \frac{\psi(x+h) - \psi(x-h)}{2h} = \psi'(x) + \psi'''(x)\frac{h^2}{6} + \psi^{\mathrm{V}}(x)\frac{h^4}{120} + \ldots, \tag{3}$$

for the first derivative so that the approximation for the second derivative becomes [12]

$$\delta^2_{h/2}\psi(x) = \frac{\psi(x+h) - 2\psi(x) + \psi(x-h)}{h^2} = \psi''(x) + \psi^{\mathrm{IV}}(x)\frac{h^2}{12} + \psi^{\mathrm{VI}}(x)\frac{h^4}{360} + \ldots. \tag{4}$$

Thus, instead of the differential equation (1) we solve the difference equation

$$\psi(x+h) + \{h^2[E - V(x)] - 2\}\psi(x) + \psi(x-h) = 0. \tag{5}$$

On choosing $h = (b-a)/N$, for sufficiently large N, and $x_j = a + jh$ we obtain the three-term recurrence relation

$$\psi_{j+1} + \{h^2[E - V(x_j)] - 2\}\psi_j + \psi_{j-1} = 0, \quad j = 1, 2, \ldots, N-1. \tag{6}$$

The boundary conditions now read $\psi_0 = \psi_N = 0$ and the approximate eigenvalues $E_n(h)$ will depend on h. We expect to obtain the exact result in the limit $h \to 0$ ($N \to \infty$). In practice our results will be affected by an error that depends on h.

According to equation (4) the error produced by the substitution of $\delta^2_{h/2}\psi(x)$ for $\psi''(x)$ is of the order of h^2 and in simple cases like the ones discussed here we expect the eigenvalue to behave in exactly the same way [12]:

$$E(h) = E(0) + a_1 h^2 + a_2 h^4 + \ldots. \tag{7}$$

However, particular boundary conditions in problems on two or more dimensions may lead to fractional powers of h [13]. In principle we can increase the accuracy of the computed eigenvalues by decreasing the mesh size h; however, if convergence is slow this may not be the most practical strategy.

3. Extrapolation

Commonly, the estimated eigenvalue $E(h)$ converges too slowly as h decreases and it is therefore convenient to accelerate the process by means of an extrapolation algorithm [12]. In what follows we develop the approach in the simplest possible way. Let us assume that we know that the error in the estimated eigenvalues is of the form

$$E(h) = E(0) + ah^\alpha + bh^\beta + \ldots, \tag{8}$$

where $\beta > \alpha > 0$. Note that we are allowing for possible fractional powers α, β, etc. The transformation

$$\Delta(\alpha, \rho, h)E(h) = \frac{E(\rho h) - \rho^\alpha E(h)}{1 - \rho^\alpha} = E(0) + b\frac{\rho^\beta - \rho^\alpha}{1 - \rho^\alpha}h^\beta + \ldots \tag{9}$$

reduces the error from order h^α to order h^β. If $0 < \rho < 1$ then $E(\rho h)$ is expected to be a better approximation to $E(0)$ than $E(h)$, but $\Delta(\alpha, \rho, h)E(h)$, based on both estimates, is an even better approximation as shown below. Since in actual applications of the shooting method one obtains estimates $E(h_j)$ for a series of decreasing values of h_j, the application of the extrapolation (9) does not require any extra calculation if we choose $h_j = \rho^j h_0$, $j = 1, 2, \ldots$. In the next section we illustrate this procedure by means of an exactly-solvable problem.

4. Exactly-solvable problem

In order to illustrate the ideas outlined in section 3 we choose a problem for which we can solve both the Schrödinger equation (1) as well as the difference equation (6) exactly. The Schrödinger equation for a particle in a one-dimensional box can be reduced to the dimensionless eigenvalue equation

$$\begin{aligned} \psi''(x) + E\psi(x) &= 0, \\ \psi(0) = \psi(1) &= 0. \end{aligned} \tag{10}$$

The exact eigenvalues and eigenfunctions are

$$\begin{aligned} E_n &= n^2\pi^2, \quad n = 1, 2, \ldots \\ \psi_n(x) &= \sqrt{2}\sin(n\pi x). \end{aligned} \tag{11}$$

On the other hand, the difference equation (6) with $V = 0$ can also be solved exactly as shown in the appendix. Its lowest eigenvalue is

$$E_1(h) = \frac{2}{h^2}[1 - \cos(\pi h)] = \pi^2 - \frac{\pi^4 h^2}{12} + \frac{\pi^6 h^4}{360} + \ldots, \tag{12}$$

where we appreciate that the error is of the order of h^2 as anticipated by equation (7). If we apply the extrapolation (9) with $\rho = 1/2$ and $\alpha = 2$ we obtain

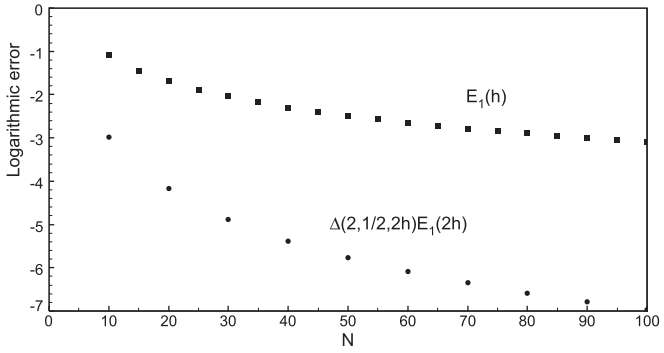

Figure 1. Logarithmic error for the approximate eigenvalue $E_1(h)$ and its first extrapolation $\Delta(2,\, 1/2,\, 2h)E_1(2h)$ for $h = 1/N$.

$$\Delta(2,\, 1/2,\, h)E_1(h) = \frac{2[15 + \cos(\pi h) - 16\cos(\pi h/2)]}{3h^2} = \pi^2 - \frac{\pi^6 h^4}{1440} + \frac{\pi^8 h^6}{64512} + \ldots, \tag{13}$$

with an error of the order of h^4. If we apply a second extrapolation $\Delta(4,\, 1/2,\, h)\Delta(2,\, 1/2,\, h)E_1(h)$ the error reduces to order h^6 and so on. For concreteness and simplicity here we restrict ourselves to just one extrapolation step.

Figure 1 shows the logarithmic error $\log|E^{\text{approx}} - E^{\text{exact}}|$ for $E_1(h)$ and $\Delta(2,\, 1/2,\, 2h)E_1(2h)$ where $h = 1/N$. Note that since $\Delta(2,\, 1/2,\, 2h)E_1(2h)$ requires the calculation of $E_1(2h)$ and $E_1(h)$ it is directly comparable to $E_1(h)$ for a given set of increasing values of N. We appreciate that the extrapolated eigenvalue is considerably more accurate that the two estimates used in its calculation.

5. Error due to approximate boundary conditions

A typical boundary condition for the one-dimensional Schrödinger equation is

$$\lim_{|x|\to\infty} \psi(x) = 0. \tag{14}$$

Since it is not possible to discretise an infinite interval for a practical numerical calculation then we resort to a finite interval like the one in equation (2). A question then arises about the error produced by such substitution. Although a rigorous analysis is probably beyond the scope of an undergraduate course it is nonetheless possible to carry out a sufficiently simple heuristic estimate of such an error.

For simplicity and concreteness we consider a parity-invariant potential $V(-x) = V(x)$ so that we can choose a symmetric finite interval around the origin

$$\varphi(-b) = \varphi(b) = 0. \tag{15}$$

Let $\psi(x)$ and $\varphi(x)$ be the solutions to the Schrödinger equation (1) with the boundary conditions (14) and (15), respectively. It follows from

$$(\varphi\psi' - \psi\varphi')' = \varphi\psi'' - \psi\varphi'' = [E(b) - E]\psi\varphi, \tag{16}$$

Table 1. Lowest eigenvalue for $V(x) = x^4$.

N	$E_0(h)$	Extrapolation
	$-3 < x < 3$	
10	1.049705767	
20	1.057701744	1.060367069
40	1.059697264	1.060362437
80	1.060195934	1.060362157
160	1.060320589	1.060362140
	$-4 < x < 4$	
80	1.060066605	
160	1.060288221	1.060362092
320	1.0603436235	1.0603620907
RPM [14]	1.0603620904841828996	

that

$$[E(b) - E]\int_{-b}^{b} \psi\varphi \, \mathrm{dx} = -\psi(b)\varphi'(b), \tag{17}$$

where E and $E(b)$ are the corresponding eigenvalues for the boundary conditions (14) and (15), respectively. In order to obtain this result we resorted to the fact that the solutions are either even or odd: $\psi(\pm x) = \pm\psi(x)$, $\psi'(\pm x) = \mp\psi'(x)$, $\varphi(\pm x) = \pm\varphi(x)$ and $\varphi'(\pm x) = \mp\varphi'(x)$. In passing we mention that this result is another useful application of the Wronskians [10, 11]. If b is sufficiently large so that it is well inside the classically forbidden region ($E < V(b)$), then $|\psi(b)\varphi'(b)|$ is exponentially small.

Let us, for example, consider the harmonic oscillator

$$V(x) = x^2. \tag{18}$$

Its ground state is well known to be $\psi_0(x) \propto \mathrm{e}^{-x^2/2}$, and assuming that $\varphi_0(x) \approx \psi_0(x)$ is valid for sufficiently large b then we have

$$E_0(b) - E_0 \approx \frac{b\mathrm{e}^{-b^2}}{\sqrt{\pi}\,\mathrm{erf}(b)}. \tag{19}$$

We conclude that the error due to the use of approximate boundary conditions is expected to be smaller than the error due to a finite mesh size h provided that b is not too small. Of course it makes no sense to decrease h too much without at some point to increase b consistently.

In addition to increasing b we can reduce the error due to finite boundary conditions by matching the inner solution to a suitable asymptotic behaviour of the wavefunction at that coordinate point [10, 11]. We do not discuss this strategy in this paper.

6. Non-trivial model

In order to test the ideas outlined in the preceding sections on a non-solvable model we consider the quartic anharmonic oscillator

$$V(x) = x^4. \tag{20}$$

Table 1 illustrates the calculation of the lowest eigenvalue using the interval $-3 < x < 3$ and mesh sizes $h = 3/N$, $N = 10, 20, 40, 80, 160$. The improvement due to extrapolation with $\alpha = 2$ and $\rho = 1/2$ is remarkable; however, for $N > 80$ it is of the order of the effect of the artificial boundary conditions and we have to increase the magnitude of the integration interval. For this reason, the same table shows similar results for the interval $-4 < x < 4$, $h = 4/N$ and $N = 80, 160, 320$. We clearly appreciate that the improvement due to extrapolation is more relevant once the error caused by the artificial boundary conditions was reduced. Table 1 does not show extrapolation results for $N = 10$ and $N = 80$ in the first and second case, respectively, because we use the results for a consecutive pair of mesh sizes h and $h/2$ in order to obtain a single extrapolated value.

Table 1 also shows a quite accurate estimate of the ground-state eigenvalue of the quartic oscillator obtained by means of the Riccati–Padé method (RPM) that consists of a rational approximation to the logarithmic derivative of the eigenfuncton. This approach exhibits an exponential rate of convergence that enables one to obtain remarkably accurate results [14].

7. Conclusions

The aim of this paper is to propose the analysis of the source of errors in the application of shooting methods in an undergraduate course on quantum mechanics. The approach followed in the preceding sections only requires elementary knowledge in Mathematics and is therefore suitable for such a course. The main equations derived in a simple and straightforward way are useful for the improvement of the results coming from the numerical solution to the Schrödinger equation. The gain in accuracy greatly justifies the relatively little time spent in the development and discussion of the subject and the student may test the algorithms on the several simple models available in most introductory textbooks on quantum mechanics.

Appendix

The solution of the difference equation (6) for $V = 0$ is well known. However, for the sake of completeness we show how to obtain the approximate eigenvalues and eigenfunctions in this appendix.

The difference equation can be written in the form

$$\psi_{j-1} + e\psi_j + \psi_{j+1} = 0, \tag{A.1}$$

where $e = h^2E - 2$. If we substitute the solution $\psi_j = Ae^{ij\theta}$ we obtain $e = -2\cos(\theta)$. Since the same result follows from $\psi_j = Be^{-ij\theta}$ we conclude that the most general solution is the linear combination $\psi_j = Ae^{ij\theta} + Be^{-ij\theta}$. From the left boundary condition $\psi_0 = 0$ we obtain $B = -A$ and from the right one $\psi_N = 0$ it follows that

$$\begin{aligned} \theta &= \theta_k = \frac{k\pi}{N}, \quad k = 1, 2, \ldots, N-1, \\ E_k(h) &= \frac{2}{h^2}[1 - \cos(k\pi h)], \quad h = \frac{1}{N}, \\ \psi_j &= C\sin(j\theta_k), \quad j = 0, 1, \ldots, N, \end{aligned} \tag{A.2}$$

where C is a normalisation factor.

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