Proceedings of the Iowa Academy of Science

Volume 71 | Annual Issue Article 57

1964

Numerical Integration of Schroedinger's Equation for a Square Well Potential Using an IBM 1620 Computer

Richard D. Adams
Upper Iowa University

Edgar Ganfield
Upper Iowa University

Gerald Sprouse
Upper Iowa University

Numerical Integration of Schroedinger's Equation for a Square Well Potential Using an IBM 1620 Computer[1]

RICHARD D. ADAMS[2], EDGAR GANFIELD[3], AND GERALD SPROUSE[4]

Abstract. For pedagogical purposes, numerical integration methods are applied to a simple eigenvalue problem in quantum mechanics. Computer programming of the problem is discussed, the effect of different choices of initial conditions is mentioned, and the sensitivity of the method to the difference interval width is discussed.

Schroedinger's time independent equation in one dimension is

$$d^2\Psi/dx^2 + 2m[E - V(x)]/h \text{ bar squared} = 0.$$

For the square potential $V(x) = V_o \quad x \leqslant -a/2, \quad x \geqslant a/2$

$$= 0 \quad -a/2 < x < a/2$$

The discrete eigenfunctions are

I. $\Psi_n(x) = [B \cos (K_1 a/2) e^{K_2 a/2}] \; e^{K_2 x} \quad x \leqslant -a/2$

$$= [B] \cos (K_1 x) \quad -a/2 < x < a/2$$

$$= [B \cos (K_1 a/2) e^{K_2 a/2}] \; e^{-K_2 x} \quad x \geqslant a/2$$

for n = 1, 3, 5, . . . odd natural numbers, and

II. $\Psi_n(x) = [-A \sin (K_1 a/2) \; e^{K_2 a/2}] \; e^{K_2 x} \quad x \leqslant -a/2$

$$= [A] \sin (K_1 x) \quad -a/2 < x < a/2$$

$$= [A \sin (K_1 a/2) \; e^{K_2 a/2}] \; e^{-K_2 x} \quad x \geqslant a/2$$

For n = 2, 4, 6, . . . even natural numbers, where

$$K_1 = \sqrt{2mE_n})/h \text{ bar squared}$$

and

$$K_2 = \sqrt{2m(V_o - E_n)}/h \text{ bar squared.}$$

The determination of the eigenvalues, E_n, involves solving the transcendental equations

$$\xi \tan \xi = \sqrt{Z^2 - \xi^2}$$

for n odd, and

$$\xi \cot \xi = \sqrt{Z^2 - \xi^2}$$

for n even, where

$$\xi = \sqrt{2mE_n a^2}/2h \text{ bar squared}$$

and

$$Z = \sqrt{2mV_o a^2}/2h \text{ bar squared}$$

This solution may be found by simple graphical or numerical

[1]The authors wish to express their gratitude to Mr. George Strawn of IBM for programming and operating the computer and to the IBM Company for their generous contribution of computer time.

[2]Assistant Professor of Physics, Upper Iowa University.
[3]Junior, Physics Department, Upper Iowa University.
[4]Instructor of Mathematics, Upper Iowa University.

techniques. The specific case of $Z = 4$ is considered for which the numerical solution of the equation

$$\xi \tan \xi = \sqrt{Z^2 - \xi^2}$$

is $E_1 = 0.098015\ V_o$ for the first eigenvalue.

The above problem provides an excellent pedagogical example for a point of departure to the use of numerical methods for solving particular cases of Schroedinger's and other equations not associated with analytical or quasi-analytical solutions.

Numerical Development

It is assumed that

$$\triangle\Psi(x)/\triangle x = d\Psi(x)/dx$$

provided $\triangle x$ is small.

This can be written as

$$\triangle\Psi(x) = \Psi_{j+1}(x) - \Psi_j(x) = \Psi'_j(x)\ \triangle x.$$

Similarly,

$$\triangle\Psi'(x)/\triangle x = d^2\Psi(x)/dx^2,$$

and from Schroedinger's equation this is

$$\triangle\Psi'(x)/\triangle x = \frac{2m}{\text{h bar squared}} [V_j(x) - E]\ \Psi(x)$$

which may be written as

$$\Psi'_{j+1}(x) - \Psi'_j(x) = \frac{2m}{\text{h bar squared}} [V_j(x) - E]\ \Psi_j(x)\ \triangle x.$$

A slight rearrangement of terms places the two equations in iterative form.

III. $\Psi_{j+1} = \Psi'_j(x)\ \triangle x + \Psi_j(x)$

IV. $\Psi'_{j+1}(x) = \frac{2m}{\text{h bar squared}} [V_j(x) - E]\ \Psi_j(x)\ \triangle x + \Psi'_j(x)$

Consider both boundary and other conditions associated with the solution. $\Psi(x)$ and $\Psi'(x)$ must be finite and continuous everywhere. In the region where $[V(x) - E] < 0$, i.e., inside the well, the eigenfunction is of oscillatory form, and in the region where $[V(x) - E] > 0$, i.e., outside the well, the eigenfunction is of decreasing exponential form. Further, the smaller the value of E, the more slowly does the eigenfunction oscillate in the interior region and the faster does it decrease in the exterior region. Thus it appears that the lowest eigenvalue, E_1, is associated with the simplest form of eigenfunction: namely, one that has a positive value at the origin, remains positive, and decreases continuously to zero.

Placement of the origin of the coordinate system such that $V(x) = V(-x)$ gives symmetry to the problem such that the eigenfunctions, Ψ_n, are of a definite parity. The Ψ_n, n odd, are of even parity, i.e., $\Psi(x) = \Psi(-x)$. The Ψ_n, n even, are of

odd partly, i.e., $\Psi(x) = -\Psi(-x)$. Thus Ψ_1 has even parity. Therefore, $\Psi_1(0)$ may be set equal to unity and $\Psi_1'(0)$ must equal zero.

Let

$$C_1 = \frac{2m}{\text{h bar squared}}[V_j(x) - E] = -64T/a^2$$

$-a/2 < x < a/2$, i.e., where $V_j(x) = 0$

and

$$C_2 = \frac{2m}{\text{h bar squared}}[V_j(x) - E] = \frac{64}{a^2}[1 - T]$$

$x \leqslant -a/2$, $v \geqslant a/2$, i.e., where $V_j(x) = V_o$

with

$$T = E/V_o\,,\quad Z = \sqrt{2mV_oa^2}/2\text{h bar squared} = 4.$$

Also, let a equal unity and

$$\triangle x = .05a/FCTR = A$$

where FCTR represents a factor through which $\triangle x$ may be varied. The significance of this factor will be apparent later.

Upon substitution, III. and IV. reduce to

$$\Psi_{j+1}(x) = \frac{.05}{FCTR}\Psi'_j(x) + \Psi_j(x)$$

and

$$\Psi'_{j+1}(x) = \frac{-3.2T\Psi_j(x)}{FCTR} + \Psi'_j(x) \quad \text{when } -a/2 < x < a/2$$

and

$$\Psi'_{j+1}(x) = \frac{3.2}{FCTR}[1-T]\Psi_j(x) + \Psi'_j(x)$$

when $x \leqslant -a/2$, $x \geqslant a/2$.

With these properties and suppositions clearly in mind, one can proceed with the systematic iteration of $\Psi(x)$ and $\Psi'(x)$, namely:

$$\Psi(0) = \Psi_o = 1$$
$$\Psi'(0) = \Psi'_o = 0$$
$$\Psi(A) = \Psi_1 = \frac{.05}{FCTR}\Psi'_o + \Psi_o$$
$$\Psi'(A) = \Psi'_1 = \frac{-3.2T\Psi_o}{FCTR} + \Psi'_o$$
$$\Psi(2A) = \Psi_2 = \frac{.05\Psi'_1}{FCTR} + \Psi_1$$
$$\Psi'(2A) = \Psi'_2 = \frac{-3.2T\Psi_1}{FCTR} + \Psi'_1$$

. . . .
. . . .
. . . .

$\Psi(x)$ and $\Psi'(x)$ are functions of the eigenvalue alone at any given point, x_i. Therefore, choose a sufficiently large value for x_i, assume a value E_1, and solve for $\Psi(x_i)$ and $\Psi'(x_i)$. Refer to the boundary and other conditions previously mentioned and correctionally assume another more feasible value for E_1. With the repetition of this procedure, one is able to converge to the correct value of the first eigenvalue and eigenfunction.

Computer Program

A 1620 digital computer was programmed to solve the problem. The FORTRAN statement was constructed in such a manner as to incorporate maximum flexibility without jeopardizing the desired ends. With this program it was possible to enter a minimum assumed value of the variable $T = E/V_o$, the increment of T, and T limit or the upper bound which restricted the variable to remain within a closed interval, namely: [T, T limit]. The programming also allowed the entry of various assumed values of Ψ'_o and FCTR. The insertion of the factor made it possible to regulate or vary the size of the increment $\triangle x$, and hence for FCTR > 1, the accuracy of the approximation $\triangle\Psi(x)/\triangle x = d\Psi(x)/dx$ was increased accordingly. The complete FORTRAN statement is given in the appendix.

Results

For the initial set of calculations, the computer printed out those values of $\Psi(x)$ and $\Psi'(x)$ corresponding to x equal to 5a/4, where T ranged over the closed interval [0.0970, 0.0990] in increments of 0.0001. In calculating with a particular T within this interval, FCTR equalled 2.0, which indicated that fifty iterative steps were taken from $x = 0$ to $x = 5a/4$. The values of $\Psi(50A)$ and $\Psi'(50A)$ for various values of T are given in Table I.

Table 1. Results of $\Psi(50A)$ and $\Psi'(50A)$ for trial values of $T = E/V_o$ within the interval [0.0970, 0.0990] in increments of 0.0001 with FCTR 2.0.

T	$\Psi(50A)$	$\Psi'(50A)$
0.09700000	1.00130710	7.60309540
0.09710000	0.91939176	6.97998070
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09810000	0.10398817	0.78112029
0.09820000	0.02282239	0.16445767
0.09830000	−0.05827484	−0.45161595
0.09840000	−0.13930308	−1.06709700
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09890000	−0.54342099	−4.13570750
0.09900000	−0.62404314	−4.74769570

From the data of Table 1, it is apparent that $\Psi(50A)$ is closest to 0^+ and $\Psi'(50A)$ is nearest to O^- for T equal to 0.0982 and 0.0983 respectively. Therefore, a fine search was made within the interval [0.0975, 0.0985] with increments of 0.0001 and a FCTR of 4.0. The results for $\Psi(100A)$ and $\Psi'(100A)$ are given in Table 2.

Table 2. Results of $\Psi(100A)$ and $\Psi'(100A)$ for trial values of $T = E/V_o$ within the interval [0.0975, 0.0985] in increments of 0.0001 with FCTR 4.0.

T	$\Psi(100A)$	$\Psi'(100A)$
0.09750000	0.57797801	4.38043020
0.09760000	0.47739225	3.61578070
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09790000	0.17619293	1.32658010
0.09800000	0.07596756	0.56500720
0.09810000	−0.02414171	−0.19559911
0.09820000	−0.12417341	−0.95553172
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09840000	−0.32396476	−2.47307750
0.09850000	−0.42370887	−3.23057290

Upon a similar analysis of this data, a fine search was made within the interval [0.09800, 0.09810] in increments of 0.00001. Again FCTR was equal to 4.0. The results of this research are given in Table 3.

Table 3. Results of $\Psi(100A)$ and $\Psi'(100A)$ for trial values of $T = E/V_o$ within the interval [0.09800, 0.09810] in increments of 0.00001 with FCTR 4.0.

T	$\Psi(100A)$	$\Psi'(100A)$
0.09800000	0.07596756	0.56500720
0.09801000	0.06596018	0.48896972
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09806000	0.01588872	0.10853251
0.09807000	0.00587890	0.03248149
0.09808000	−0.00413833	−0.04362493
0.09809000	−0.01414263	−0.11963226
0.09810000	−0.02414171	−0.19559911

Similarly, a fine search was made within the interval, [0.098070, 0.098080] in increments of 0.000001 with a FCTR of 4.0. The results are given in Table 4.

After the analysis of Table 4, the last search was made within the interval [0.09800, 0.09806] with increments of 0.00001 and a FCTR of 8.0. The results for $\Psi(200A)$ and $\Psi'(200A)$ are given in Table 5.

Table 4. Results of $\Psi(100A)$ and $\Psi'(100A)$ for trial values of $T = E/V_o$ within the interval [0.098070, 0.098080] in increments of 0.000001 with FCTR 4.0.

T	$\Psi(100A)$	$\Psi'(100A)$
0.09807000	0.00587890	0.03248149
0.09807100	0.00488311	0.02491588
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09807400	0.00187359	0.00205086
0.09807500	0.00086841	−0.00558604
0.09807600	−0.00012858	−0.01316079
0.09807700	−0.00114129	−0.02085491
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
. . . . .	. . . . .	. . . . .
0.09807900	−0.00312314	−0.03591202
0.09808000	−0.00413833	−0.04362493

Table 5. Results of $\Psi(200A)$ and $\Psi'(200A)$ for trial values of $T = E/V_o$ within the interval [0.09800, 0.09806] in increments of 0.00001 with FCTR 8.0.

T	$\Psi(200A)$	$\Psi'(200A)$
0.09800000	0.04254389	0.30923889
0.09801000	0.03132518	0.22399946
0.09802000	0.02010450	0.13874596
0.09803000	0.00885197	0.05325137
0.09804000	−0.00236170	−0.03194704
0.09805000	−0.01357742	−0.11716006
0.09806000	−0.02478886	−0.20233951

It is to be noted that by increasing FCTR, i.e., decreasing $\triangle x$, the computed value of E_1 converges to the value obtained by a conventional method. Therefore, the result of Table 5, namely: $E_1 = 0.09803V_o$, where $E = TV_o$, definitely indicates that the iterative solution is in agreement with the solution obtained by conventional means ($E_1 = 0.098015V_o$). Furthermore, after properly normalizing equation I., the values of $\Psi(100A)$ and $\Psi'(100A)$ are 0.000106 and −0.00809 respectively; whereas, the corresponding computer results with $T = 0.098075$ for $\Psi(100A)$ and $\Psi'(100A)$ are 0.00087 and −0.00559.

Results For $\Psi'(0) \neq 0$

Consideration of parity indicates that $\Psi'(0) = 0$. However, it is interesting to compare the values obtained for E_1 by assuming $\Psi'(0) \neq 0$ with the previous results. See Table 6.

Note that from the symmetry of the problem, $\Psi(+100A)$ for $\Psi'(0) = {}^{+}0.1$ equals $\Psi(-100A)$ for $\Psi'(0) = {}^{-}0.1$ and similarly for $\Psi'(0) = {}^{+}0.2$ and ${}^{-}0.2$ respectively. When the improper value of $\Psi'(0)$ is assumed, no value for E_1 will satisfy the conditions on $\Psi(+100A)$ and $\Psi(-100A)$ simultaneously. However, the average of the best values for $E_1{}^{+}$ and $E_1{}^{-}$ is quite close to the value obtained for E_1 when $\Psi'(0) = 0$. This indicates

a method for determining the best value for $\Psi'(0)$ when a definite parity or symmetry is lacking.

Table 6. Approximate values obtained for T with FCTR = 1 and various assumed values for $\Psi'(0)$.

$\Psi'(0)$	$T = E_1/V_o$
+0.2	= 0.108
+0.1	= 0.103
−0.1	= 0.095
−0.2	= 0.091

APPENDIX

```
FORTRAN STATEMENT
    1 FORMAT (5F10.0)
    2 ACCEPT 1, T,TLIM,TINCR,PR1,FCTR
      M = 10.0*FCTR
      N = 15.0*FCTR
    5 PS = 1.0
      PR = PR1
      DO 10 1 = 1,M
      PS1 = .05/FCTR*PR +PS
      PR = − 3.2*T/FCTR*PS+PR
   10 PS = PS1
      DO 20 1 = 1,N
      PSI = .05/FCTR*PR + PS
      PR = (3.2−3.2*T)/FCTR*PS + PR
   20 PS = PS1
      PRINT 30, T,PS,PR
   30 FORMAT (     3F14.8)
      T = T + TINCR
      IF(T−TLIM) 5,5,2
      END
```

In translating the problem to FORTRAN, the following representations were made:

1. M = number of points at which $\Psi(x)$ and $\Psi'(x)$ are calculated for $0 < x < a/2$.
2. N = number of points at which $\Psi(x)$ and $\Psi'(x)$ are calculated for $a/2 \leqslant x \leqslant 5a/4$
3. PS = $\Psi(x)$
4. PR = $\Psi'(x)$
5. T limit = TLIM
6. T increment = TINCR