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# Shooting methods for the Schrödinger equation

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**Abstract.** A simple stable shooting method for the Schrödinger equation is described and is shown to work with various integrators, including the Numerov one. Quantum mechanical techniques are extended to apply to problems for which $E$ is not a traditional eigenvalue and are shown to permit the extraction of useful information even from an unstable shooting method.

## 1. Introduction

In the mathematical literature which deals with techniques for the solution of two-point boundary value problems the test problem

$$-D^2\psi + x^2\psi = E\psi \tag{1}$$

with $E=-1$, $\psi(0)=1$ and $\psi(5)=0$ has been studied by several authors (e.g. Holt 1964, Osborne 1969, Roberts and Shipman 1971, Gupta and Agarwal 1985). These authors have pointed out that simple shooting methods starting at $x=0$ do not suffice to find $\psi(x)$ beyond $x\sim 3.5$, because the shooting methods become unstable. The present work describes several original techniques which have been developed by looking at this mathematical problem from the point of view of a physicist who interprets the equations in terms of quantum mechanics.

The guiding principles involved can be summarised as follows. Equation (1) is the harmonic oscillator Schrödinger equation, with $E$ held at a value which is not an eigenvalue. The solution function will thus have a non-zero initial slope $\psi'(0)=G$ whereas if $E$ were a traditional eigenvalue we would have $\psi'(0)=0$ (for an even-parity state). In the half-space $0<x<\infty$ we can either fix $E$ and find the associated $G$, or fix $G$ and find the associated $E$. Only the case $G=0$ will give the usual even-parity eigenvalues associated with the full space $-\infty<x<\infty$. However, we can formally regard the $E$ for any $G$ as an eigenvalue for a Schrödinger equation in the full space with the potential $x^2+2G\,\delta(x)$. The delta function potential produces a slope discontinuity of $2G\psi(0)$ at $x=0$ and so gives $\psi'(0)=G$ as the right-hand slope for an even-parity function with $\psi(0)=1$. It was the exploration of these intuitive ideas which led to the methods of this work, and several techniques which have so far only been used for the special quantum mechanical case $G=0$ were found to be applicable to the more general boundary value problem treated in the mathematical literature.

Section 2 describes a simple shooting method for equation (1), and points out that with the right approach the instability of the method can be turned to computational advantage, even though $\psi(x)$ at large $x$ cannot be found. Section 3 describes a simple power series method which can compute $G$ or $E$ accurately but which again illustrates

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the difficulty of finding $\psi(x)$ at large $x$. Section 4 describes a new shooting technique which allows $\psi(x)$ to be computed accurately over the whole region for any $E$ and which can be used with various traditional integrating methods, including the Numerov one. The new method uses only one auxiliary variable, whereas Gupta and Agarwal (1985), in attempting something similar, devised a technique requiring three auxiliary variables. It is interesting to note that (as kindly pointed out by a referee) the method of § 4 represents a modern computational application of some classical mathematics from the theory of difference equations; the invariance theorem used in that section is equivalent to a special case of a theorem due to Heymann (1892). Section 5 of the present work describes how some techniques used for quantum mechanical problems can be modified to calculate various quantities which depend on the solution function $\psi(x)$, without using the explicit $\psi(x)$ in the calculations. Section 6 gives a brief discussion of the methods developed in the previous sections.

Following Osborne (1969) we should point out that the instabilities studied here and in the cited literature are not those which are due to computational rounding error; they are those caused by the extreme sensitivity of the actual solution function $\psi(x)$ to the values of $E$ and $G$. Even if $\psi(x)$ could be computed with unlimited accuracy, the slightest mismatch of the initial conditions would introduce into it a growing exponential component which would become dominant at large $x$. Indeed, it is only because this component *can* be calculated with fair accuracy that some of the interpolatory methods described in §§ 2 and 3 can be used at all to estimate $E$ or $G$.

## 2. Simple forward shooting

Throughout this paper we shall discuss a generalised form of equation (1), so that our methods are of wide applicability. We study the equation

$$-D^2\psi + V\psi = E\psi \tag{2}$$

with $V$ a smooth potential function. The boundary conditions are $\psi(0) = 1$, $\psi(L) = 0$. The most simple finite difference simulation of the differential equation (2) is provided by slicing the region $0 < x < L$ into strips of fixed width $h$ and using the recurrence relation

$$\psi(x+h) = [2 + h^2(V(x) - E)]\psi(x) - \psi(x-h) \tag{3}$$

which must be supplemented by the starting equation

$$\psi(h) = \tfrac{1}{2}[2 + h^2(V(0) - E)]\psi(0) + hG \tag{4}$$

to produce a solution with $\psi'(0) = G$. Equations (3) and (4) can be used in two ways: $E$ can be fixed while $G$ is varied to make $\psi(L)$ zero or $G$ can be fixed while $E$ is varied to make $\psi(L)$ zero. The calculation can be performed efficiently on a microcomputer using the techniques described by Killingbeck (1985b). Table 1 shows some results for the test problem with $V = x^2$ and $L = 5$, using two neighbouring $G$ values and a fixed $E$ value of $-1$. The results show that the sensitivity of $\psi(x)$ to the $G$ value increases with $x$. The values for the ratio of the two $\psi$ indicate asymptotic behaviour, with only a very small tail of $\psi$ remaining at larger $x$. However, the $\psi$ values in this tail cannot be calculated with any certainty. The two $\psi$ values at $x = 5$ imply that a $G$ value of $-1.128\,463$ would make $\psi(5)$ zero, and the last column of table 1 shows

**Table 1.** $\psi(x)$ values for $V = x^2$, $E = -1$, with $L = 5$ and $h = 0.025$, using (3) and (4).

| $G$ | −1.1285 | −1.1284 | $\psi$ ratio | Interpolated $\psi$ |
|---|---|---|---|---|
| $x$ | | | | |
| 1 | 0.259 299 | 0.259 422 | 1.000 47 | 0.259 344 |
| 2 | 0.034 325 | 0.034 977 | 1.018 97 | 0.034 566 |
| 3 | −0.000 955 | 0.007 011 | −7.344 10 | 0.001 992 |
| 4 | −0.097 294 | 0.166 086 | −1.707 05 | 0.000 157 |
| 4.5 | −0.813 995 | 1.388 501 | −1.705 79 | 0.000 929 |
| 5 | −8.736 66 | 14.902 7 | −1.705 77 | 0[a] |

[a] Rendered formally zero by choice of weighting factors.

the resulting $\psi(x)$ values, as obtained by linear interpolation from the results of the first two columns. The method based on equations (3) and (4) has a discretisation error with a leading term of $h^2$ type, but at $h = 0.025$ this error does not significantly affect the $\psi(x)$ values obtained, as is confirmed by the results obtained in the next two sections. The instability of the forward shooting method has a computational benefit in that it allows $G$ (or $E$) to be found accurately (for a given $h$). Further, the interpolated $G$ (or $E$) can be calculated as soon as the $\psi$ ratio has stabilised, so that it is not always necessary to integrate all the way up to $x = L$.

## 3. Power series shooting

If the potential $V$ in equation (2) is a power series with the general term $V_n x^n$ then substitution of the ansatz

$$\psi = \exp(-\tfrac{1}{2}\beta x^2) \sum_0^\infty A_n x^n \tag{5}$$

into (2) produces the recurrence relation

$$(N+1)(N+2)A_{N+2} = [(2N+1)\beta - E]A_N - \beta^2 A_{N-2} + \sum_M V_M A_{N-M} \tag{6}$$

with the initial values

$$\psi(0) = 1 = A_0 \qquad G = \psi'(0) = A_1. \tag{7}$$

The series involved converges quickly and $\beta$ can be adjusted to speed up convergence. The use of this approach to calculate quantum mechanical eigenvalues has been discussed by Killingbeck (1985a), but it is clear that the test $\psi(L) = 0$ can be used to find $\psi'(0) = G$ (with $E$ fixed) or $E$ (with $G$ fixed). To make $\psi(L)$ zero only requires that the sum of the series be zero, so the exponential factor in (5) is only used explicitly if $\psi(x)$ is quoted for $x < L$. We should note that table 4 of Gupta and Agarwal (1985), which compares $\psi(x)$ values obtained by different methods, is misleading, since it fails to allow for the fact that some authors re-define $\psi(x)$ to incorporate a factor $\exp(-\frac{1}{2}\beta x^2)$, usually with $\beta = 1$.

Table 2 shows some results for the test problem for which table 1 gave the finite difference results. The results for $\psi(5)$ indicate that $G = -1.128\,379$ is required to make $\psi(5)$ zero. Once $G$ is fixed, of course, the $\psi(x)$ for any $x$ can be computed, but we show results for the same $x$ values used in table 1. The general trends in table 2

**Table 2.** $\psi(x)$ values for $V = x^2$, with $E = -1$, $L = 5$ and $\beta = 0$, using (6) and (7). (About 80 terms required for convergence.)

| $G$ | −1.1284 | −1.1283 | $\psi$ ratio | Interpolated $\psi$ |
|---|---|---|---|---|
| $x$ | | | | |
| 1 | 0.259 317 | 0.259 440 | 1.000 47 | 0.259 343 |
| 2 | 0.034 428 | 0.035 080 | 1.018 93 | 0.034 565 |
| 3 | 0.000 327 | 0.008 304 | 25.4256 | 0.001 976 |
| 4 | −0.054 989 | 0.209 190 | −3.804 21 | 0.000 489 |
| 4.5 | −0.460 808 | 1.751 14 | −3.800 16 | 0.003 702 |
| 5 | −4.954 08 | 18.826 6 | −3.800 22 | 0 |

[a] Rendered formally zero by choice of weighting factors.

are the same as those in table 1. $\psi(x)$ is again difficult to estimate beyond $x \sim 3.5$. The values of $\psi(1)$ and $\psi(2)$ in the two tables agree closely, which shows that the discretisation error in the finite difference method does not affect them much, despite the fact that it shifts the $G$ estimate from −1.128 379 to −1.128 463.

## 4. An accurate shooting method

We have recently devised and tested a simple form of shooting which provides accurate $\psi(x)$ values at all $x$ and does not require the specification of $G$; indeed, it produces the $G$ value as one of the results. The new method uses an auxiliary variable $\phi$ and in this respect was inspired by the work of Gupta and Agarwal (1985), although they needed three auxiliary variables. The argument used to derive the equations is reminiscent of those which use the concept of the Wronskian in the theory of differential equations. First we write the finite difference recurrence relation (3) in the symbolic form

$$\psi(N+2) = F(N+1)\psi(N+1) - \psi(N) \tag{8}$$

since the particular form of $F$ does not affect the argument. Using the convention $x = Nh$ we use the initial value $\psi(0) = 1$ in (8) but do not have to give a value for $\psi(1) \equiv \psi(h)$ to initiate the calculation. Instead we introduce the auxiliary recurrence relation

$$\phi(N+1) = F(N+1)\phi(N) - \phi(N-1) \tag{9}$$

with the initial values $\phi(0) = 1$, $\phi(-1) = 0$. Multiplying (8) by $\phi(N)$ and (9) by $\psi(N+1)$, we can show that the quantity

$$W(N) = \psi(N)\phi(N) - \psi(N+1)\phi(N-1) \tag{10}$$

has the property $W(N) = W(N+1)$, i.e. is $N$ independent. However, $W(N)$ has the value 1 at $N = 0$. Suppose now that $\psi(N_0) = 0$, as we would require to ensure that $\psi(L)$ is zero with $L = N_0 h$. From (10) we find that $W(N_0 - 1) = \psi(N_0 - 1)\phi(N_0 - 1)$, and thus conclude that the last two $\psi$ values are given by

$$\psi(N_0) = 0 \qquad \psi(N_0 - 1) = 1/\phi(N_0 - 1). \tag{11}$$

Having obtained these two $\psi$ values we can then use them in (8), running it backwards to find the $\psi(N)$ down to $\psi(-1)$ and estimating $G$ from the finite difference formula

$$2h\psi'(0) \simeq \psi(1) - \psi(-1). \tag{12}$$

The algebra described here is straightforward, as is that in the derivation of equations (3) and (4). What matters computationally is the stability of the recurrence relations involved. We found that the new method is highly stable and table 3 shows some results for the standard test case used in tables 1 and 2. Comparison of the second column of values in table 3 with the results in table 1 shows clearly how well the simple shooting method of § 2 is stabilised by using the auxiliary recurrence relation. The last column in table 3 was obtained using the Numerov method in the simplified form recently discussed by Killingbeck (1986). The vital step is to note that in the Numerov method the quantity

$$\psi_N(x) = [1 - \tfrac{1}{12}h^2(V(x) - E)]\psi(x) \tag{13}$$

obeys the recurrence relation (3) but with an extra term $\frac{1}{12}h^4(V(x)-E)^2$ added inside the square bracket in (3). This merely changes the form of the function $F(N)$ in equation (8) and so the $\psi_N(x)$ values with $\psi_N(0) = 1$ are obtained from the calculation. The correct $\psi(x)$ values then follow by applying the conversion formula (13) at the end of the shooting process. Killingbeck (1986) discussed various possible choices for the function which appears in the square bracket of equation (3) and they could all be used in conjunction with the stabilised shooting technique described here.

**Table 3.** $\psi(x)$ values for $V = x^2$, with $E = -1$, $L = 5$, using (9), (10) and (11).

| | Simple method[a] | | Numerov |
|---|---|---|---|
| $x$ | $N_0 = 100$ | $N_0 = 200$ | $N_0 = 100$ |
| 1 | 0.259 350 8 | 0.259 344 6 | 0.259 342 6 |
| 2 | 0.034 572 0 | 0.034 566 0 | 0.034 564 1 |
| 3 | 0.001 991 6 | 0.001 989 3 | 0.001 988 5 |
| 4 | 0.000 046 2 | 0.000 046 0 | 0.000 046 0 |
| 4.5 | 0.000 004 91 | 0.000 004 88 | 0.000 004 87 |
| 5 | 0 | 0 | 0 |
| $G$ | −1.128 714[a] | −1.128 463[a] | −1.128 378[b] |

[a] Richardson extrapolation gives $G = -1.128\,379$.
[b] Using a fourth-order difference formula for $G$.

**Table 4.** Results obtained by the new technique (Numerov version) for the case $V = x^2$, $L = 10$, $E = 1$, $N_0 = 200$.

| $x$ | $\psi(x)$ | $\exp(-x^2/2)$ |
|---|---|---|
| 9 | 2.5793 E − 18 | 2.5768 E − 18 |
| 8 | 1.2671 E − 14 | 1.2664 E − 14 |
| 7 | 2.2903 E − 11 | 2.2897 E − 11 |
| 6 | 1.5232 E − 8 | 1.5230 E − 8 |
| 5 | 3.7268 E − 6 | 3.7267 E − 6 |
| 4 | 3.3547 E − 4 | 3.3546 E − 4 |
| 3 | 1.1109 E − 2 | 1.1109 E − 2 |
| 2 | 1.3534 E − 1 | 1.3534 E − 1 |
| 1 | 6.0653 E − 1 | 6.0653 E − 1 |
| 0 | 1 E0 | 1 E0 |

Numerical tests confirm that the Numerov version of the technique described here gives a truncation error of leading order $h^4$ in $\psi(x)$. It is clear that this technique, based on a simple three-term recurrence relation, is a much more simple way to achieve $h^4$ accuracy than those which calculate the eigenvalues of large pentadiagonal matrices (e.g. Fack and Vanden Berghe 1985). To illustrate clearly the stability of the technique we show in table 4 some results for the case $V=x^2$, $E=1$, $L=10$; the computed $\psi(x)$ agree with the exact analytical solution over a range of many orders of magnitude. To check that the stability of the method does not depend crucially on the monotonicity of the potential function we also tested the method on potentials such as $-5x^2+x^4$ and $(x-5)^2$ and obtained highly accurate results.

## 5. Further calculations

If the potential function $V(x)$ has even parity then the initial condition $G=0$ plus the test $\psi(L)=0$ will yield quantum mechanical eigenvalues for even-parity states. Using the methods of §§ 2 and 3 the $G$ value can be set at zero and the $E$ values which would make $\psi(L)$ zero can be found by interpolation from the $\psi(L)$ values at several trial $E$ values (by analogy with the procedures used to set up tables 1 and 2). The method of § 3 is most conveniently set up to yield $\psi$ and $G$ when $E$ is given, and so eigenvalues are found by varying $E$ until the resulting $G$ is zero. Since the initial condition used is $\psi(0)=1$, it might seem that the method is suitable only for even-parity eigenvalues. However, computer experiment revealed that $G(E)$ has a singularity as $E$ passes through odd-parity eigenvalues, so that the eigenvalues for both parities can be found by varying $E$ to find the zeros of the quantity $G(1+G^2)^{-1}$. For example, the Numerov integrator with $L=7$ and $N_0=200$ gives the correct energies 1.232 351, 3.507 388, 5.589 779 and 7.648 202 for the potential $x^2+x^2(1+x^2)^{-1}$, which Fack and Vanden Berghe (1986) treated by a pentadiagonal matrix approach.

The function $\psi(x)$ as computed in § 3 has the initial value $\psi(0)=1$, whereas in quantum mechanics we would usually require that the integral of $\psi^2$ over the interval 0 to $L$ should equal 1. As pointed out in the introduction, $\psi(x)$ can be regarded as an eigenfunction for a potential which includes a delta function type of term at the origin. We can use the arguments devised by Killingbeck (1985b) to conclude that the square of the normalised wavefunction at the origin is given by

$$\psi^2(0)=\frac{\partial E}{\partial G}=\left(\frac{\partial G}{\partial E}\right)^{-1} \tag{14}$$

even when $G$ is non-zero (i.e. $E$ is not a traditional quantum mechanical eigenvalue). Equation (14) can be used in conjuction with all three methods of this paper. The method of § 3 allows the integral of $\psi^2$ to be calculated explicitly and so gives an independent check of the validity of (14). However, even with the method of § 3 it is easier to vary $E$, find $\partial G/\partial E$ and thus $\psi^2(0)$ and then get the normalised $\psi(x)$ by scaling the original table which uses the initial condition $\psi(0)=1$.

If the potential $V(x)$ has a small term $\lambda x^2$ added to it, then the arguments given by Killingbeck (1985b) lead to the conclusion

$$\langle x^2\rangle=\left(\frac{\partial E}{\partial \lambda}\right)_G=-\left(\frac{\partial G}{\partial \lambda}\right)_E\left(\frac{\partial G}{\partial E}\right)_\lambda^{-1} \tag{15}$$

and so $\langle x^2 \rangle$ can be found by using the three methods of this paper, monitoring the response of $E$ or $G$ as the other quantities are varied slightly. The method of § 3, of course, allows $\langle x^2 \rangle$ to be estimated directly (if desired) from the relevant integrals, but the indirect methods based on equation (15) will work even with the first two methods, which do not give an accurate $\psi(x)$ for all $x$. This seems to be a remarkable result, but we conjecture that the explanation is that the instability of forward shooting only sets in in the tail region of $\psi$ and so the lost information about $\psi(x)$ makes negligible difference to the integrals defining $\langle x^2 \rangle$. This is consistent with the fact that accurate $E$ values can be found by integrating only up to the onset of instability, as discussed in § 1, so that application of the energy-based equation (15) leads to accurate expectation values. Clearly, the use of $x^2$ here is purely illustrative; the expectation value of any function $f(x)$ can be found by similar numerical procedures. We checked that for the case $V = x^2$, $L = 5$, $E = 1$ the use of (14) and (15) with the methods of §§ 2 and 3 gave the correct $\psi^2(0)$ and $\langle x^2 \rangle$ values, 1.128 38 and $\frac{1}{2}$, respectively. When $E$ is changed to $-1$, we found that $\psi^2(0)$ becomes 2.557 11 and $\langle x^2 \rangle$ becomes 0.221 357. These results are reasonable, since tables 3 and 4 show that at $E = -1$ the function $\psi$ is concentrated nearer to the origin than it is at $E = 1$.

## 6. Conclusion

The stable shooting method described in this paper makes possible the accurate determination of the solution function $\psi(x)$ over the whole region of integration and is applicable for any $E$ value, whether or not $E$ is a traditional quantum mechanical eigenvalue for the potential $V(x)$. The method provides the $\psi(N_0)$ and $\psi(N_0 - 1)$ values for inward integration directly, without use of the WKB approximations used by other workers (e.g. Cooley 1961, Wicke and Harris 1976). The method of § 3 provides accurate $G$ or $E$ values for power law potentials even though it shows the same kind of instability as the simple forward shooting method of § 2. The indirect methods of § 5 make it possible to extract some useful information even from methods which are unstable for the purpose of calculating $\psi(x)$ throughout the whole range.

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