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Matrix Numerov Method for Solving Schrödinger's Equation

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Abstract

We recast the well-known Numerov method for solving Schrödinger's equation into a representation of the kinetic energy operator on a discrete lattice. With just a few lines of Mathematica code, it is simple to calculate and plot accurate eigenvalues and eigenvectors for a variety of potential problems. We illustrate the method by calculating high accuracy solutions for the $|x|$ potential.

I. INTRODUCTION

With modern high level programming and visualization environments such as Mathematica, Matlab, and Python, it is possible and desirable to use computational methods to illustrate and illuminate many basic physics principles with a minimum of programming overhead. This latter point is key: if the programming is too difficult and/or time consuming, the focus shifts from the physics to the programming.

A case in point is the solution of boundary value problems for the 1D Schrödinger equation. One typically starts at one boundary with an assumed value for the energy, then integrates to the other boundary where the boundary conditions are tested. A new guess is generated, and the process is repeated until the desired level of accuracy is obtained.[1] Using the Numerov method, the numerical integration can be done with relatively high accuracy even with large step sizes.[1–3] Though straightforward, this process is tedious to program to solve for a large number of eigenstates.

An alternative approach that gives a large number of eigenstates simultaneously is to expand the wave function in a set of orthogonal basis states that satisfy the appropriate boundary conditions. By truncating the basis set, the Hamiltonian can be diagonalized with built-in matrix routines. The resulting eigenvectors can be used to generate a superposition of the basis states to represent the spatial wave function.

A particularly attractive hybrid approach is to discretize the wave function on a (linear) lattice. This is equivalent to expanding in a basis set of Dirac δ functions centered at the lattice points. The eigenvectors are then simply lists of the values of the various eigenfunctions at the lattice points. This allows straightforward visualization of the eigenfunctions, as demonstrated recently on time-dependent problems.[4]

In the discretized approach, the potential energy operator is simply a diagonal matrix of the potential energy evaluated at each lattice point. The kinetic energy operator, being a differential operator, is more difficult to realize. The purpose of this paper is to show how the Numerov method can be used to represent the kinetic energy operator on the lattice in a straightforward manner, allowing for high accuracy solutions to be obtained with very straightforward programs using matrix diagonalization.

II. MATRIX NUMEROV REPRESENTATION OF THE HAMILTONIAN

The Numerov method is a specialized integration formula for numerically integrating differential equations of the form

$$\psi''(x) = f(x)\psi(x). \tag{1}$$

For the time-independent 1-D Schrodinger equation, $f(x) = -2m(E - V(x))/\hbar^2$. On a lattice of points x_i evenly spaced by a distance d, the integration formula is

$$\psi_{i+1} = \frac{\psi_{i-1}\left(12 - d^2 f_{i-1}\right) - 2\psi_i\left(5d^2 f_i + 12\right)}{d^2 f_{i+1} - 12} + O(d^6), \tag{2}$$

where, for example, $\psi_i = \psi(x_i)$. This can be rearranged into the form

$$-\frac{\hbar^2}{2m}\frac{(\psi_{i-1} - 2\psi_i + \psi_{i+1})}{d^2} + \frac{V_{i-1}\psi_{i-1} + 10V_i\psi_i + V_{i+1}\psi_{i+1}}{12} = E\frac{(\psi_{i-1} + 10\psi_i + \psi_{i+1})}{12}. \tag{3}$$

Now, if we represent ψ as the column vector $(\ldots\psi_{i-1}, \psi_i, \psi_{i+1}\ldots)$, and define matrices $A = (\mathbb{I}_{-1} - 2\mathbb{I}_0 + \mathbb{I}_1)/d^2$, $B = (\mathbb{I}_{-1} + 10\mathbb{I}_0 + \mathbb{I}_1)/12$, $V = \mathrm{diag}(\ldots V_{i-1}, V_i, V_{i+1}\ldots)$, where $\mathbb{I}_p$ is a matrix of 1s along the pth diagonal, and zeros elsewhere, this becomes the matrix equation

$$-\frac{\hbar^2}{2m}A\psi + BV\psi = EB\psi. \tag{4}$$

Multiplying by B^{-1}, we get

$$-\frac{\hbar^2}{2m}B^{-1}A\psi + V\psi = E\psi. \tag{5}$$

Clearly, the first term is the Numerov representation of the kinetic energy operator.

On an N-point grid, the boundary conditions are implemented by taking $N \times N$ sub matrices of A and B. This corresponds to the condition $\psi_0 = \psi_{N+1} = 0$; effectively we have placed the potential of interest inside an infinite-walled box. Alternatively, one can use periodic boundary conditions, with $A_{1,N} = A_{N,1} = 1/d^2$, and $B_{1,N} = B_{N,1} = 1/12$.

We choose the grid in the following manner, valid for finding bound state solutions to attractive potentials. It is easy to extend the following advice to other cases. Suppose we wish to find all the states with $E < E_m$ above the potential minimum. The minimum local deBroglie wavelength is therefore $\lambda = h/\sqrt{2mE_m}$. We have found that sufficient accuracy is generally obtained by taking the grid spacing d corresponding to about 1 point per radian, i.e. $d = \lambda/2\pi$. The number of grid points needed can be estimated by finding the outer turning points x_t, $V(x_t) = E_m$, and allowing for an extra 2λ in the classically forbidden region. Thus $N = 2(x_t/d + 4\pi)$, rounded to the nearest integer.

III. EXAMPLE: $|x|$ POTENTIAL

The "linear" potential $V(x) = b|x|$ is analytically solvable[5] and so is useful for comparison to the numerical calculations. Introducing scaled variables $s = x(mb/\hbar^2)^{1/3}$ and $\epsilon = E(m/b^2\hbar^2)^{1/3}$, we get

$$\frac{-1}{2}B^{-1}A\psi + |s|\psi = \epsilon\psi. \tag{6}$$

Following the guidelines for selecting the grid, we pick a grid spacing $d_s = 1/\sqrt{2\epsilon_m}$ in order to find accurate results for states up to energy ϵ_m. The turning point is $s_t = \epsilon_m$, so with the additional two deBroglie wavelengths outside the turning point we get $N = 2(4\pi + s_t/d_s)$. A Mathematica code for solving this problem is shown in Fig. 1. The grid used is $d_s = 0.158$, $N = 278$, and the program runs in typically 0.1 s of CPU time.

```
(*Potential, desired max energy*)
V[s_] := Abs[s]; em = 20.;
(*determine grid*)
st = FindRoot[V[s] == em, {s, em}][[1, 2]]; ds = 1 / Sqrt[2 em];
n = Round[2 (st / ds + 4 π)]; s = Table[-ds (n + 1) / 2 + ds i, {i, n}];
(*Numerov approximation to KE matrix*)
one[n_, d_] := DiagonalMatrix[1 + 0 Range[n - Abs[d]], d];
B = (one[n, -1] + 10 one[n, 0] + one[n, 1]) / 12.;
A = (one[n, -1] - 2 one[n, 0] + one[n, 1]) / ds^2;
KE = -Inverse[B].A / 2;
(*Hamiltonian*)
H = KE + DiagonalMatrix[V[s]];
(*Energies, wavefunctions*)
{eval, evec} = Eigensystem[H];
```

FIG. 1. Full Mathematica code for solving the potential problem $V = |s|$. The energy of the mth state can be accessed by the command `eval[[-m]]`, and the corresponding list of wave function values at the grid points `s` is `evec[[-m]]`.

A comparison of the exact and matrix Numerov results for some of the energy levels is given in Table I. It is remarkable that such high accuracy results can be achieved with a simple program. An even simpler program might be accomplished by using a simple 3-point approximation to the second derivative, obtained by setting $B = 1$. The results are also

shown in Table I and are of similar quality to the Numerov method for small n, but give clearly less accurate results for large n. Figure 2 compares the Numerov and exact wave functions for $n = 50$.

	$n=1$	2	3	4	10	20	50
Exact	0.808617	1.85576	2.57810	3.24461	6.30526	10.1822	18.9469
Numerov	0.809907	1.85574	2.57848	3.24454	6.30487	10.1806	18.9364
3-pt	0.808854	1.85286	2.57278	3.23576	6.27166	10.0938	18.6344

TABLE I. Comparison of exact and numerical results for the quantized energies (in scaled units, see text) of the linear potential. The numerical results are calculated on an $N = 278$ point grid with a spacing of 0.158 in scaled distance units.

We have used the matrix Numerov method to solve a variety of problems. These include the harmonic oscillator, particle in a box, hydrogen atom, and the partner super potential to the particle in a box.[6] With periodic boundary conditions, we have solved the cosine potential and the periodic square well. We have also simulated a double-well potential to demonstrate tunneling. Among these, the hydrogen atom is the most challenging due to its singularity at $x = 0$ and the rapid increase of the classical turning point with principal quantum number. Codes for a few of these examples are available online.[7]

IV. CONCLUSIONS

While there are other related methods, examples being b-splines[8] and the Fourier grid representation[9], that may be superior for accurate calculation of energies and wave functions by experts, we feel that the simplicity of the matrix Numerov method introduced here makes it ideal for classroom and course work settings as a tool for helping students grow comfortable with the notion of the wave function and eigenvalue problems. The method, though illustrated here for the prominent 1-D Schrödinger equation, is of course useful for any Numerov-type problem. We have used it to solve for diffusion modes of simple geometries, for example.

We have also experimented with variable mesh grids, which can be useful for certain problems such as the hydrogen atom where a variable mesh grid can improve the accuracy. However, this adds new complexities that detract from what we feel is the main advantage

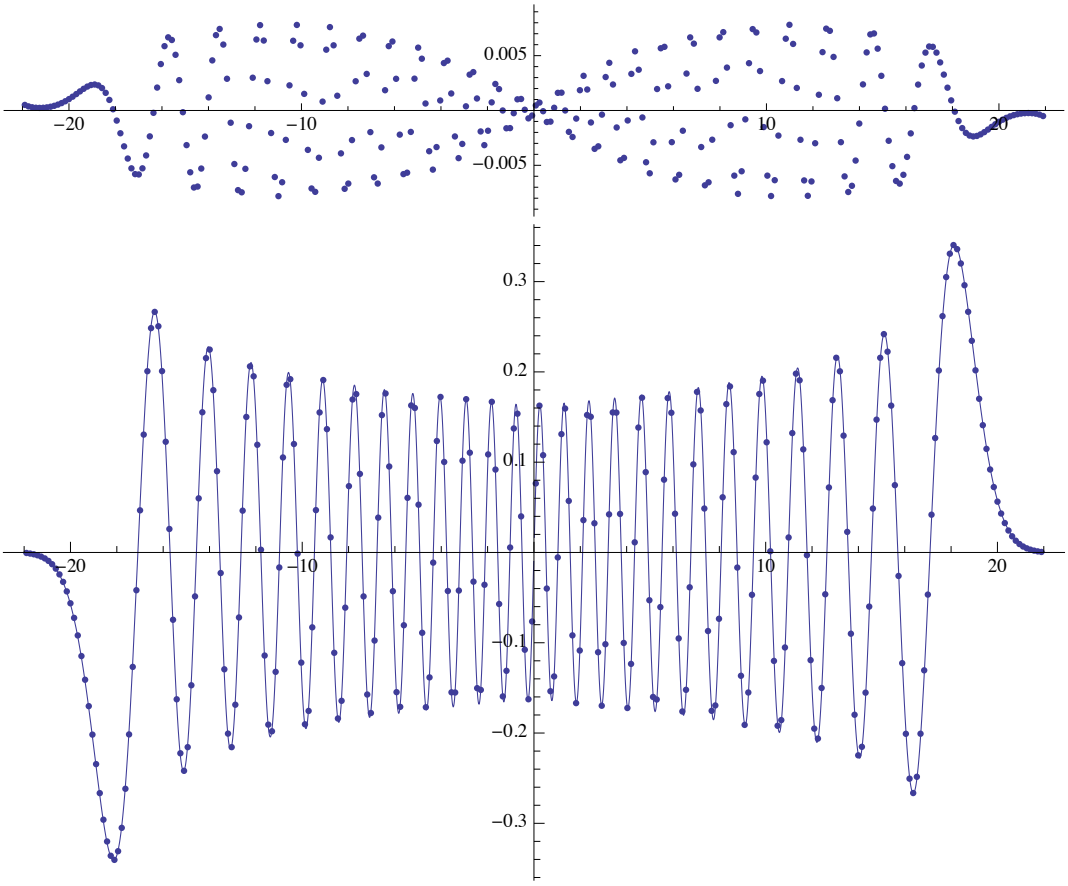

FIG. 2. The lower graph shows the analytical Airy function solution to the Schrödinger equation for the $n = 50$ state of a linear potential, compared to the Numerov method eigenfunction (dots). The upper graph shows the difference between the analytical and Numerov wave functions.

of the method: attainment of very high accuracy for minimum programming complexity and computer time.

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[1] J.M. Blatt, "Practical points concerning the solution of the Schrödinger equation", J. Comput. Phys., 1 (1967), pp. 382396.

[2] P. C. Chow, "Computer solutions to the Schrödinger equation," Am. J. Phys. 40, 730734 (1972).

[3] R. H. Landau, M. J. Paez, and C. C. Bordeianu, *A Survey of Computational Physics* (Princeton U. P., Princeton, NJ, 2008).

[4] M. Belloni and W. Christian, "Time development in quantum mechanics using a reduced Hilbert space approach" Am. J. Phys. 76, 385 (2008).

[5] J. J. Sakurai, J. J. Napolitano, "Modern Quantum Mechanics" (Addison Wesley, 2010).

[6] A. Gangopadhyaya, J. V. Mallow, and C. Rasinariu, *Supersymmetric Quantum Mechanics: An Introduction*, (2011).

[7] See <http://www.physics.wisc.edu/∼tgwalker/NumerovExamples/> for the code of Fig. 1 and some worked examples.

[8] A. Derevianko, E. Luc-Koenig, F. Masnou-Seeuws, "Application of B-splines in determining the eigenspectrum of diatomic molecules: robust numerical description of halo-state and Feshbach molecules", Can. J. Phys. 87, 67 (2009)

[9] C. C. Marston and G. G. Balint-Kurti, "The Fourier grid Hamiltonian method for bound state eigenvalues and eigenfunctions", J. Chem. Phys. 91, 3571 (1989).