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Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods

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The solution of the two-dimensional time-independent Schrödinger equation is considered by partial discretization. The discretized problem is treated as an ordinary differential equation problem and Numerov type methods are used to solve it. Specifically the classical Numerov method, the exponentially and trigonometrically fitting modified Numerov methods of Vanden Berghe et al. [Int. J. Comp. Math 32 (1990) 233–242], and the minimum phase-lag method of Rao et al. [Int. J. Comp. Math 37 (1990) 63–77] are applied to this problem. All methods are applied for the computation of the eigenvalues of the two-dimensional harmonic oscillator and the two-dimensional Henon–Heils potential. The results are compared with the results produced by full discterization.

KEY WORDS: Numerov method, minimum phase-lag, two-dimensional Schrödinger equation, partial discretization

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1. Introduction

The time-independent Schrödinger equation is one of the basic equations in quantum mechanics [1]. Plenty of methods have been developed for the solution

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of the one-dimensional time-independent Schrödinger equation. A well known class of methods for the solution of the Schrödinger equation are Numerov-type methods.

The two-dimensional problem has been treated in the literature by means of discretization of both variables x and y, this transforms the problem into an eigenvalue problem of a block tridiagonal matrix (see [2–4]). In this work we partially discretize with respect to the variable y and transform the partial differential equation into a system of ordinary differential equations. Then we apply the classical Numerov-method, the exponentially fitted and the trigonometrically fitted modified Numerov method Raptis et al. [5], Vanden Berghe et al. [6,7]. Also a Numerov type methods with an extra layer the minimum phase-lag Chawla et al. [8,9].

The two-dimensional time-independent Schrödinger equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + (2E - 2V(x,y))\psi(x,y) = 0, \tag{1}$$

$$\psi(x,\pm\infty) = 0, \quad -\infty < x < \infty,$$
$$\psi(\pm\infty,y) = 0, \quad -\infty < y < \infty.$$

where E is the energy eigenvalue, $V(x,y)$ is the potential and $\psi(x,y)$ the wave function. The wave functions $\psi(x,y)$ assymptotically approaches zero away from the origin.

We consider

$$x \in [-R_x, R_x] \quad \text{and} \quad y \in [-R_y, R_y]$$

then the boundary conditions are

$$\psi(x,-R_y) = 0 \qquad \text{and} \qquad \psi(x,R_y) = 0$$
$$\psi(-R_x,y) = 0 \qquad \text{and} \qquad \psi(R_x,y) = 0.$$

2. Partial discretization

We consider partition of the interval $[-R_y, R_y]$

$$-R_y = y_{-N},\ y_{-N+1},\ \ldots,\ y_{-1},\ y_0,\ y_1,\ \ldots,\ y_{N-1},\ y_N = R_y,$$

where $y_{j+1} - y_j = h_y = R_y/N$.

We approximate the partial derivative

$$\frac{\partial^2\psi}{\partial y^2} = \frac{\psi(x,y_{j+1}) - 2\psi(x,y_j) + \psi(x,y_{j-1})}{h_y^2}$$

and substitute into equation (1)

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{1}{h_y^2}\psi(x, y_{j+1}) - B(x, y_j)\psi(x, y_j) - \frac{1}{h_y^2}\psi(x, y_{j-1}) \tag{2}$$

with

$$\psi(-R_x, y_j) = 0 \qquad \text{and} \qquad \psi(R_x, y_j) = 0$$

for $j = -N+1, \ldots, 0, \ldots, N-1$, and

$$B(x, y_j) = 2\left(E - V(x, y_j) - \frac{1}{h_y^2}\right).$$

We define the $k = 2N - 1$ length vector

$$\Psi(x) = \begin{pmatrix} \psi(x, y_{-N+1}) \\ \psi(x, y_{-N+2}) \\ \vdots \\ \psi(x, y_0) \\ \vdots \\ \psi(x, y_{N-2}) \\ \psi(x, y_{N-1}) \end{pmatrix}$$

then equation (1) can be written as

$$\frac{\partial^2 \Psi}{\partial x^2} = -S(x)\Psi(x) \tag{3}$$

with

$$\Psi(-R_x) = 0 \qquad \text{and} \qquad \Psi(R_x) = 0,$$

where $S(x)$ is a $k \times k$ matrix

$$S(x) = \begin{pmatrix} B(x, y_{-N+1}) & 1/h_y^2 & & & \\ 1/h_y^2 & B(x, y_{-N+2}) & 1/h_y^2 & & \\ \ddots & \ddots & \ddots & & \\ & 1/h_y^2 & B(x, y_{N-2}) & 1/h_y^2 & \\ & & 1/h_y^2 & B(x, y_{N-1}) & \end{pmatrix}$$

another way to see $S(x)$ is

$$S(x) = 2EI - 2V(x) + \frac{1}{h_y^2}M$$

and $V(x)$ is a diagonal matrix with diagonal elements

$$V(x, y_{-N+1}),\ V(x, y_{-N+2}),\ \ldots,\ ,\ V_(x, y_{N-1})$$

and the matrix M is tridiagonal with diagonal elements -2 and off diagonal elements 1.

3. Application of Numerov-type methods

Now we consider x in the interval $[-R_x, R_x]$ with boundary conditions

$$\Psi(-R_x) = 0, \qquad \Psi(R_x) = 0.$$

we take a partition of the above interval of length $2N + 1$

$$-R_x = x_{-N},\ x_{-N+1},\ \ldots,\ x_{-1},\ x_0,\ x_1,\ \ldots,\ x_{N-1},\ x_N = R_x$$

where $x_{j+1} - x_j = h_x = R_x/N$.
We define

$$\Psi^n = \Psi(x_n), \quad \text{for} \quad n = -N+1, \ldots, 0, \ldots, N-1$$

the $k = (2N - 1)$ length vector $\Psi(x)$ evaluated at x_n.

3.1. Numerov-type methods

The classical Numerov method as well as the exponetially and trigonometrically fitted methods of Raptis et al. [5] and Vanden Berghe et al. [6,7] are written as

$$\psi_{n+1} - 2\psi_n + \psi_{n-1} = h^2 (b_0 f_{n+1} + b_1 f_n + b_0 f_{n-1}) \tag{4}$$

for the classical Numerov method the coefficients are

$$b_0 = \frac{1}{12}, \quad \text{and} \quad b_1 = \frac{10}{12}$$

for the exponentially fitted method

$$b_0 = \frac{1}{w^2h^2} - \frac{e^{wh}}{(1 - e^{wh})^2} \quad \text{and} \quad b_1 = \frac{1 + e^{2wh}}{(1 - e^{wh})^2} - \frac{2}{w^2h^2}$$

for the trigonometrically fitted method

$$b_0 = \frac{1}{2 - 2\cos(wh)} - \frac{1}{(wh)^2} \quad \text{and} \quad b_1 = \frac{2}{(wh)^2} - \frac{\cos(wh)}{1 - \cos(wh)}.$$

We apply to equation (3)

$$\Psi^{n+1} - 2\Psi^{n} + \Psi^{n-1} = -h_x^2 \left(b_0 S(x_{n+1})\Psi^{n+1} + b_1 S(x_n)\Psi^{n} + b_0 S(x_{n-1})\Psi^{n-1} \right). \quad (5)$$

Substitution of $S(x)$ to (5) gives the following generalized eigenvalue problem

$$\begin{aligned} \Psi^{n+1} - 2\Psi^{n} + \Psi^{n-1} = & -2h_x^2 E \left(b_0 \Psi^{n+1} + b_1 \Psi^{n} + b_0 \Psi^{n-1} \right) \\ & +2h_x^2 \left(b_0 V_{n+1} \Psi^{n+1} + b_1 V_n \Psi^{n} + b_0 V_{n-1} \Psi^{n-1} \right) \\ & -b_0 \frac{h_x^2}{h_y^2} M \left(\Psi^{n+1} + \Psi^{n} + \Psi^{n-1} \right). \end{aligned} \quad (6)$$

We consider the matrices A, B, C, and V.

$$A = \begin{pmatrix} -2I_k & I_k & & \\ I_k & -2I_k & I_k & \\ & \ddots & \ddots & \ddots \\ & & I_k & -2I_k \end{pmatrix}, \qquad B = \begin{pmatrix} b_1 I_k & b_0 I_k & & \\ b_0 I_k & b_1 I_k & b_0 I_k & \\ & \ddots & \ddots & \ddots \\ & & b_0 I_k & b_1 I_k \end{pmatrix} \quad (7)$$

and C is a block diagonal matrix with each block equal M. The diagonal matrix V has blocks

$$V(x_{-N+1}),\ V(x_{-N+2}),\ \ldots,\ V(x_{N-1}).$$

Now let the $l = k^2 = (2N-1)^2$ length vector

$$\Psi = \left(\Psi^{-N+1}, \Psi^{-N+2}, \ldots, \Psi^{0}, \ldots, \Psi^{N-2}, \Psi^{N-1} \right)^T.$$

Collecting all equations (6) we have

$$A\Psi = -2h_x^2 E B\Psi + 2h_x^2 B V \Psi - \frac{h_x^2}{h_y^2} C B \Psi$$

or in the more general form as

$$(P + E h_x^2 Q)\,\Psi = 0,$$

where

$$\begin{aligned} P &= A - 2h_x^2 B V + \frac{h_x^2}{h_y^2} C B, \\ Q &= 2B. \end{aligned}$$

3.2. Numerov-type methods with an extra layer

It is known that the classical Numerov method has phase lag $h^4/480$, the Chawla and Rao method has phase lag $h^6/12096$. The method is

$$\begin{aligned} \hat{y}_n &= y_n - \alpha h^2 (f_{n+1} - 2f_n + f_{n-1}) \\ y_{n+1} - 2y_n + y_{n-1} &= h^2 (b_0 f_{n+1} + b_1 \hat{f}_n + b_0 f_{n-1}) \end{aligned} \tag{8}$$

for Chawla and Rao minimum phase-lag method ($h^6/12096$ instead of $h^4/480$)

$$\alpha = \frac{1}{200}, \quad b_0 = \frac{1}{12}, \quad b_1 = \frac{10}{12}.$$

We apply to equation (3)

$$\begin{aligned} &\Psi^{n+1} - 2\Psi^n \ + \ \Psi^{n-1} \\ &\quad = -h_x^2 \left(b_0 S(x_{n+1})\Psi^{n+1} + b_1 S(x_n)\Psi^n + b_0 S(x_{n-1})\Psi^{n-1}\right) \\ &\qquad -\alpha b_0 h_x^4 S(x_n) \left(S(x_{n+1})\Psi^{n+1} - 2S(x_n)\Psi^n + S(x_{n-1})\Psi^{n-1}\right). \end{aligned} \tag{9}$$

Substitution of $S(x)$ from (8) gives the following generalized eigenvalue problem

$$(P \ + \ E\, h^2\, Q \ - \ E^2\, h^4\, R)\, \Psi = 0.$$

where

$$\begin{aligned} P &= A - 2b_0 h_x^2 BV + b_0 \frac{h_x^2}{h_y^2} CB \\ &\qquad \alpha b_0 h_x^2 \left(DA - 2\frac{h_x^2}{h_y^2}(VCA + CAV) \right) + \alpha b_0 h_x^4 VAV \\ Q &= 2b_0 B \ + \ 4\alpha b_1 \frac{h_x^2}{h_y^2} CA \ - \ 4\alpha b_1 h_x^2 (AV + VA) \\ R &= -4\alpha b_1 A \end{aligned}$$

D is a block diagonal matrix with each block equal to M^2.

Matrices P, Q, R are real, symmetric and sparse, they are very large even for small N (e.g., $l = 1521$ for $N = 20$). In order to manage to work as we increase N we treat them as sparse matrices in terms of storage and computational.

4. Numerical results

We applied all numerical methods developed above to the calculation of the eigenvalues of the two-dimensional harmonic oscillator and the Henon–Heiles potential.

Results are compared with those produced using the full discretization technique.

4.1. *Two-dimensional harmonic oscillator*

The potential of the two-dimensional harmonic oscillator is

$$V(x, y) = \frac{1}{2}(x^2 + y^2).$$

The exact eigenvalues are given by

$$E_n = n + 1, \quad n = n_x + n_y, \quad n_x, n_y = 0, 1, 2, \ldots$$

In table 1 we compare the results produced by full discretization (Meth1), Numerov method (Meth2), trigonometrically-fitted Numerov method (Meth3) and Numerov method with minimum phase lag (Meth4). All computations were performed with $h_x = h_y = 0.1$, we had to increase the interval from $[-5.5, 5.5]$ for the first eigenvalues to $[-8.5, 8.5]$ for higher eigenvalues.

All the new methods applied here perform similarly up to the 10th state eigenvalue. The errors produced by these methods (maximum absolute error 10^{-3}) are much smaller than the corresponding errors of full discretization (maximum absolute error 0.05).

For higher state eigenvalues the full discretization method failed to produce accurate results. The minimum phase lag method and the trigonometrically fitted method continue to give very accurate results (maximum absolute error up to 0.5×10^{-3}) while the classical Numerov method lost accuracy (maximum absolute error 0.5×10^{-2}.

4.2. *Two-dimensional Henon–Heiles potential*

The Henon–Heiles potential is

$$V(x, y) = \frac{1}{2}(x^2 + y^2) + (0.0125)^{1/2}\left(x^2 y - \frac{y^3}{3}\right).$$

The eigenvalues of the two dimensional Henon–Heiles potential computed are given in table 2.

All methods *Meth2, Meth3, Meth4* give very accurate results for this potential compared to the eigenvalues given in Davis and Heller [10].

Table 1
The eigenvalues of the harmonic oscillator.

	Meth1	Meth2	Meth3	Meth4
E_0	0.999243	0.999687	0.999687	0.999687
E_1	1.997728	1.999685	1.999688	1.999687
E_2	2.996214	2.999678	2.999689	2.999687
E_3	3.993181	3.999663	3.999691	3.999687
E_4	4.990149	4.999637	4.999695	4.999687
E_5	5.985595	5.999598	5.999702	5.999689
E_6	6.981041	6.999553	6.999722	6.999700
E_7	7.974963	7.999549	7.999807	7.999773
E_8	8.968885	8.999824	8.999733	8.999689
E_9	9.961280	9.999232	9.999750	9.999685
E_{10}	10.953675	10.999077	10.999773	10.999686
E_{11}	11.944548	11.998901	11.999813	11.999700
E_{12}	12.935791	12.998747	12.999917	12.999773
E_{13}	13.985601	13.998784	13.999855	13.999675
E_{14}	14.984086	14.998074	14.999892	14.999671
E_{15}	15.981054	15.997717	15.999936	15.999667
E_{16}	16.976500	16.997314	16.999989	16.999665
E_{17}		17.996872	17.999841	17.999675
E_{18}		18.996425	19.000098	18.999735
E_{19}		19.996089	19.999920	19.999633
E_{20}		20.996209	20.999968	20.999621
E_{21}		21.997668	21.999723	21.999608
E_{22}		22.994645	23.000081	22.999593
E_{23}		23.994417	24.000147	23.999580

Table 2
The eigenvalues of Henon–Heiles potential.

	Meth1	Meth2	Davis–Heller
E_0	0.9978	0.9986	0.9986
E_1	1.9879	1.9901	1.9901
E_2	2.9512	2.9562	2.9562
E_2	2.9815	2.9853	2.9853
E_3	3.9176	3.9259	3.9260
E_3	3.9749	3.9822	3.9824
E_3	3.9783	3.9856	3.9858
E_4	4.8572	4.8700	4.8701
E_4	4.8880	4.8986	4.8986
E_4	4.9749	4.9860	4.9863
E_5	5.7993	5.8174	5.8170
E_5	5.8497	5.8679	5.8670
E_5	5.8642	5.8812	5.8814
E_5	5.9753	5.9912	5.9913

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