Numerical Solution of a Two-Dimensional Time-Independent Schrödinger Equation by Using Symplectic Schemes

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ABSTRACT: Symplectic schemes are extended to the solution of a two-dimensional time-independent Schrödinger equation. The Schrödinger equation is first transformed into a Hamiltonian canonical equation and then the numerical method is developed to solve the numerical solution of the two-dimensional time-independent Schrödinger equation. This called the symplectic scheme–matrix eigenvalue method (SSMEM). This method is applied to calculations of the two-dimensional harmonic oscillator and the two-dimensional Henon–Heils potential. It is shown that the numerical results of the two-dimensional harmonic oscillator by using the SSMEM tend to the exact ones monotonically with decreasing space step length and the numerical eigenvalues of the two-dimensional Henon–Heils potential by using the SSMEM are lower than those by using the Gaussian basis set method. © 2001 John Wiley & Sons, Inc. Int J Quantum Chem 83: 303–309, 2001

Key words: canonical equation; symplectic scheme; symplectic scheme–matrix eigenvalue method

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Introduction

The time-independent Schrödinger equation is one of the basic equations of quantum mechanics. Its solutions are required in the studies of atomic and molecular structure and spectra, molecular dynamics, and quantum chemistry. Recently, we developed two kinds of numerical methods to solve the one-dimensional time-independent Schrödinger equation by using symplectic schemes [1]. These two methods are the symplectic scheme–matrix eigenvalue method (SSMEM) and the symplectic scheme-shooting method (SSSM). As we all know, Numerov's method is traditional for solving the time-independent Schrödinger equation. Avdelas, Konguetsof, and Simos [2] gave a generalization of Numerov's method for the numerical solution of the Schrödinger equation in two dimensions. In their work, the symplectic schemes were extended to the numerical solution of the two-dimensional time-independent Schrödinger equation. We first transform the two-dimensional time-independent Schrödinger equation into a Hamiltonian canonical equation by means of investigating the symplectic property and by means of the Legendre transformation of many variables, and then we verify that the variation of the solution of the canonical equation is always a symplectic transformation. Thus the symplectic schemes are reasonable algorithms for solving the Hamiltonian canonical equation, and the canonical equation is worked out by using the symplectic schemes. The SSME method has been developed for solving the eigenvalues and eigenfunctions. In the SSMEM, the symplectic schemes are converted into a group of algebraic equations whose coefficient matrix is a real symmetric matrix, and the eigenvalues are obtained by solving the matrix eigenvalue problem. This method is applied to computations of the eigenvalues of the two-dimensional harmonic oscillator and the two-dimensional Henon–Heils potential. The numerical results of the two-dimensional harmonic oscillator by using the SSMEM tend to the exact ones monotonically with decreasing space step length and the numerical eigenvalues of the two-dimensional Henon–Heils potential by using the SSMEM are lower than those by using the Gaussian basis set method.

In the following section, the Hamiltonian canonical equation of a two-dimensional Schrödinger equation is deduced and the symplectic property of the solutions of the canonical equation is illustrated. In the third section, the symplectic schemes are outlined, the canonical equation is worked out, and the method for solving the eigenvalues is developed. Numerical results and conclusions are given in the last section.

Symplectic Form of the Two-Dimensional Time-Independent Schrödinger Equation

In atomic units, the two-dimensional time-independent Schrödinger equation may be written in the form

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

$$\psi(x,\pm\infty) = 0, \qquad -\infty < x < +\infty, \tag{2}$$

$$\psi(\pm\infty, y) = 0, \qquad -\infty < y < +\infty, \tag{3}$$

where E is the energy eigenvalue, $V(x,y)$ is the potential, and $\psi(x,y)$ is the wave function. Let $-R_y$ and R_y, respectively, be the left and right boundaries in the y direction, suppose R_y is finite, and take N as a sufficiently large positive integer. We denote the space step $\Delta y = R_y/N$, $y_j = j\Delta y$, $j = -N, -N+1, \ldots, -1, 0, 1, \ldots, N-1, N$. Substituting the symmetry difference quotient for the partial derivative $\partial^2\psi/\partial y^2$, we have

$$\frac{\partial^2\psi}{\partial y^2} = \frac{\psi(x,y_{j-1}) - 2\psi(x,y_j) + \psi(x,y_{j+1})}{\Delta y^2}, \tag{4}$$

and considering the boundary conditions (2), we have

$$\psi(x,-R_y) = 0, \qquad \psi(x,+R_y) = 0. \tag{5}$$

Inserting Eq. (4) into Eq. (1), we obtain

$$\begin{aligned}\frac{d^2\psi(x,y_j)}{dx^2} &= -\frac{1}{\Delta y^2}\psi(x,y_{j-1}) - B(x,y_j)\psi(x,y_j) \\ &\quad - \frac{1}{\Delta y^2}\psi(x,y_{j+1}), \\ &\qquad j = -N+1, \ldots, -1, 0, 1, \ldots, N-1,\end{aligned} \tag{6}$$

where $B(x,y_j) = 2[E - V(x,y_j) - 1/\Delta y^2]$. If we introduce the boundary conditions Eq. (5) into Eq. (6) and let

$$\begin{aligned}\psi = \big[&\psi(x,y_{-N+1}), \psi(x,y_{-N+2}), \ldots, \psi(x,y_0), \ldots, \\ &\psi(x,y_{N-2}), \psi(x,y_{N-1})\big]^T,\end{aligned} \tag{7}$$

$$\begin{aligned}\varphi = \dot\psi = \big[&\dot\psi(x,y_{-N+1}), \dot\psi(x,y_{-N+2}), \ldots, \dot\psi(x,y_0), \ldots, \\ &\dot\psi(x,y_{N-2}), \dot\psi(x,y_{N-1})\big]^T,\end{aligned} \tag{8}$$

where the superscript T denotes the transposed matrix, then Eq. (6) can be rewritten in the form of matrix as

$$\dot{\varphi} = -S\psi, \qquad \dot{\psi} = \varphi, \tag{9}$$

where the overdot denotes the derivative with respect to x,

$$S(x) = \begin{bmatrix} B(x, y_{-N+1}) & \frac{1}{\Delta y^2} & & & \\ \frac{1}{\Delta y^2} & B(x, y_{-N+2}) & \frac{1}{\Delta y^2} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{\Delta y^2} & B(x, y_{N-2}) & \frac{1}{\Delta y^2} \\ & & & \frac{1}{\Delta y^2} & B(x, y_{N-1}) \end{bmatrix}, \tag{10}$$

and $S(x)$ is a $(2N-1)$-order tridiagonal symmetric matrix, $S^T = S$. Equation (9) can be rewritten as the matrix form

$$\dot{z} = Gz, \qquad z = \begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \qquad G = J^{-1}C,$$
$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad C = \begin{pmatrix} 1 & 0 \\ 0 & S \end{pmatrix}. \tag{11}$$

It is easy to verify that G is an infinitesimal symplectic matrix and its exponential transformation $\exp(\int_0^x G(x)\,dx)$ is a symplectic matrix [3–9], so Eq. (9) can be viewed formally as the Hamiltonian canonical equation, and its Hamiltonian function is

$$H = \tfrac{1}{2} z^T C z = \tfrac{1}{2}\varphi^T\varphi + \tfrac{1}{2}\psi^T S\psi. \tag{12}$$

The fundamental theorem of the Hamiltonian formalism says that the solution $z(x)$ of the canonical equation (9) can be generated by a one-parameter group $g_H^{0x} = \exp(\int_0^x G(x)\,dx)$, depending on the given Hamiltonian H, of canonical transformation, such that

$$z(x) = g_H^{0x} z(0). \tag{13}$$

That is to say, the solution of canonical equation (9) from x_1 to another x_2 is a symplectic transformation

$$g_H^{x_1x_2} : \begin{pmatrix} \varphi(x_2) \\ \psi(x_2) \end{pmatrix} = g_H^{x_1x_2} \begin{pmatrix} \varphi(x_1) \\ \psi(x_1) \end{pmatrix}.$$

The spatial distribution of the Hamiltonian canonical equation (9) preserves symplectic product conservation. In this sense, we say that the two-dimensional time-independent Schrödinger equation (1) has a symplectic form. Therefore, the symplectic algorithm is the reasonable method for solving the Schrödinger equation.

We also obtain the canonical equation of the two-dimensional time-independent Schrödinger equation (1) by means of the Legendre transformation of many variables. If we denote $\psi_j = \psi(x, y_j)$, then Eq. (6) can be rewritten in the form

$$\ddot{\psi}_j + \frac{\partial u}{\partial \psi_j} = 0, \qquad j = -N+1, \ldots, -1, 0, 1, \ldots, N-1, \tag{14}$$

where

$$u(x, \psi) = \frac{1}{2}\sum_j \left[\frac{1}{\Delta y^2}\psi_{j-1}\psi_j + B(x)\psi_j^2 + \frac{1}{\Delta y^2}\psi_{j+1}\psi_j\right] = \frac{1}{2}\psi^T S(x)\psi$$

and $\psi = (\psi_{-N+1}, \ldots, \psi_{N-1})^T$ is the vector variable. If x is regarded as the time variable, and $\psi(x)$ and $u(x, \psi)$ are, respectively, regarded as the generalized coordinates and the formal potential function, then $\dot{\psi}(x)$ and $\ddot{\psi}(x)$ are the generalized velocities and the generalized accelerations, respectively. Thus Eq. (14) is the formal Newtonian equation for many-particle interactions with the unit of mass moving in a functional space. In this sense, if the Lagrange function

$$L(\psi, \dot{\psi}, x) = T - u = \tfrac{1}{2}\dot{\psi}^T\dot{\psi} - \tfrac{1}{2}\psi^T S(x)\psi$$

is regarded as a function of the vector variable $\dot{\psi}$, it is a positive quadratic form in $\dot{\psi}$. Therefore, Eq. (14) can be transformed into the canonical equation by means of Legendre transformation of many variables [1, 4]. The Legendre transformation of $L(\psi, \dot{\psi}, x)$ is

$$H(\psi, \varphi, x) = \varphi^T\dot{\psi} - L(\psi, \dot{\psi}, x), \tag{15}$$

$$\frac{\partial}{\partial \dot{\psi}}\left(\varphi^T\dot{\psi} - L(\psi, \dot{\psi}, x)\right) = 0. \tag{16}$$

Equation (16) gives that $\varphi = \partial L/\partial\dot{\psi} = \dot{\psi}$. Substituting φ into Eq. (15), we can obtain the Hamiltonian function. The Hamiltonian function we obtained in such a way is precisely Eq. (12), and the corresponding Hamiltonian canonical equation is precisely Eq. (9).

From the preceding discussion, we see that the two-dimensional time-independent Schrödinger equation can be transformed into a Hamiltonian canonical equation by investigating the symplectic property or by means the Legendre transformation of many variables.

Symplectic Schemes and Numerical Method

Let $-R_x$ and R_x, respectively, be the left and right boundaries in the x direction, suppose R_x is finite, and that M is a sufficiently large positive integer. We denote the space step $\Delta x = R_x/M$, $x_n = n\,\Delta x$, $n = -M, -M+1, \ldots, -1, 0, 1, \ldots, M-1, M$. Then the boundary conditions (3) can be written as

$$\psi(-R_x, y_j) = 0, \qquad \psi(+R_x, y_j) = 0, \qquad j = -N+1, \ldots, -1, 0, 1, \ldots, N-1. \tag{17}$$

Let us now consider the two-dimensional eigenvalue problem with the boundary conditions (17). Denoting $\psi^n = \psi(x_n, y)$, $\varphi^n = \varphi(x_n, y)$, $\psi_j^n = \psi(x_n, y_j)$, $\varphi_j^n = \varphi(x_n, y_j)$, and $S^{n+1/2} = S(x_n + \Delta x/2, y)$, we can formulate explicit symplectic schemes. For example, the first-order explicit symplectic scheme reads [10]

$$\varphi^{n+1} = \varphi^n - \Delta x\, S^{n+1/2}\psi^n, \qquad \psi^{n+1} = \psi^n + \Delta x\, \varphi^{n+1}; \tag{18}$$

the second-order explicit symplectic scheme reads

$$\begin{aligned} p &= \varphi^n, \qquad q = \psi^n + \tfrac{1}{2}\Delta x\, y, \\ \varphi^{n+1} &= p - \Delta x\, S^{n+\frac{1}{2}} q, \qquad \psi^{n+1} = q + \tfrac{1}{2}\Delta x\, \varphi^{n+1}. \end{aligned} \tag{19}$$

We give the numerical method for solving the eigenvalue problem (9) with the boundary conditions (17) by using the symplectic schemes.

For the sake of simplicity, we use the first-order symplectic scheme (18) to illustrate the method. Eliminating φ^n and φ^{n+1} in the scheme (18), we obtain

$$\psi^{n-1} + \left[\Delta x^2 S^{n+1/2} - 2I\right]\psi^n + \psi^{n+1} = 0, \qquad (n = -M+1, \ldots, -1, 0, 1, \ldots, M-1). \tag{20}$$

Introducing the boundary conditions (17) to Eq. (20), we obtain a group of algebraic equations, which is written in the form of matrix as

$$\left[A + 2\,\Delta x^2 E I\right]\Psi = 0, \tag{21}$$

where I is the unit matrix, $\Psi = [\psi^{-M+1}, \psi^{-M+2}, \ldots, \psi^{M-2}, \psi^{M-1}]^T$ is a matrix that consists of the wave function on different mesh points,

$$A = \begin{bmatrix} \Delta x^2 U^{-M+1+1/2} - 2I & I & & & \\ I & \Delta x^2 U^{-M+2+1/2} - 2I & I & & \\ & \ddots & \ddots & \ddots & \\ & & I & \Delta x^2 U^{M-2+1/2} - 2I & I \\ & & & I & \Delta x^2 U^{M-1+1/2} - 2I \end{bmatrix}, \tag{22}$$

and

$$U^{n+1/2} = \begin{bmatrix} -2\left[V(x_{n+1/2}, y_{-N+1}) + \frac{\Delta x}{\Delta y}\right] & \frac{\Delta x}{\Delta y} & & & \\ \frac{\Delta x}{\Delta y} & -2\left[V(x_{n+1/2}, y_{-N+2}) + \frac{\Delta x}{\Delta y}\right] & \frac{\Delta x}{\Delta y} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{\Delta x}{\Delta y} & -2\left[V(x_{n+1/2}, y_{N-2}) + \frac{\Delta x}{\Delta y}\right] & \frac{\Delta x}{\Delta y} \\ & & & \frac{\Delta x}{\Delta y} & -2\left[V(x_{n+1/2}, y_{N-1}) + \frac{\Delta x}{\Delta y}\right] \end{bmatrix}. \tag{23}$$

$U^{n+1/2}$ is a $(2N-1)$-order tridiagonal symmetric matrix and A is a $(2M-1)(2N-1)$-order real symmetric matrix. The eigenvalues $E_0, E_1, \ldots$ and the corresponding wave functions $\Psi_0 = (0, \psi_{0j}^{-M+1}, \ldots, \psi_{0j}^{M-1}, 0)^T$, $\Psi_1 = (0, \psi_{1j}^{-M+1}, \ldots, \psi_{1j}^{M-1}, 0)^T$, $\ldots$ ($j = -N+1, \ldots, -1, 0, 1, \ldots, N-1$) can be obtained by solving the matrix eigenvalue problem (21) for Ψ. The matrix eigenvalue problem (21) by using the first-order symplectic scheme (18) is similar to the one by using the second-order symmetry finite difference method.

For the second-order symplectic scheme (19), we change the roles of the two equations (9): A similar matrix eigenvalue problem can be obtained by using the foregoing procedure above. Now in Eq. (23), the diagonal elements of the matrix $U^{n+1/2}$ are $-[(V^{n-1+1/2} + V^{n+1/2}) + 2\Delta x/\Delta y]$, $n = -M+1, \ldots, -1, 0, 1, \ldots, M-1$.

By using the second-order symplectic scheme (19), we improve the matrix A in Eq. (22) of the matrix eigenvalue problem (21).

Numerical Results and Discussion

To illustrate the preceding algorithm, we apply the algorithm to calculations of the eigenvalues of the two-dimensional harmonic oscillator and the two-dimensional Henon–Heiles potential.

TWO-DIMENSIONAL HARMONIC OSCILLATOR

The potential of the two-dimensional harmonic oscillator is taken to be

$$V(x,y) = \tfrac{1}{2}x^2 + \tfrac{1}{2}y^2, \qquad (24)$$

with the boundary conditions (2) and (3). The exact eigenvalues of the two-dimensional harmonic oscillator are given by

$$E_n = n + 1, \qquad n = n_x + n_y, \qquad n_x, n_y = 0, 1, 2, \ldots. \qquad (25)$$

To compute the eigenvalues of the lower excitation states, we take $R_x = R_y = 5.5$. For different M and N, the eigenvalues obtained from the second-order symplectic scheme (19) are listed in Table I together with the exact values. For the ground state, with the increase of M and N, the absolute errors are, respectively, 0.004 (for $M = N = 20$), 0.002 (for $M = N = 60$), and 0.001 (for $M = N = 70$). For the first excitation state, with the increase of M and N, the absolute errors are, respectively, 0.005 (for $M = N = 20$), 0.003 (for $M = N = 60$), and 0.002 (for $M = N = 70$), i.e., with the increase of M and N, the absolute error is smaller and smaller. This verifies that our method is stable and convergent. From Table I, we can see that the numerical results by using the second-order symplectic scheme (19) (SSMEM) tend to the exact ones monotonically with the increase of M and N (or decrease of the space step length Δx and Δy).

TWO-DIMENSIONAL HENON–HEILES POTENTIAL

We also applied our method to calculations of the eigenvalues of the two-dimensional Henon–Heiles potential. The potential is taken to be of the form

$$V(x,y) = \frac{1}{2}(x^2 + y^2) + (0.0125)^{1/2}\left(x^2 y - \frac{y^3}{3}\right). \qquad (26)$$

This potential was considered in Refs. [11–13]. In our computation, we take $R_x = R_y = 5.5$. For ($M = 60, N = 60$) and ($M = 70, N = 70$), the numerical results by using the second-order symplectic scheme are given in Table II and compared to the results of Davis and Heller [11]. The table shows that numerical eigenvalues by using the SSMEM are lower than those Davis and Heller, who used the Gaussian basis set method (except the first eigenvalue). From Table II, we can see again that the numerical results by using the second-order symplectic scheme (19) (SSMEM) tend to the values of Davis and Heller monotonically with the increase of M and N. This again veritices that our method is stable and convergent.

For the two-dimensional Hamiltonian form $H = p_x^2/2 + p_y^2/2 + V(x,y)$, Davis and Heller's basis set is separable in x and y,

$$G_{ij}(x,y) = g_i(x) g_j(y),$$

TABLE I
The eigenvalues of the two-dimensional harmonic oscillator.

n	n_x	n_y	Symplectic $M = 20, N = 20$	Symplectic $M = 60, N = 60$	Symplectic $M = 70, N = 70$	Exact
0	0	0	1.004	1.002	1.001	1.000
1	0	1	1.995	1.997	1.998	2.000
1	1	1	1.995	1.997	1.998	2.000
2	0	2	2.976	2.989	2.992	3.000
2	1	1	2.976	2.989	2.992	3.000
2	2	0	2.985	2.993	2.995	3.000
3	0	3	3.947	3.976	3.983	4.000
3	1	2	3.947	3.976	3.983	4.000
3	2	1	3.966	3.985	3.989	4.000
3	3	0	3.966	3.985	3.989	4.000

TABLE II
The eigenvalues of the two-dimensional Henon–Heiles potential.

Symmetry	Symplectic $M = 60$, $N = 60$	Symplectic $M = 70$, $N = 70$	Davis and Heller
A	1.000	0.999	0.9986
E	1.988	1.989	1.9901
A	2.948	2.950	2.9562
E	2.979	2.980	2.9853
E	3.909	3.914	3.9260
A	3.968	3.972	3.9824
A	3.972	3.975	3.9858
A	4.843	4.850	4.8701
E	4.877	4.883	4.8986
E	4.963	4.969	4.9863
E	5.779	5.790	5.8170
A	5.831	5.841	5.8670
A	5.845	5.855	5.8814
E	5.958	5.967	5.9913
A	6.691	6.705	6.7379
E	6.723	6.734	6.7649
E	6.806	6.819	6.8534

where

$$g_i(x) = \left(\frac{2\alpha_x}{\pi}\right)^{1/4} \exp\left[-\alpha_x(x - x_i)^2 + ip_{xi}x\right],$$
$$g_j(y) = \left(\frac{2\alpha_y}{\pi}\right)^{1/4} \exp\left[-\alpha_y(y - y_j)^2 + ip_{yj}y\right].$$

The parameters α_x and α_y are real and chosen so that the Gaussian centered at $x_i = 0$, $y_i = 0$, $p_{xi} = 0$, $p_{yi} = 0$ is the ground state wave function for the harmonic part of the Hamiltonian. This gives $\alpha_x = \alpha_y = 1/2$ for the Henon–Heiles potential (26).

In summary, the symplectic schemes are extended to the numerical solution of the two-dimensional time-independent Schrödinger equation. The Schrödinger equation is first transformed into a Hamiltonian canonical equation by means of the symplectic property and by means of the Legendre transformation of many variables. The numerical method SSMEM is developed for solving the eigenvalues. In SSMEM, the symplectic schemes are converted into a group of algebraic equations whose coefficient matrix is a real symmetric matrix and the eigenvalues are obtained by solving the matrix eigenvalue problem. This method is applied to calculations of the eigenvalues of two-dimensional harmonic oscillators and two-dimensional Henon–Heiles potentials. The numerical results of the two-dimensional harmonic oscillator by using the SSMEM tend to the exact ones monotonically with the increase of M and N (or decrease of the space step length), and the numerical eigenvalues of the two-dimensional Henon–Heils potential by using the SSMEM are lower than those by using the Gaussian basis set method.

From our computation, we see that more computer time needs to be spent with the increase of M and N. If we increase M and N (or decrease the space step length), the numerical results of the two-dimensional harmonic oscillator by using the SSMEM approach the exact ones more and the numerical results of the two-dimensional Henon–Heils potential by using the SSMEM approach those by using the Gaussian basis set method more, but the order of the matrix (22) increases rapidly and more and more computer time needs to be spent. To solve this problem completely, we are considering the following future research:

1. The matrix (22) is a $(2M - 1)(2N - 1)$-order real symmetric matrix, and computer storage is at least $[(2M - 1)(2N - 1)]^2$. Because the matrix (22) is sparse, the computer storage reduces to $5(2M - 1)(2N - 1)$. More computer time needs to be spent. Therefore, we are trying to use some kind of dimensionality reduction technique or parallel computation to solve the matrix eigenvalue problem (21).
2. Recently, the multisymplectic algorithm for solving the multisymplectic Hamiltonian partial differential equation was presented [14, 15]. One of the nice features of the multisymplectic structure of certain partial differential equation is that it is a strictly local concept and it can be formulated as a conservation law involving differential two forms. It is thus also a very natural generalization of the conservation of symplecticity for canonical Hamiltonian systems. The multisymplectic scheme also can be applied to the stationary problem (1)–(3).
3. We have found a direct method for solving the two-dimensional Schrödinger equation similar to the symplectic scheme-shooting method for solving the one-dimensional Schrödinger equation [1]. It is a simpler and more effective method for this kind of problem; high-order symplectic schemes can be used easily in this method. We are practicing it.

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