



A Flexible Symplectic Scheme for Two-Dimensional Schrödinger Equation with Highly Accurate RBFs Quasi-Interpolation

Shengliang Zhang^a, Liping Zhang^{b,*}

^aCollege of Economics and Management, Nanjing Forestry University, Nanjing, PR China.

^bDepartment of Mathematics, Zhejiang University of Technology, Hangzhou 310023, PR China.

Abstract. Based on highly accurate multiquadric quasi-interpolation, this study suggests a meshless symplectic procedure for two-dimensional time-dependent Schrödinger equation. The method is high-order accurate, flexible with respect to the geometry, computationally efficient and easy to implement. We also present a theoretical framework to show the conservativeness and convergence of the proposed method. As the numerical experiments show, it not only offers a high order accuracy but also has a good performance in the long time integration.

1. Introduction

This study aims to develop a meshless symplectic algorithm for two-dimensional Schrödinger equation

$$-i \cdot \partial_t w = \partial_{xx} w + \partial_{yy} w + \rho(x, y)w, \quad (1)$$

where $i = \sqrt{-1}$ and $\rho(x, y)$ is a potential function. The equation has many real-life applications in physical sciences and engineering fields, such as the modeling of quantum devices [1], electromagnetic wave propagation [13], underwater acoustics [21] and design of certain optoelectronic devices [10]. Moreover, it has been used in many quantum dynamics calculations (see [11] and references therein). In application, it is hard to obtain an analytic formula for E.q (1), since usually the analytical solution is not available. This leads to a practical need to develop numerical procedure to simulate the solution, some numerical methods have been developed by [7, 12, 20], for example.

On the other hand, the equation can be viewed as an infinite dimensional Hamiltonian system, which possesses a symplectic structure (cf. [4, 14, 19]). It is now well known from the development of algorithms for Hamiltonian systems that 'geometric integration' is an important guiding principle. Hence, robust numerical algorithms for Hamiltonian partial differential equations (PDEs) should preserve the symplectic structure. A standard method, to obtain symplectic algorithms for Hamiltonian PDEs, involves two steps. First, spatial discretization transforms Hamiltonian PDEs into a finite-dimensional Hamiltonian system

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*Corresponding author: Liping Zhang

Email address: zhanglp@zjut.edu.cn (Liping Zhang)

(ordinary differential equations, ODEs). In the second step, the resulting system of ODEs is evolved by using symplectic integrators. In this numerical procedure, the key for success is to ensure that the obtained semi-discrete system is associated with a finite dimensional Hamiltonian system. Several spatial discretization approaches can be adopted, such as finite difference method (FDM) by [4, 8, 9], finite element method (FEM) by [28], Fourier pseudospectral method by [14] and wavelet collocation method by [29]. However, most of those methods require equally-spaced grids, which is difficult for problems with very complicated and irregular geometries.

More recently, a meshless symplectic algorithm for Hamiltonian PDEs with radial basis functions (RBFs) interpolation is developed by [23]. In a subsequent, [24] suggests a symplectic scheme for two-dimensional Schrödinger equation. However, RBFs interpolation method suffers from a serious ill-conditioning problem due to the use of the RBFs as a global interpolation, and the results are sensitive to a shape parameter c [6, 16]. To avoid solving a large scaled linear system of equations, RBFs quasi-interpolation method thereby has caught the attentions of many researchers. In the recent literature [25], the authors present a meshless symplectic algorithm for nonlinear wave equation with the help of cubic multiquadric quasi-interpolation. By using the technique proposed by [25], this study will develop a meshless symplectic procedure for two-dimensional time-dependent Schrödinger equation. The method has a number of advantages over existing approaches, including:

(I). The method is highly accurate and flexible. Compared to traditional methods, cubic multiquadric quasi-interpolation often offers a highly accurate approximation to the objective function. Moreover, the method is meshfree, it can be used for the problem with the irregularly spaced points;

(II). The method possesses a long-time tracking capability for solving Schrödinger equation. Since the method is symplectic, it can preserve structural properties of the original problem's flow as long as the intermediate problems' flow do;

(III). The method is computationally efficient. Because it does not require solving a resultant full matrix, the ill-conditioning problem arising when using RBFs as a global interpolant can be avoided.

The layout of the paper is as follows. Section 2 provides a brief introduction to cubic multiquadric quasi-interpolation. In section 3, Hamiltonian form of the continuous problem is introduced. A spatial discretization approach by using cubic multiquadric quasi-interpolation is illustrated, and the resulting semi-discrete system is proven to be a finite-dimensional Hamiltonian system. In section 4, evolving the semi-discrete system by classical symplectic integrator in time, one can get the expected symplectic algorithms. In section 5, some numerical examples are given to verify the effectiveness of the method. The last section is dedicated to a brief conclusion.

2. Cubic multiquadric quasi-interpolation

In this section, a brief overview of cubic multiquadric quasi-interpolation is given, more details can be found in [2, 3, 22, 26]. Specifically, consider a points sequence

$$\mathbf{x} = \cdots < x_{j-1} < x_j < x_{j+1} < \cdots, \quad h := \max_j (x_j - x_{j-1})$$

where $x_{\pm j} \rightarrow \pm\infty$ as $j \rightarrow \pm\infty$. The cubic multiquadric quasi-interpolation of a function $f(x)$ is defined by

$$(\mathcal{L}f) = \sum f(\xi_j) \Psi_j(x), \quad (2)$$

where $\xi_j = (x_{j-1} + x_j + x_{j+1})/3$ ($\xi_j = x_j$ when the points are uniformly distributed),

$$\Psi_j(x) = \Psi(x - x_j) = \frac{\psi_{j+1}(x) - \psi_j(x)}{2(x_{j+2} - x_{j-1})} - \frac{\psi_j(x) - \psi_{j-1}(x)}{2(x_{j+1} - x_{j-2})}$$

and $\psi_j(x)$ are the following linear combinations of cubic multiquadric function, i.e

$$\psi_j(x) = \psi(x - x_j) = \frac{(\phi_{j+1} - \phi_j)/(x_{j+1} - x_j) - (\phi_j - \phi_{j-1})/(x_j - x_{j-1})}{x_{j+1} - x_{j-1}},$$

with $\phi(x) = \sqrt{(x^2 + c^2)^3}$ and $\phi_j = \phi(x - x_j)$. As discussed in [2, 22, 26], cubic multiquadric quasi-interpolation operator possesses shape-preserving and high-order approximation properties. Moreover, for any $\delta > 0$, one can find a positive integer M , satisfying

$$1 - \sum_{j=i-M}^{j=i+M} \Psi_j(x) < \delta, \quad \sum_{j=i-M}^{j=i+M} \frac{\partial \Psi_j(x)}{\partial x} < \delta, \quad \sum_{j=i-M}^{j=i+M} \frac{\partial^2 \Psi_j(x)}{\partial x^2} < \delta, \quad i \in \mathbb{Z}. \tag{3}$$

for any fixed $x = x_i$. This implies that the matrices $\Psi = (\Psi_j(x_i))$, $\Psi_1 = \left(\frac{\partial \Psi_j(x_i)}{\partial x}\right)$ and $\Psi_2 = \left(\frac{\partial^2 \Psi_j(x_i)}{\partial x^2}\right)$ can be treated as bounded matrices with bandwidth of $2M + 1$, which is computationally efficient in numerical procedure.

2.1. Cubic multiquadric quasi-interpolation tensor-product approximation

For a single variable function $f(x)$, we can approximate it by using cubic multiquadric quasi-interpolation operator $(\mathcal{L}f)(x)$, and rearrange the scheme as

$$f^*(x) = (\mathcal{L}f)(x) = \sum_j \left[\frac{f_{j+1} - f_j}{\xi_{j+1} - \xi_j} - \frac{f_j - f_{j-1}}{\xi_j - \xi_{j-1}} \right] \frac{\psi_j(x)}{6}.$$

Meanwhile, the second derivative of $f(x)$ can be approximated by

$$f''(x) \approx (f^*)''(x) = \sum_j \left[\frac{f_{j+1} - f_j}{\xi_{j+1} - \xi_j} - \frac{f_j - f_{j-1}}{\xi_j - \xi_{j-1}} \right] \frac{\psi_j''(x)}{6}.$$

Notice

$$\psi_j(x) = \frac{(\phi_{j+1} - \phi_j)/(x_{j+1} - x_j) - (\phi_j - \phi_{j-1})/(x_j - x_{j-1})}{x_{j+1} - x_{j-1}} \approx \frac{\phi_j''(x)}{2},$$

hence $\frac{\psi_j''(x)}{6} \approx \frac{\phi_j^{(4)}(x)}{12}$. Therefore, the approximation can be written in a matrix form

$$F_{xx} \approx \Phi \Lambda F,$$

where $F_{xx} = [\dots, f''(x_i), \dots]^T$, $F = [\dots, f(x_j), \dots]^T$, $\Phi = \left(\frac{\phi_j^{(4)}(x_i)}{12}\right)$, and the symmetric matrix

$$\Lambda := \begin{pmatrix} \ddots & & & & & \\ & \alpha_j & & & & \\ \alpha_j & -(\alpha_j + \beta_j) & & \beta_j & & \\ & & \beta_j & & \ddots & \\ & & & & & \ddots \end{pmatrix} \tag{4}$$

with $\alpha_j = \frac{1}{\xi_j - \xi_{j-1}}$ and $\beta_j = \frac{1}{\xi_{j+1} - \xi_j}$.

The approximation for a function $f(x, y)$ of two variables, can be obtained by using tensor-product approach. Denote $F = [\dots, f(x_i, y_j), \dots]^T$, $\partial_{xx}F$ and $\partial_{yy}F$ can be thereby approximated by

$$\partial_{xx}F \approx (\Phi \Lambda \otimes \mathbf{I})F, \quad \partial_{yy}F \approx (\mathbf{I} \otimes \Phi \Lambda)F, \tag{5}$$

where \otimes denotes the Kronecker tensor-product, \mathbf{I} is the identity matrix, $\partial_{xx}F = [\dots, \partial_{xx}f(x_i, y_j), \dots]^T$ and $\partial_{yy}F = [\dots, \partial_{yy}f(x_i, y_j), \dots]^T$.

2.2. Cubic multiquadric function

The important property of cubic multiquadric function $\phi(x) = \sqrt{(x^2 + c^2)^3}$ is prepared by the following lemma, which can be found from Theorem 2.1 of [25].

Lemma 2.1. For a large enough real number M and the scattered knots

$$-\infty < -M = x_{-N} < x_{-N+1} < \dots < x_0 < x_1 < \dots < x_N = M < +\infty \quad h := \max_j(x_j - x_{j-1}),$$

if $f(x), g(x) \in C^2(\mathbb{R})$, $\int |f(x)|dx < \infty$, $\int |g(x)|dx < \infty$, $\int f^2(x)dx < \infty$ and $\int g^2(x)dx < \infty$, then the following inequality

$$|\int_{-\infty}^{\infty} f(x)g(x)dx - F^T \Phi^{-1}G| \leq O(h^\ell)$$

holds, where $F = [\dots, f(x_j), \dots]^T$, $G = [\dots, g(x_j), \dots]^T$, ℓ is the approximation order of second derivative by using cubic multiquadric quasi-interpolation, and $\Phi = \left(\frac{\phi_j^{(4)}(x_i)}{12}\right)_{i,j=-N}^N$.

Remark 2.2. Φ is a positive definite matrix, since $\phi^{(4)}(x)$ is a positive definite function [25]. As the lemma shows, Φ^{-1} plays the same role with the matrix $X := \text{diag}(\Delta_j)$ in numerical quadrature, where $\Delta_j = \frac{x_{j+1} - x_{j-1}}{2}$. That is

$$F^T \Phi^{-1}G = \sum_j f(x_j)g(x_j) \frac{x_{j+1} - x_{j-1}}{2} + O(h^\ell).$$

3. Hamiltonian form of the continuous problem and spatial discretization method

3.1. Hamiltonian form of the continuous problem

Let $w(x, y, t) = v(x, y, t) + iu(x, y, t)$, where $u(x, y, t)$ and $v(x, y, t)$ are real-valued functions, by separating the real part from the imaginary, one can obtain a Hamiltonian form for E.q (1),

$$\begin{cases} \partial_t u = \partial_{xx}v + \partial_{yy}v + \rho(x, y)v, \\ \partial_t v = -\partial_{xx}u - \partial_{yy}u - \rho(x, y)u. \end{cases} \tag{6}$$

Hamiltonian functional (which usually refers to the energy of the system)

$$H(u, v) = \frac{1}{2} \iint (|\nabla u|^2 + |\nabla v|^2 - \rho(x, y)(u^2 + v^2)) dx dy \tag{7}$$

is invariant with respect to time if the function u and v possesses a fast decay as $\mathbf{x} = (x, y) \rightarrow \infty$, or satisfies a zero boundary conditions. The derivation is as follows. Multiplying the equations (6) by $\partial_t v$ and $\partial_t u$ respectively, and subtracting both equations, the result can be rewritten as a divergence. Then, considering the integral over the domain Ω , it is immediately deduced that $\frac{dH}{dt} = 0$, from the divergence theorem.

Furthermore, denote $\delta H/\delta u$, $\delta H/\delta v$ the variational derivatives with respect to u and v respectively, then E.q (6) can be rearranged as a standard Hamiltonian system

$$\begin{cases} \partial_t u = -\delta H/\delta v \\ \partial_t v = \delta H/\delta u, \end{cases} \tag{8}$$

where

$$\iint \delta H/\delta u \cdot \eta dx dy \triangleq \lim_{\epsilon \rightarrow 0} \frac{H(u + \epsilon \eta, v) - H(u, v)}{\epsilon}$$

and

$$\iint \delta H / \delta v \cdot \eta dx dy \triangleq \lim_{\epsilon \rightarrow 0} \frac{H(u, v + \epsilon \eta) - H(u, v)}{\epsilon}$$

for variations η with vanishing boundary variation. The symplectic structure of this system

$$\omega = \iint \mathbf{d}u \wedge \mathbf{d}v dx dy \tag{9}$$

is also invariant with respect to time, where \wedge denotes the wedge product and \mathbf{d} is the differential operator. More details about Hamiltonian PDEs can be found in [4, 14, 19], etc.

A systematic approach to construct a symplectic scheme for Hamiltonian PDEs is the method-of-line, a standard procedure starts with the discretization of the equation in space and then in time. To preserve the symplectic structure, the spatial discretization is required to be able to preserve the symmetric property of second-order derivatives [5]. Several approaches can be adopted, such as the finite difference method [4], finite element method [28], Fourier pseudospectral method [14] and wavelet collocation method [29] when collocating with a uniform grid. However sometimes the sampling data points are scattered, it's hard to settle it by using the traditional methods which depend on a suitable generation of meshes. Multiquadric quasi-interpolation is meshfree, it can be used for the problem with the irregularly spaced points. In this paper, a cubic multiquadric quasi-interpolation method will be employed for spatial discretization for two-dimensional Schrödinger equation.

3.2. Cubic multiquadric quasi-interpolation for space discretization

In this section, cubic multiquadric quasi-interpolation method is used for space discretization. According to the approximation formulas (5), we can evaluate the second order spatial derivatives of u and v of (6) by

$$\nabla^2 U = \partial_{xx} U + \partial_{yy} U \sim (\Phi \Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi \Lambda) U, \quad \nabla^2 V = \partial_{xx} V + \partial_{yy} V \sim (\Phi \Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi \Lambda) V,$$

where $U = [\dots, u(x_i, y_j, t), \dots]^T$, $V = [\dots, v(x_i, y_j, t), \dots]^T$ and ∇ is the gradine operator. Then a semi-discretization system arises

$$\begin{cases} U_t = (\Phi \Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi \Lambda) V + \rho V \\ V_t = -(\Phi \Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi \Lambda) U - \rho U, \end{cases} \tag{10}$$

where $\rho = \text{diag}([\dots, \rho(x_i, y_j), \dots]^T)$. Because Φ is a positive definite matrix (see Remark 2.2), there exists one and only one positive definite matrix P satisfying $\Phi = P^2$. By employing transformations

$$\tilde{U} = (P^{-1} \otimes P^{-1}) U, \quad \tilde{V} = (P^{-1} \otimes P^{-1}) V, \tag{11}$$

the system (10) will be

$$\begin{cases} \tilde{U}_t = (P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P) \tilde{V} + \rho \tilde{V} \\ \tilde{V}_t = -(P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P) \tilde{U} - \rho \tilde{U}. \end{cases} \tag{12}$$

Notice that the coefficient matrices are all symmetric, then the system (12) is a finite-dimensional Hamiltonian system with respect to \tilde{U} and \tilde{V} [5]. Where the Hamiltonian

$$\begin{aligned} 2H(\tilde{U}, \tilde{V}) &= -\langle \tilde{V}, (P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P) \tilde{V} \rangle - \langle \tilde{V}, \rho \tilde{V} \rangle \\ &\quad -\langle \tilde{U}, (P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P) \tilde{U} \rangle - \langle \tilde{U}, \rho \tilde{U} \rangle \end{aligned} \tag{13}$$

and the symplectic structure $J = \mathbf{d}\tilde{U} \wedge \mathbf{d}\tilde{V}$.

Next we will prove that, by means of cubic multiquadric quasi-interpolation method, not only the Hamiltonian function (7) but also the symplectic structure (9) can be approximated by the corresponding discretization $H(\tilde{U}, \tilde{V})$ and J .

Theorem 3.1. *Hamiltonian function of the finite-dimensional Hamiltonian system (12) is an approximant of infinite-dimensional Hamiltonian (6)'s, i.e.*

$$\begin{aligned} H(u, v) &= \iint (|\nabla u|^2 + |\nabla v|^2 - \rho(x, y)(u^2 + v^2)) dx dy \\ &= 2H(\tilde{U}, \tilde{V}) + O(h^\ell). \end{aligned}$$

Proof. Because

$$\begin{aligned} 2H(\tilde{U}, \tilde{V}) &= -\langle \tilde{V}, (P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P)\tilde{V} \rangle - \langle \tilde{V}, \rho \tilde{V} \rangle \\ &\quad -\langle \tilde{U}, (P \otimes P)(\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)(P \otimes P)\tilde{U} \rangle - \langle \tilde{U}, \rho \tilde{U} \rangle \\ &= -\langle V, (\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)V \rangle - \langle \Phi^{-1} \otimes \Phi^{-1} V, \rho V \rangle \\ &\quad -\langle U, (\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)U \rangle - \langle \Phi^{-1} \otimes \Phi^{-1} U, \rho U \rangle. \end{aligned}$$

Notice the definition (4) of Λ , and according to Lemma (2.1), we have

$$\begin{aligned} &-\langle V, (\Lambda \otimes \Phi^{-1} + \Phi^{-1} \otimes \Lambda)V \rangle - \langle \Phi^{-1} \otimes \Phi^{-1} V, \rho V \rangle \\ &= \frac{1}{2} \sum_j \sum_i \left(\left(\frac{v(x_i, y_j) - v(x_{i-1}, y_j)}{x_i - x_{i-1}} \right)^2 + \left(\frac{v(x_{i+1}, y_j) - v(x_i, y_j)}{x_{i+1} - x_i} \right)^2 \right) (x_{i+1} - x_i) \frac{y_{j+1} - y_{j-1}}{2} \\ &+ \frac{1}{2} \sum_i \sum_j \left(\left(\frac{v(x_i, y_j) - v(x_i, y_{j-1})}{y_j - y_{j-1}} \right)^2 + \left(\frac{v(x_i, y_{j+1}) - v(x_i, y_j)}{y_{j+1} - y_j} \right)^2 \right) (y_{j+1} - y_j) \frac{x_{i+1} - x_{i-1}}{2} \\ &- \sum_j \sum_i \rho(x_i, y_j) v(x_i, y_j)^2 \frac{x_{i+1} - x_{i-1}}{2} \frac{y_{j+1} - y_{j-1}}{2} + O(h^\ell) \\ &= \iint (|\nabla v|^2 - \rho(x, y)v^2) dx dy + O(h^\ell). \end{aligned}$$

The derivation of the other part of $H(u, v)$ approximating by $H(\tilde{U}, \tilde{V})$'s can be obtained in a similar way. Then we complete the proof of the theorem. \square

To discuss the symplecticness of (12), we start by preparing the follow lemma:

Lemma 3.2. [18] *If f and g are vector-valued functions and S a real-valued matrix, we have the following equality*

$$d(Sf) \wedge dg = df \wedge d(S^T g),$$

where \wedge denotes the wedge product.

Theorem 3.3. *The symplectic structure of the finite-dimensional Hamiltonian system (12) is an approximant of infinite-dimensional Hamiltonian (6)'s, i.e.*

$$\iint du \wedge dv dx dy = d\tilde{U} \wedge d\tilde{V} + O(h^\ell).$$

Proof. By the above Lemma 2.1 and Lemma 3.2, we have

$$\begin{aligned} d\tilde{U} \wedge d\tilde{V} &= d(P^{-1} \otimes P^{-1})U \wedge d(P^{-1} \otimes P^{-1})V \\ &= dU \wedge d(\Phi^{-1} \otimes \Phi^{-1})V \\ &= \iint du \wedge dv dx dy + O(h^\ell). \end{aligned}$$

\square

4. Time discretization for two-dimensional Schrödinger equation

The finite-dimensional Hamiltonian system (12) can be discretized in time by many symplectic integrators. The separable Hamiltonian which consists of a sum of quadratic kinetic energies

$$H(u, v) = \mathcal{V}(u) + \mathcal{T}(v)$$

is often discretized by using splitting schemes. In fact, splitting symplectic integrators preserve structural properties of the original problem’s flow as long as the intermediate problems’ flow do. Symplectic methods do, in general, nearly preserve the energy, i.e. a modified energy is preserved up to an exponentially small error term [15, 27]. The good performance of the symplectic integrators in the long time integration of Hamiltonian ODEs systems is well showed in [17, 18, 27], etc. In this work, for the sake of simplicity, we use *the staggered Störmer-Verlet scheme*

$$\begin{aligned} u^{n+1} &= u^n + \tau \nabla_v \mathcal{T}(v^{n+\frac{1}{2}}) \\ v^{n+\frac{1}{2}} &= v^{n-\frac{1}{2}} - \tau \nabla_u \mathcal{V}(u^n), \end{aligned} \tag{14}$$

where $(u^n, v^{n+\frac{1}{2}}) = (u(t^n), v(t^{n+\frac{1}{2}}))$ and $t^n = t^0 + n\tau$ ($\tau = \Delta t$). This scheme is second-order symplectic with respect to a staggered symplectic structure (e.g.[18]), i.e,

$$\omega = \mathbf{d}u^n \wedge \mathbf{d}v^{n+\frac{1}{2}},$$

where $\mathbf{d}u^n$ and $\mathbf{d}v^{n+\frac{1}{2}}$ are solutions of the discrete variational equation associated with (14), then

$$\omega^{n+1} = \omega^n.$$

By integrating (12) or equivalently integrating (10) with *the staggered Störmer-Verlet scheme*, the following symplectic algorithm can be obtained

$$\begin{cases} U^{n+1} = U^n + \tau(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)V^{n+1/2} + \tau\rho V^{n+1/2} \\ V^{n+1/2} = V^{n-1/2} - \tau(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)U^n - \tau\rho U^n, \end{cases} \tag{15}$$

where $U^n = \{u(x_i, y_j, t^n)\}$ and $V^{n+\frac{1}{2}} = \{v(x_i, y_j, t^{n+\frac{1}{2}})\}$. Moreover, we can get

$$\begin{cases} \frac{U^{n+1} - U^{n-1}}{2\tau} = (\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda) \frac{V^{n+1/2} + V^{n-1/2}}{2} + \rho \frac{V^{n+1/2} + V^{n-1/2}}{2} \\ \frac{V^{n+1/2} - V^{n-1/2}}{\tau} = -(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)U^n - \rho U^n. \end{cases} \tag{16}$$

Now, the convergence of the symplectic scheme (15) is investigated. Define the truncation error

$$\begin{aligned} T_u^n &\triangleq \frac{U^{n+1} - U^{n-1}}{2\tau} - (\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda) \frac{V^{n+1/2} + V^{n-1/2}}{2} - \rho \frac{V^{n+1/2} + V^{n-1/2}}{2} \\ &\quad - \left(\partial_t U^n - \partial_{xx} V^n - \partial_{yy} V^n - \rho V^n \right), \end{aligned} \tag{17}$$

$$T_v^n \triangleq \frac{V^{n+1/2} - V^{n-1/2}}{\tau} + (\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)U^n + \rho U^n - \left(\partial_t V^n + \partial_{xx} U^n + \partial_{yy} U^n + \rho U^n \right), \tag{18}$$

and denote $\|\cdot\|$ the L^2 norm, then the following theorems are obtained.

Theorem 4.1. *Suppose $u(x, y, t), v(x, y, t) \in H_0^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2)$, for any $t \in [0, T]$, $u(x, y, t), v(x, y, t) \in C^4(\mathbb{R}^2)$, $\mathcal{V}(x, y) \in \mathbb{R}^2$. Then the truncation errors satisfy*

$$\|T_u^n\| \leq O(\tau^2 + h^\ell), \quad \|T_v^n\| \leq O(\tau^2 + h^\ell)$$

where ℓ is the approximation order of $\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda$ simulating the operator $\partial_{xx} + \partial_{yy}$.

Proof. Let $U^n = [\dots, u(x_i, y_j, t_n), \dots]^T$, $V^n = [\dots, v(x_i, y_j, t_n), \dots]^T$ be the solution of (6). Based on Taylor expansion, the following equation can be obtained

$$U^{n+1} - U^{n-1} = 2\tau\partial_t U^n + O(\tau^3)$$

and

$$V^{n+\frac{1}{2}} + V^{n-\frac{1}{2}} = 2V^n + O(\tau^2).$$

In addition, notice $\Phi\Lambda \otimes \mathbf{I}$ and $\mathbf{I} \otimes \Phi\Lambda$ are approximants of ∂_{xx} and ∂_{yy} , the approximation order is ℓ . According to E.q (17), the truncation error thereby goes as

$$T_u^n = O(\tau^2 + h^\ell).$$

Similarly, we can get $T_v^n = O(\tau^2 + h^\ell)$ by E.q (18). \square

Theorem 4.2. Suppose $u(x, y, t), v(x, y, t)$ satisfy the same conditions as in Theorem 4.1. Denote

$$U_{true}^n = [\dots, u_{true}(x_i, y_j, t_n), \dots]^T, U^n = [\dots, u(x_i, y_j, t_n), \dots]^T, \varepsilon_u^n = U_{true}^n - U^n,$$

$$V_{true}^n = [\dots, v_{true}(x_i, y_j, t_n), \dots]^T, V^n = [\dots, v(x_i, y_j, t_n), \dots]^T, \varepsilon_v^n = V_{true}^n - V^n.$$

Then the global error estimates of the scheme (15) at time T satisfy

$$\|\varepsilon_u(T)\| = \|\varepsilon_u^L\| \leq C^*O(\tau^2 + h^\ell), \quad \|\varepsilon_v(T)\| = \|\varepsilon_v^L\| \leq C^{**}O(\tau^2 + h^\ell)$$

where $L = T/\tau$, denotes the total steps and C^*, C^{**} are positive constants.

The proof of the theorem 4.2 can be similarly obtained as Theorem 3.3 in [29] with a minor modification, where for ε_u^L we replace $\langle -B_2\varepsilon^{n+1/2}, \varepsilon^{n+1/2} \rangle \geq 0$ by

$$\begin{aligned} \langle -(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)\varepsilon_v^{n+1/2}, \varepsilon_v^{n+1/2} \rangle &= \langle -(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)(V_{true}^{n+1/2} - V^{n+1/2}), V_{true}^{n+1/2} - V^{n+1/2} \rangle \\ &\approx -\langle \nabla^2 V_{true}^{n+1/2} - \nabla^2 V^{n+1/2}, V_{true}^{n+1/2} - V^{n+1/2} \rangle \\ &= \langle \nabla(V_{true}^{n+1/2} - V^{n+1/2}), \nabla(V_{true}^{n+1/2} - V^{n+1/2}) \rangle \geq 0. \end{aligned}$$

and for ε_v^L , by

$$\begin{aligned} \langle -(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)\varepsilon_u^n, \varepsilon_u^n \rangle &= \langle -(\Phi\Lambda \otimes \mathbf{I} + \mathbf{I} \otimes \Phi\Lambda)(U_{true}^n - U^n), U_{true}^n - U^n \rangle \\ &\approx -\langle \nabla^2 U_{true}^n - \nabla^2 U^n, U_{true}^n - U^n \rangle \\ &= \langle \nabla(U_{true}^n - U^n), \nabla(U_{true}^n - U^n) \rangle \geq 0. \end{aligned}$$

Remark 4.3. Compared with the classic symplectic algorithm by using FDM which usually possesses the error $O(\tau^2 + h^2)$, the proposed symplectic scheme possesses $O(\tau^2 + h^\ell)$, where usually ℓ is larger than 2 [22, 26].

5. Numerical example

In this section, we give two examples to describe the efficiency of the cubic multiquadric quasi-interpolations method for solving two-dimensional time-dependent Schrödinger equation. In our computations, the following approach is adopted to handle the boundary. For the data points $\{x_j\}_{j=0}^N$, take four extra artificial endpoints, satisfying

$$x_{-2} < x_{-1} < x_0 < x_1 < \dots < x_N < x_{N+1} < x_{N+2},$$

the radial basis function is chosen to be

$$\phi_j(x) = \begin{cases} (x - x_j)^3, & \text{for } -2 \leq j \leq 1, \\ \sqrt{((x - x_j)^2 + c^2)^3}, & \text{for } 2 \leq j \leq N - 2, \\ (x_j - x)^3, & \text{for } N - 1 \leq j \leq N + 2. \end{cases}$$

Example 5.1. Consider E.q (1) with the potential function

$$\rho(x, y) = 3 - 2 \tanh^2(x) - 2 \tanh^2(y), \tag{19}$$

the initial condition

$$w(x, y, 0) = \frac{i}{\cosh(x) \cosh(y)}, \tag{20}$$

and the boundary conditions

$$\begin{aligned} w(0, y, t) &= \frac{i \exp(it)}{\cosh(y)}, & w(1, y, t) &= \frac{i \exp(it)}{\cosh(1) \cosh(y)}, \\ w(x, 0, t) &= \frac{i \exp(it)}{\cosh(x)}, & w(x, 1, t) &= \frac{i \exp(it)}{\cosh(x) \cosh(1)}, \end{aligned} \tag{21}$$

where the computational domain $\Omega = \{(x, y) : 0 \leq x, y \leq 1\}$. As shown in [7], the exact solution of the problem is

$$w(x, y, t) = \frac{i \exp(it)}{\cosh(x) \cosh(y)}. \tag{22}$$

The problem is calculated till $t = 100$. The root mean square error (RMS-error) and the max error (MAX-error) are defined as

$$\sqrt{\frac{1}{(N + 1)^2} \sum_i \sum_j (u_{true}(x_i, y_j, t_n) - u(x_i, y_j, t_n))^2}$$

and

$$\max_{i,j} |u_{true}(x_i, y_j, t_n) - u(x_i, y_j, t_n)|,$$

where $(N + 1)^2$ is the number of collocation points. In Table.1 we report the results for the solution at $t = 1$ with $\tau = 0.001$ (in order to investigate the space accuracy of the proposed algorithm, a very small τ is chosen), a shape parameter of $c = 0.3h$, $(N + 1) \times (N + 1)$ uniform points in Ω . While in Table.2 we use the nonuniform data points with $\{x_i : x_i = \frac{1}{2} \cos \frac{i\pi}{N} + \frac{1}{2}\}_{i=0}^N$ and $\{y_j : y_j = \frac{1}{2} \cos \frac{j\pi}{N} + \frac{1}{2}\}_{j=0}^N$. Figure.1 shows the graphs of numerical and analytical solutions at $t = 100$.

Table.1 The accuracy of the multiquadric quasi-interpolation method collocating with the uniform data points at $t = 1s$

N	Imaginary part		Real part		CPU(s)
	RMS-error	rate	RMS-error	rate	
6	2.83×10^{-3}		3.08×10^{-3}		1
11	6.56×10^{-4}	2.11	6.42×10^{-4}	2.26	3
16	2.37×10^{-4}	2.51	2.55×10^{-4}	2.27	10
21	1.05×10^{-4}	2.83	1.17×10^{-4}	2.71	13
26	5.12×10^{-5}	3.22	5.53×10^{-5}	3.36	18

Table.2 The accuracy of the multiquadric quasi-interpolation method collocating with the nonuniform data points at $t = 1s$

N	Imaginary part		Real part		CPU(s)
	RMS-error	rate	RMS-error	rate	
6	3.12×10^{-3}		3.25×10^{-3}		1
11	6.67×10^{-4}	2.22	6.75×10^{-4}	2.26	4
16	2.69×10^{-4}	2.24	2.71×10^{-4}	2.25	11
21	1.16×10^{-4}	2.92	1.21×10^{-4}	2.80	16
26	5.44×10^{-5}	3.34	5.57×10^{-5}	3.40	19

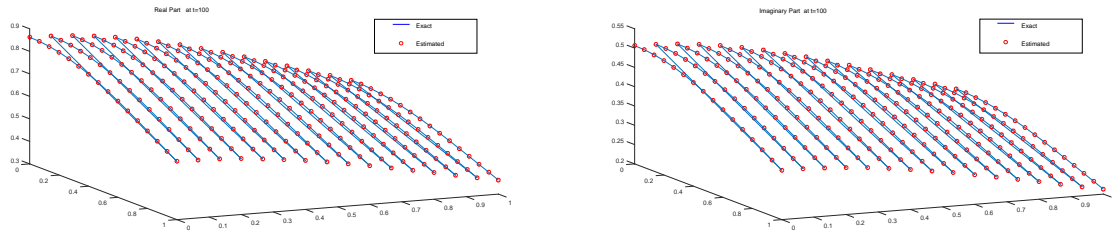


Figure 1: Real and imaginary parts of numerical and analytical solutions at $t = 100$ with $N = 16$ and $c = 0.3h$

Remark 5.2. As Table.1 and Table.2 show, no matter collocating with uniform points and nonuniform data points, the errors decrease rapidly when N gets bigger, which verifies Theorem 4.2. Figure.1 implies the algorithm has a good behavior in long-time simulation.

Example 5.3. Consider E.q (1) again, and set the potential function

$$\rho(x, y) = 1 - \frac{2}{x^2} - \frac{2}{y^2}, \tag{23}$$

the initial condition

$$w(x, y, 0) = x^2y^2, \tag{24}$$

and the boundary conditions

$$\begin{aligned} w(1, y, t) &= y^2 \exp(it), & w(2, y, t) &= 4y^2 \exp(it), \\ w(x, 1, t) &= x^2 \exp(it), & w(x, 2, t) &= 4x^2 \exp(it). \end{aligned} \tag{25}$$

We take the computational domain $\Omega = [1, 2] \times [1, 2]$. The analytical solution of the problem is presented in [20]

$$w(x, y, t) = x^2y^2 \exp(it). \tag{26}$$

It is solved till $t = 100$ too. In Table.3, we give RMS-error and MAX-error for the real and imaginary parts of the solution at some different time points, with $\tau = 0.01$, $N = 21$ and $c = 0.5h$. As shown in Table.3, the RMS-error and MAX-error are also small till $t = 100$, which confirms Theorem 4.2 again. Moreover, cubic multiquadric quasi-interpolation method takes less CPU time (the CPU time is 90s after 10000 time steps), which tells us the method is efficient for solving time-dependent Schrödinger equation.

Table.3 Numerical error of the multiquadric quasi-interpolation method collocating with the uniform data points, $N = 21$

t	Imaginary part		Real part		CPU(s)
	RMS-error	MAX-error	RMS-error	MAX-error	
5	2.03×10^{-5}	4.16×10^{-5}	3.11×10^{-5}	4.66×10^{-5}	5
15	4.24×10^{-5}	4.89×10^{-5}	5.01×10^{-5}	5.70×10^{-5}	8
25	6.98×10^{-5}	7.17×10^{-5}	7.22×10^{-5}	7.43×10^{-5}	20
50	9.09×10^{-5}	9.56×10^{-5}	9.28×10^{-4}	1.03×10^{-4}	37
100	2.06×10^{-4}	3.83×10^{-4}	2.60×10^{-4}	3.13×10^{-4}	90

6. Conclusions

Based on highly accurate radial basis functions quasi-interpolation, this study illustrates a meshless symplectic algorithm for two-dimensional time-dependent Schrödinger equation. The method is based on a combination of cubic multiquadric quasi-interpolation and symplectic integrators. The idea is discretizing the system (6) with cubic multiquadric quasi-interpolation and then integrating the semi-discretized system

by splitting symplectic integrators. The paper also provides a systematic theoretical framework to show the conservativeness and convergence of the proposed method. Numerical results confirm the proposed scheme is easy to implement with the nonuniform knots, high-order accurate, computationally efficient and possesses a long-time tracking capability for solving time-dependent Schrödinger equation.

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