Research Article

Linear Barycentric Rational Method for Solving Schrodinger Equation

Peichen Zhao ¹ and Yongling Cheng ²

¹School of Mathematics and Statistics, Heze University, Heze 274015, China

²College of Science, North China University of Science and Technology, Tangshan 063210, China

Correspondence should be addressed to Yongling Cheng; chengyongling1129@163.com

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A linear barycentric rational collocation method (LBRCM) for solving Schrodinger equation (SDE) is proposed. According to the barycentric interpolation method (BIM) of rational polynomial and Chebyshev polynomial, the matrix form of the collocation method (CM) that is easy to program is obtained. The convergence rate of the LBRCM for solving the Schrodinger equation is proved from the convergence rate of linear barycentric rational interpolation. Finally, a numerical example verifies the correctness of the theoretical analysis.

1. Introduction

Schrodinger equation (SDE) is widely used in atomic physics, nuclear physics and solid physics, quantum mechanics, and so on. SDE is only applicable to nonrelativistic particles with low velocity, and there is no description of particle spin. In this paper, we are concerned with solving the numerical solution of the SDE:

$$i\hbar \frac{\partial \varphi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \varphi(x, t)}{\partial x^2} + V(x, t)\varphi(x, t) + f(x, t), \quad (1)$$

$$\varphi(x, 0) = g_1(x), \varphi(x, t) = g_2(x), x \in (a, b), \quad (2)$$

$$\varphi(a, t) = h_1(t), \varphi(b, t) = h_2(t), \quad 0 < t < T, \quad (3)$$

where $\hbar$ is reduced Planck constant and m denotes quality. In [1], the fractional Schrodinger–Choquard equation with blow-up criteria and instability of normalized standing waves is studied. In [2], the finite-difference time-domain (FDTD) method is studied to solve SDE. In [3], nonlinear magnetic Schrodinger–Poisson type equation is studied. In [4], high-order multiscale discontinuous Galerkin method

for one-dimensional stationary SDEs with oscillating solutions is presented. In [5], sixth-order nonlinear SDE is concerned by factorization formula and an analytical method. In [6], nonlinear SDEs are solved by the iterative method. In [7], the two-dimensional Klein–Gordon SDEs are solved by linear compact alternating direction implicit (CADI) scheme.

For getting the equidistant node of the barycentric formula, Floater [8–10] has proposed a reasonable interpolation method; in particular, equidistant distribution nodes and the quasi-equidistant nodes have high numerical stability and accuracy of interpolation [11, 12]. In [13, 14], the linear barycentric rational collocation method (LBRCM) have been used to solve the integro-differential equation. Wang et al. [15–17] have expanded the application fields of the collocation method (CM), such as initial value problems, plane elasticity problems, and nonlinear problems. LBRCM for solving heat conduction equation and biharmonic equation are studied in [18, 19].

In this paper, a LBRCM for solving SDE is proposed. According to the barycentric interpolation method (BIM) of rational polynomial and Chebyshev polynomial, the matrix form of the collocation method that is easy to program is obtained. The convergence rate of the LBRC method for

solving the telegraph equation is proved from the convergence rate of linear barycentric rational interpolation (LBRI). Finally, a numerical example verifies the correctness of the theoretical analysis.

The remaining of this paper is planned as follows. Section 2 presents the differentiation matrices, CM for SDE, and the matrix form of CM. In Section 3, the convergence rate is proved. Finally, a numerical example verifies the theoretical analysis.

2. Differentiation Matrices of SDE

We partition the interval $[a, b]$ and $[0, T]$ into $a = x_0 < x_1 < \dots < x_m = b$ and $0 = t_0 < t_1 < \dots < t_n = T$ with $h_i = x_i - x_{i-1}$, $i = 0, 1, \dots, m$, and $\tau_j = t_j - t_{j-1}$, $j = 0, 1, \dots, n$, for the uniform partition with $h = (b - a)/m$ and $\tau = T/n$. For $\Omega = [a, b] \times [0, T]$ with (x_i, t_j) , $i = 0, 1, \dots, m$ and $j = 0, 1, \dots, n$ will be the uniform partition.

Consider the barycentric interpolation function (BIF) as

$$\varphi(x_i, t) = \varphi(x_i), \quad i = 0, 1, \dots, m, \quad (4)$$

and its barycentric interpolation approximation is

$$\varphi(x, t) = \sum_{i=0}^m \sum_{j=0}^n r_i(x) r_j(t) \varphi_{ij}, \quad (5)$$

where

$$r_i(x) = \frac{w_i/(x - x_i)}{\sum_{k=0}^m w_k/(x - x_k)}, \quad (6)$$

$$w_i = \sum_{k_1 \in J_i} (-1)^{i-d_1} \prod_{h_1=k_1, h_1 \neq i}^{k_1+d_1} \frac{1}{|x_i - x_{h_1}|},$$

where $J_i = \{k_1 \in I_m: i - d_1 \leq k_1 \leq i\}$, $I_m = \{0, \dots, m - d_1\}$, and

$$r_j(t) = \frac{w_j/(t - t_j)}{\sum_{k=0}^n w_k/(t - t_k)}, w_j = \sum_{k_2 \in J_j} (-1)^{j-d_2} \prod_{h_2=k_2, h_2 \neq j}^{k_2+d_2} \frac{1}{|t_j - t_{h_2}|}, \quad (7)$$

where $J_j = \{k_2 \in I_n: j - d_2 \leq k_2 \leq j\}$, $I_n = \{0, \dots, n - d_2\}$ is the basis function, and φ_{ij} is the value at point $\varphi(x_i, t_j)$. Combining equations (1) and (5), we obtain

$$i(I_m \otimes D^{(1)}) \begin{bmatrix} \varphi_0 \\ \vdots \\ \varphi_m \end{bmatrix} + (C^{(2)} \otimes I_n) \begin{bmatrix} \varphi_0 \\ \vdots \\ \varphi_m \end{bmatrix} - I_n \begin{bmatrix} \varphi_0 \\ \vdots \\ \varphi_m \end{bmatrix} = \begin{bmatrix} f_0 \\ \vdots \\ f_m \end{bmatrix}, \quad (8)$$

and then, we have

$$[iI_m \otimes D^{(1)} + (C^{(2)} \otimes I_n) - I_m \otimes I_n] \Phi = F, \quad (9)$$

and

$$L\Phi = F, \quad (10)$$

where

$$L = iI_m \otimes D^{(1)} + (C^{(2)} \otimes I_n) - I_m \otimes I_n, \quad (11)$$

and

$$D_{ij}^{(1)} = \begin{cases} \frac{w_j/w_i}{t_i - t_j}, & i \neq j, \\ -\sum_{k \neq i} D_{ik}^{(1)}, & i = j, \end{cases} \quad (12)$$

and

$$C_{ij}^{(1)} = \begin{cases} \frac{w_j/w_i}{x_i - x_j}, & i \neq j, \\ -\sum_{k \neq i} C_{ik}^{(1)}, & i = j, \end{cases} \quad (13)$$

$$C_{ij}^{(2)} = \begin{cases} 2C_{ij}^{(1)} \left(D_{ii}^{(1)} - \frac{1}{x_i - x_j} \right), & i \neq j, \\ -\sum_{k \neq i} C_{ik}^{(2)}, & i = j, \end{cases}$$

and $\otimes$ is Kronecher product of matrix. In the following, we define the Kronecher product of matrix $A = (a_{ij})_{m \times n}$ and $B = (b_{ij})_{k \times l}$ as

$$A \otimes B = (a_{ij} b_{kl})_{m \cdot k \times n \cdot l} \quad (14)$$

where

$$a_{ij} B = \begin{bmatrix} a_{ij} b_{11} & a_{ij} b_{12} & \dots & a_{ij} b_{1l} \\ a_{ij} b_{21} & a_{ij} b_{22} & \dots & a_{ij} b_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ a_{ij} b_{k1} & a_{ij} b_{k2} & \dots & a_{ij} b_{kl} \end{bmatrix}. \quad (15)$$

3. Convergence Rate and Error Analysis

The barycentric rational interpolants of function (BRIF) $\phi(x)$ with $r(x)$ and its error convergence rate is

$$e(x) := \varphi(x) - r_n(x) = (x - x_i) \dots \cdot (x - x_{i+d}) \varphi[x_i, x_{i+1}, \dots, x_{i+d}, x], \quad (16)$$

and

$$e(x) = \frac{\sum_{i=0}^{n-d} \lambda_i(x) (\varphi(x) - r_n(x))}{\sum_{i=0}^{n-d} \lambda_i(x)} = \frac{A(x)}{B(x)} = O(h^{d+1}), \quad (17)$$

where

$$A(x) := \sum_{i=0}^{n-d} (-1)^i \varphi[x_i, x_{i+1}, \dots, x_{i+d}, x], \quad (18)$$

and

$$B(x) = \sum_{i=0}^{n-d} \lambda_i(x), \quad (19)$$

where

$$\lambda_i(x) = \frac{(-1)^i}{(x - x_i) \cdots (x - x_{i+d})}. \quad (20)$$

The following Lemma was proved by Jean-Pau Berrut in [11].

Lemma 1 (see [11]), For $e(x)$ defined in (16), we have

$$\begin{cases} |e(x)| \leq Ch^{d+1}, & \varphi \in C^{d+2}[a, b], \\ |e'(x)| \leq Ch^d, & \varphi \in C^{d+3}[a, b], \\ |e''(x)| \leq Ch^{d-1}, & \varphi \in C^{d+4}[a, b], d \geq 1. \end{cases} \quad (21)$$

For the BRIF $\varphi(x, t)$ with $r(x, t)$, we can get the barycentric rational interpolation (BRI):

$$r_n(x, t) = \frac{\sum_{i=0}^m \sum_{j=0}^n w_{ij} / [(x - x_i)(t - t_j)] \varphi_{ij}}{\sum_{i=0}^m \sum_{j=0}^n w_{ij} / (x - x_i)(t - t_j)}, \quad (22)$$

where

$$w_{ij} = \sum_{k_1 \in J_i} \sum_{k_2 \in J_j} (-1)^{i-d_1+j-d_2} \prod_{h_1=k_1, h_1 \neq i}^{k_1+d_1} \frac{1}{|x_i - x_{h_1}|} \prod_{h_2=k_2, h_2 \neq j}^{k_2+d_2} \frac{1}{|t_j - t_{h_2}|}, \quad (23)$$

$$\begin{aligned} \text{and } J_i &= \{k_1 \in I_m: i - d_1 \leq k_1 \leq i\}, I_m = \{0, \dots, m - d_1\}, \\ J_j &= \{k_2 \in I_n: j - d_2 \leq k_2 \leq j\}, I_n = \{0, \dots, n - d_2\}. \end{aligned} \quad (24)$$

By the error term of Newton–Cotes rule for two-dimensional function, we have

$$\begin{aligned} e(x, t) &:= \varphi(x, t) - r(x, t) = \varphi(x, t) - r_n(x, t) \\ &= (x - x_i) \cdots (x - x_{i+d_1}) \varphi[x_i, x_{i+1}, \dots, x_{i+d_1}, x] \\ &\quad + (t - t_j) \cdots (t - t_{j+d_2}) \varphi[t_j, t_{j+1}, \dots, t_{j+d_2}, t]. \end{aligned} \quad (25)$$

The following theorem has been proved in reference by Li in [18].

Theorem 1. For $e(x, t)$ defined in (25) and $\varphi(x, t) \in C^{d_1+2}[a, b] \times C^{d_2+2}[0, T]$, we have

$$|e(x, t)| \leq C(h^{d_1+1} + \tau^{d_2+1}). \quad (26)$$

Corollary 1. For $e(x, t)$ defined in (25),

$$\begin{cases} |e_x(x, t)| \leq C(h^{d_1} + \tau^{d_2+1}), & \varphi(x, t) \in C^{d_1+3}[a, b] \times C^{d_2+2}[0, T], \\ |e_t(x, t)| \leq C(h^{d_1+1} + \tau^{d_2}), & \varphi(x, t) \in C^{d_1+2}[a, b] \times C^{d_2+3}[0, T], \\ |e_{xx}(x, t)| \leq C(h^{d_1-1} + \tau^{d_2+1}), & \varphi(x, t) \in C^{d_1+4}[a, b] \times C^{d_2+2}[0, T], \quad d_1 \geq 1. \end{cases} \quad (27)$$

This corollary can be obtained similarly as Theorem 1, where we omit it.

Let $\varphi(x, t)$ be the solution of (1) and $\varphi(x_m, t_n)$ be the numerical solution; then, we have

$$D\varphi(x_m, t_n) = f(x, t), \quad (28)$$

and

$$\lim_{m, n \rightarrow \infty} D\varphi(x_m, t_n) = f(x, t). \quad (29)$$

According to the above lemma, the following theorem can be proved.

Theorem 2. Let $\varphi(x_m, t_n): D\varphi(x_m, t_n) = f(x, t)$ and $f(x) \in C[a, b]$; we have

$$|\varphi(x, t) - \varphi(x_m, t_n)| \leq C(h^{d_1-1} + \tau^{d_2}). \quad (30)$$

Proof. As

TABLE 1: Convergence rate of equidistant nodes with different $d_1 = 7$ and $t = 2$.

n	$d_2 = 2$		$d_2 = 3$		$d_2 = 4$		$d_2 = 5$	
8×8	$6.1237e-01$		$8.7824e-01$		$7.4433e-01$		$1.1222e+00$	
16×16	$1.7534e-01$	1.8042	$1.0471e-01$	3.0682	$3.0341e-02$	4.6166	$4.9307e-02$	4.5084
32×32	$3.3624e-02$	2.3826	$6.6239e-03$	3.9826	$2.3415e-03$	3.6957	$7.0714e-04$	6.1236
64×64	$6.0006e-03$	2.4863	$4.5724e-04$	3.8567	$1.1369e-04$	4.3643	$1.0298e-05$	6.1016

TABLE 2: Convergence rate of equidistant nodes with different $d_2 = 7$ and $t = 2$.

n	$d_1 = 2$		$d_1 = 3$		$d_1 = 4$		$d_1 = 5$	
8×8	1.6771		1.6716		1.6795		1.6782	
16×16	$1.5313e-02$	6.7751	$1.6007e-02$	6.7064	$1.6217e-02$	6.6944	$1.6091e-02$	6.7045
32×32	$1.4665e-03$	3.3843	$7.1109e-05$	7.8144	$8.4703e-05$	7.5809	$7.2416e-05$	7.7957
64×64	$1.8040e-04$	3.0231	$2.9783e-06$	4.5775	$6.9138e-07$	6.9368	$2.4334e-07$	8.2172

TABLE 3: Convergence rate of quasi-equidistant nodes with different $d_1 = 7$ and $t = 2$.

n	$d_2 = 2$		$d_2 = 3$		$d_2 = 4$		$d_2 = 5$	
8×8	$5.1334e-01$		$3.7631e-01$		$1.1156e-01$		$1.2259e-01$	
16×16	$2.8133e-02$	4.1896	$1.1572e-02$	5.0232	$4.8063e-03$	4.5368	$2.5873e-03$	5.5663
32×32	$2.8913e-03$	3.2825	$5.4800e-04$	4.4003	$1.4573e-04$	5.0435	$2.1084e-05$	6.9392
64×64	$3.2935e-04$	3.1340	$3.0820e-05$	4.1523	$4.1594e-06$	5.1308	$2.5797e-07$	6.3528

TABLE 4: Convergence rate of quasi-equidistant nodes with different $d_2 = 7$ and $t = 2$.

n	$d_1 = 2$		$d_1 = 3$		$d_1 = 4$		$d_1 = 5$	
8×8	$2.8707e-01$		$2.8566e-01$		$2.8297e-01$		$2.8323e-01$	
16×16	$1.0263e-02$	4.8059	$5.7980e-04$	8.9445	$5.0888e-04$	9.1191	$5.0644e-04$	9.1274
32×32	$6.1791e-04$	4.0539	$2.9283e-06$	7.6293	$1.1254e-06$	8.8207	$1.0428e-06$	8.9237
64×64	$7.9511e-05$	2.9582	$1.3835e-06$	1.0817	$1.4398e-06$	—	$4.3847e-06$	—

FIGURE 1: Error estimate of equidistant nodes with $t = 2$, $m = n = 19$, and $d_1 = d_2 = 8$.

$$\begin{aligned}
& D\varphi(x, t) - D\varphi(x_m, t_n) \\
&= i\varphi_t(x, t) - \varphi(x, t) + i\varphi_{xx}(x, t) - [i\varphi_t(x_m, t_n) - \varphi(x_m, t_n) + i\varphi_{xx}(x_m, t_n)] \\
&= i[\varphi_t(x, t) - \varphi_t(x_m, t_n)] + [-\varphi(x, t) + \varphi(x_m, t_n)] + i[\varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n)] \\
&:= iR_1(x, t) + R_2(x, t) + iR_3(x, t),
\end{aligned} \tag{31}$$

FIGURE 2: Error estimate of quasi-equidistant nodes with $t = 2$, $m = n = 19$, and $d_1 = d_2 = 8$.TABLE 5: Convergence rate of equidistant nodes with different $d_1 = 7$ and $t = 1$.

n	$d_2 = 2$		$d_2 = 3$		$d_2 = 4$		$d_2 = 5$	
8×8	$1.7995e-03$		$4.6557e-04$		$1.5050e-04$		$1.4417e-04$	
16×16	$5.5795e-04$	1.6894	$6.5769e-05$	2.8235	$1.1394e-05$	3.7235	$1.5421e-06$	6.5467
32×32	$1.1570e-04$	2.2698	$5.2988e-06$	3.6337	$4.9129e-07$	4.5355	$2.8309e-08$	5.7675
64×64	$2.1482e-05$	2.4291	$4.7396e-07$	3.4828	$2.3083e-08$	4.4117	$5.7039e-10$	5.6332

TABLE 6: Convergence rate of equidistant nodes with different $d_2 = 7$ and $t = 1$.

n	$d_1 = 2$		$d_1 = 3$		$d_1 = 4$		$d_1 = 5$	
8×8	$1.6168e-03$		$5.1505e-04$		$1.7042e-04$		$9.0483e-05$	
16×16	$1.9952e-04$	3.0185	$2.1403e-05$	4.5888	$8.2906e-06$	4.3615	$1.2726e-06$	6.1518
32×32	$2.5369e-05$	2.9754	$1.2042e-06$	4.1516	$2.4768e-07$	5.0649	$1.4595e-08$	6.4461
64×64	$3.4030e-06$	2.8982	$7.6096e-08$	3.9842	$8.0774e-09$	4.9384	$3.4093e-10$	5.4198

TABLE 7: Convergence rate of quasi-equidistant nodes with different $d_1 = 7$ and $t = 1$.

n	$d_2 = 2$		$d_2 = 3$		$d_2 = 4$		$d_2 = 5$	
8×8	$2.1572e-03$		$2.1324e-04$		$2.9588e-05$		$1.1861e-05$	
16×16	$1.7804e-04$	3.5989	$6.5585e-06$	5.0230	$9.5692e-07$	4.9505	$7.8014e-08$	7.2482
32×32	$1.2864e-05$	3.7907	$4.1551e-07$	3.9804	$3.2481e-08$	4.8807	$1.0198e-09$	6.2574
64×64	$1.3676e-06$	3.2336	$2.2121e-08$	4.2314	$8.0913e-09$	2.0051	$2.4516e-08$	-

TABLE 8: Convergence rate of quasi-equidistant nodes with different $d_2 = 7$ and $t = 1$.

n	$d_1 = 2$		$d_1 = 3$		$d_1 = 4$		$d_1 = 5$	
8×8	$2.1937e-03$		$5.6367e-04$		$7.8737e-05$		$6.3534e-06$	
16×16	$1.6769e-04$	3.7094	$3.6712e-06$	7.2625	$5.9101e-07$	7.0577	$8.7629e-08$	6.1800
32×32	$1.4478e-05$	3.5339	$1.2449e-07$	4.8821	$1.2882e-08$	5.5198	$4.5441e-10$	7.5913
64×64	$7.0525e-06$	1.0376	$6.1937e-07$	—	$2.2631e-07$	—	$1.0710e-06$	—

we have

$$\begin{aligned} R_1(x, t) &= \varphi_t(x, t) - \varphi_t(x_m, t_n), \\ R_2(x, t) &= \varphi(x, t) - \varphi(x_m, t_n), \\ R_3(x, t) &= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n). \end{aligned} \quad (32)$$

As, for $R_3(x, t)$, we have

$$\begin{aligned} R_3(x, t) &= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t_n) \\ &= \varphi_{xx}(x, t) - \varphi_{xx}(x_m, t) + \varphi_{xx}(x_m, t) - \varphi_{xx}(x_m, t_n) \\ &= \frac{\sum_{i=0}^{m-d_1} (-1)^i \varphi_{xx}[x_i, x_{i+1}, \dots, x_{i+d_1}, x, t]}{\sum_{i=0}^{m-d_1} \lambda_i(x)} \\ &\quad + \frac{\sum_{j=0}^{n-d_2} (-1)^j \varphi_{xx}[t_j, t_{j+1}, \dots, t_{j+d_2}, x_m, t]}{\sum_{j=0}^{n-d_2} \lambda_j(t)} \\ &= e_{xx}(x, t_n) + e_{xx}(x_m, t_n). \end{aligned} \quad (33)$$

By the corollary, we obtain

$$|R_3(x, t)| \leq |e_{xx}(x, t_n) + e_{xx}(x_m, t_n)| \leq C(h^{d_1+1} + \tau^{d_2+1}). \quad (34)$$

Similarly, for $R_2(x, t)$ and $R_1(x, t)$, we have

$$R_1(x, t) = \varphi_t(x, t) - \varphi_t(x_m, t_n) = e_t(x, t_n) - e_t(x_m, t_n), \quad (35)$$

$$|R_1(x, t)| \leq |e_t(x, t_n) + e_t(x_m, t_n)| \leq C(h^{d_1+1} + \tau^{d_2}), \quad (36)$$

and

$$R_2(x, t) = \beta |\varphi(x, t) - \varphi(x_m, t_n)| \leq C(h^{d_1+1} + \tau^{d_2+1}). \quad (37)$$

Combining the identity equations (31), (34), (36), and (37), the conclusion of theorem is obtained.

4. Numerical Examples

Example 1. The SDE $a = 0, b = 1, t = 2$, and

$$f(x, t) = 0, \quad (38)$$

under condition $g_1(x) = \sqrt{2} \sin(\pi x)$; the analysis solution is

$$\varphi(x, t) = \sqrt{2} e^{-i\pi^2 t/2} \sin(\pi x). \quad (39)$$

Tables 1 and 2 show the errors of the LBRCM for equidistant nodes of space variables and time variables.

Tables 3 and 4 show the errors of the LBRCM for quasi-equidistant nodes of space variables and time variables.

Example 2. The SDE $a = 0, b = 1, t = 1$, and

$$f(x, t) = (x^2 - 2) e^{i\pi^2 t/4} \cos\left(\frac{\pi x}{2}\right) + 2\pi \sin\left(\frac{\pi x}{2}\right), \quad (40)$$

under condition $g_1(x) = x^2 \cos(\pi x/2)$; the analysis solution is

$$\varphi(x, t) = e^{-t} \sin x. \quad (41)$$

In Figures 1 and 2, the error estimate of equidistant and quasi-equidistant nodes with $t = 2, m = n = 19$, and $d_1 = d_2 = 8$ is presented. It can be seen from Figure 2 that the barycentric rational interpolation collocation method has higher accuracy in both quasi-equidistant and equidistant nodes conditions.

Tables 5 and 6 show the errors of the LBRCM for equidistant nodes of space variables and time variables.

Tables 7 and 8 show the errors of the LBRCM for quasi-equidistant nodes of space variables and time variables.

5. Conclusion

In this paper, the LBRCM have been constructed to solve SDE, while the time variable and space variable are obtained at the same time. Numerical solution confirms the theorem analysis.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

This manuscript was written by Peicheng Zhao and Yongling Cheng. Some checks of grammar were given by Yongling Cheng.

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