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High-order split-step exponential methods for solving coupled nonlinear Schrödinger equations

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Abstract. Numerical integration schemes for coupled time-dependent nonlinear Schrödinger equations are examined using exponential splitting step methods. Exponentiation of the nonlinear potential term is reduced to the exponential of a kinetic energy term which can be calculated by fast Fourier transforms. High-order iteration schemes involving a minimum number of product operators are shown to yield highly accurate amplitude and phase. These new splitting methods are shown to be highly efficient both with respect to accuracy and integration time.

1. Introduction

Current research in many areas of physics, such as fluid dynamics, nonlinear optics, plasma physics, etc, requires studies of the solutions of nonlinear Schrödinger equations (NLSEs) [1]. In particular, systems of coupled NLSEs serve as examples of interaction between nonlinear modes [2–3] for which branching bifurcations can occur [4]. Recent developments in the theory of interaction of atoms with intense laser fields requires solutions of Maxwell–Schrödinger equations [5–7]. In the non-resonant case, these can be reduced to coupled NLSEs [1].

Previous studies of NLSEs have focused on simple non-coupled equations for which stable solutions exist. Various discretization schemes have been examined in order to preserve integrability [8] or higher-order conservation laws [9–11]. In particular, split-step exponential methods have been recently examined for the single NLSE [10, 12]. In such a method, one solves separately the linear and nonlinear parts of the NLSE.

The split exponential method of solving coupled linear Schrödinger equations (LSEs) has been very valuable in order to treat time-dependent excitation of quantum systems. Thus, multiphoton transitions in molecules can be treated as systems of coupled LSEs [13, 14], since molecules are intrinsically multilevel systems. Pulse propagation in such multilevel systems leads to new general sine–Gordon equations [15]. We have recently shown that highly accurate solutions of systems of LSEs can be obtained by using high-order split exponential methods [16, 17]. Such exponential splitting methods go back to earlier work by mathematicians (Strang [18], Burstein and Mirin [19] and, recently, Sheng [20]) for solving hyperbolic and parabolic partial differential equations. In particular, as noticed earlier by Burstein and Mirin [19], phase accuracy of the numerical solution is very sensitive to the order of the integration schemes. This has been confirmed in our recent high-order extensions of the exponential methods to coupled LSEs [16, 17].

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In the present paper, we apply the split-step exponential methods to two coupled NLSEs, for which exact solutions are known in the integrable case. We will show that the exponential of the nonlinear potential term can be evaluated as a kinetic energy exponential by means of fast Fourier transforms (FFTs). The accuracy of both amplitude and phase is reported for various orders of accuracy of the integration schemes.

2. Split exponential operator method

We wish to examine solutions of the two coupled NLSEs

$$\begin{aligned} &i\varphi_{1t} + iv_1\varphi_{1,x} + \varphi_{1,xx} + 2(R_{11}|\varphi_1|^2 + R_{12}|\varphi_2|^2)\varphi_1 = 0 \\ &i\varphi_{2t} + iv_2\varphi_{2,x} + \varphi_{2,xx} + 2(R_{21}|\varphi_1|^2 + R_{22}|\varphi_2|^2)\varphi_2 = 0. \end{aligned} \tag{1}$$

Such a system of equations determines the dynamics of envelope waves with components (φ_1, φ_2) and phase velocities (v_1, v_2) in a nonlinear medium with the nonlinearity parameters R [2–4]. Integrability of these coupled equations for particular values of the parameters v and R leads to stable, analytic solutions called *solitons*. We use these exact analytic solutions to evaluate the accuracy of our integration schemes.

We write the coupled equations (1) in the general form

$$i\frac{\partial\varphi}{\partial t} = (A + B)\varphi \tag{2}$$

where A contains all spatial derivatives $(\partial/\partial x, \partial^2/\partial x^2)$ and B contains all potential terms $V(x, t)$, i.e. functions of x and t. For time-independent potentials $B = V(x)$, the exact solution of equation (2) is given by

$$\varphi(x, t + \Delta t) = \exp[\lambda(A + B)]\varphi(x, t) \tag{3}$$

where $\lambda = i\Delta t$. Expressing $\exp[\lambda(A+B)]$ as products of exponentials of A and B generates high-order approximations to equation (3). Various authors have examined high-order product schemes [16–23]. In the case of Schrödinger equations, since the integration time step λ is imaginary, symmetric products automatically conserve the energy L^2 norm of the total function [16, 17, 22–24]. These are called unitary schemes because $S^*(\lambda)S(\lambda) = 1$ at all times. We therefore enumerate below various product formulae which preserve unitarity of the total function $\varphi(x, t)$:

$$S_2(\lambda) = e^{\lambda A}e^{\lambda B} \tag{4}$$

$$S_3(\lambda) = e^{\lambda A/2}e^{\lambda B}e^{\lambda A/2} \tag{5}$$

$$S_5(\lambda) = S_3(\omega\lambda)S_3[(1 - 2\omega)\lambda]S_3(\omega\lambda) \tag{6}$$

where $2\omega^3 + (1 - 2\omega)^3 = 0$,

$$S_7(\lambda) = S_3(\omega_3\lambda)S_3(\omega_2\lambda)S_3(\omega_1\lambda)S_3(\omega_0\lambda)S_3(\omega_1\lambda)S_3(\omega_2\lambda)S_3(\omega_3\lambda) \tag{7}$$

where

$$\omega_3 = 0.784\,513\,610\,477\,560\text{E}0$$
$$\omega_2 = 0.235\,573\,321\,335\,9357\text{E}0$$
$$\omega_1 = -0.117\,767\,998\,418\,87\text{E}1$$
$$\omega_0 = 1 - 2(\omega_1 + \omega_2 + \omega_3)$$

and

$$S_9(\lambda) = S_3(\omega_7\lambda)S_3(\omega_6\lambda)S_3(\omega_5\lambda)S_3(\omega_4\lambda)S_3(\omega_3\lambda)S_3(\omega_2\lambda)S_3(\omega_1\lambda)S_3(\omega_0\lambda)S_3(\omega_1\lambda)$$
$$\times S_3(\omega_2\lambda)S_3(\omega_3\lambda)S_3(\omega_4\lambda)S_3(\omega_5\lambda)S_3(\omega_6\lambda)S_3(\omega_7\lambda) \tag{8}$$

where

$$\omega_7 = 0.629\,030\,650\,210\,433\text{E}0$$
$$\omega_6 = 0.136\,934\,946\,416\,6871\text{E}1$$
$$\omega_5 = -0.106\,458\,714\,789\,183\text{E}1$$
$$\omega_4 = 0.166\,335\,809\,963\,315\text{E}1$$
$$\omega_3 = -0.167\,896\,928\,259\,640\text{E}1$$
$$\omega_2 = -0.155\,946\,803\,821\,447\text{E}1$$
$$\omega_1 = 0.311\,790\,812\,418\,427\text{E}0$$
$$\omega_0 = 1 - 2(\omega_1 + \omega_2 + \omega_3 + \omega_4 + \omega_5 + \omega_6 + \omega_7).$$

The accuracy of each scheme is given by the leading errors:

$$\begin{aligned}\exp[\lambda(A+B)] &= S_2(\lambda) + \mathrm{O}(\lambda^2)\\ &= S_3(\lambda) + \mathrm{O}(\lambda^3)\\ &= S_5(\lambda) + \mathrm{O}(\lambda^5)\\ &= S_7(\lambda) + \mathrm{O}(\lambda^7)\\ &= S_9(\lambda) + \mathrm{O}(\lambda^9).\end{aligned} \tag{9}$$

S_2 has two exponential operators, S_3 has three, S_5 has seven, S_7 has 15, and S_9 has 31. According to Suzuki [22, 23], all the formulae (4)–(8) have a minimal number of exponential operators for the indicated leading errors.

It is clear that all symmetric products (equations (5)–(8)) give leading errors which are of *odd* order with respect to the integration step λ. This is due to the fact that symmetric products maintain unitarity after every integration step as we show now. The product of two such operators or propagators has an nth-order leading error:

$$S_n(\lambda_1)S_n(\lambda_2) = \exp[(A+B)(\lambda_1+\lambda_2)] + C_n(\lambda_1^n + \lambda_2^n) + \cdots \tag{10}$$

where C_n is the coefficient of the order n correction of each propagator S_n, i.e. $C_n\lambda^n$. Thus since $S^*(\lambda) = S(-\lambda)$ for Hermitian operators A, B, then setting $\lambda_1 = -\lambda_2$ and using the fact that the unitarity condition $S^*S = 1$ must hold, we readily obtain that $C_n = 0$ for n *even* and $C_n \neq 0$ for n *odd*. Hence all leading errors involve odd powers of the order only. Thus S_2 (equation (4)), which is not symmetric, has an even-power leading error.

The unitary exponential product representations for $\exp[\lambda(A + B)]$ enumerated above apply to time-independent potential matrices B only. Thus, iteration of equations (3) using the product scheme (5)–(8) allows for efficient numerical integration of time-independent LSEs. In general, it was found that S_7 was the most efficient in producing the highest accuracy for a given integration time for both amplitude and phase of linear solutions $\varphi(x, t)$ of both single and coupled equations. Furthermore, phase accuracy was generally found to be poor at the low-order accuracy level (S_3), so that for proper phase description, higher-accuracy schemes such as S_5 and beyond were found to be essential [16, 17].

For time-dependent potential matrices $B = V(x, t)$, integrations of $\exp[B]$ itself over the time interval need to be addressed consistently [17, 24]. This problem was previously addressed for B linear, i.e. independent of $\varphi(x, t)$. We next treat this problem in detail for the single NLSE in order to illustrate the subtleties involved when B is nonlinear, i.e. it depends on $\varphi(x, t)$.

3. The formal solution of the NLSE and approximations

We consider the single (uncoupled) NLSE

$$i\varphi_t + \varphi_{xx} + q|\varphi|^2 = 0 \tag{11}$$

(φ is a complex-valued function, q a real parameter, $i^2 = -1$), with the initial condition

$$\varphi(x, 0) = g(x) \qquad x \in \mathbb{R}.$$

Equation (11) has the formal solution to third-order accuracy [17]

$$\varphi(t + \Delta t) = \exp\left[i\int_t^{t+\Delta t} (\partial^2/\partial x^2 + q|\varphi|^2)\,dt\right]\varphi(t) + O(\Delta t^3). \tag{12}$$

In [16] and [17], we proved that formulae (5)–(8) can be used to approximate (12) with the same order of leading errors as in (9). By assuming $|\varphi|^2$ is a constant value at t only, this gives low-order approximations which have been used in previous work on NLSEs [10, 12]. We next show how to improve such approximations. Using the middle point formula [25], we have

$$\int_t^{t+\Delta t} |\varphi|^2\,dt = \Delta t|\varphi(t + \Delta t/2)|^2 + O(\Delta t^3). \tag{13}$$

Next we estimate $|\varphi(t + \Delta t/2)|^2$. Using a Taylor expansion, we readily obtain

$$\varphi(t + \Delta t) = \varphi(t) + \Delta t\varphi_t(t) + O(\Delta t^2). \tag{14}$$

Substituting equation (11) into equation (14), we next get

$$\varphi(t + \Delta t/2) = \varphi(t) + i\Delta t(\varphi_{xx}(t) + q|\varphi(t)|^2\varphi(t))/2 + O(\Delta t^2). \tag{15}$$

Using the conjugate to equation (15), we obtain

$$\begin{aligned}|\varphi(t+\Delta t/2)|^2 &= \varphi(t+\Delta t/2)\varphi^*(t+\Delta t/2)\\ &= (\varphi(t)+\mathrm{i}\Delta t\varphi_{xx}(t)/2)(\varphi^*(t)-\mathrm{i}\Delta t\varphi^*_{xx}(t)/2)+\mathrm{O}(\Delta t^2)\\ &= \exp(\mathrm{i}\Delta t\partial^2/\partial x^2/2)\varphi(t)^*\exp(-\mathrm{i}\Delta t\partial^2/\partial x^2/2)\varphi(t)+\mathrm{O}(\Delta t^2)\\ &= |\exp(\mathrm{i}\Delta t\partial^2/\partial x^2/2)\varphi(t)|^2+\mathrm{O}(\Delta t^2). \end{aligned} \tag{16}$$

Thus a high-order estimate of the potential integral is obtained, i.e.

$$\int_t^{t+\Delta t}|\varphi|^2\,\mathrm{d}t = \Delta t|\exp(\mathrm{i}\Delta t\partial^2/\partial x^2/2)\varphi(t)|^2+\mathrm{O}(\Delta t^3). \tag{17}$$

What we have therefore shown is that to $\mathrm{O}(\Delta t^2)$ accuracy the nonlinear potential term in the exact propagation scheme (12) can be replaced by the kinetic energy term only, i.e. it allows us to sum to all orders the gradient corrections to $\varphi(t)$. This should be particularly useful for non-smooth soliton envelopes.

Thus with $A = \partial^2/\partial x^2$, and B equal to equation (17), clearly by further use of the iteration formulae (5)–(8) in equation (17), one can generate formulae of higher-order accuracy. This higher-order procedure can obviously save computation time, since equation (17) is calculated in the previous time step at each iteration and involves single FFTs as shown next. This is a considerable improvement over previous exponential schemes for NLSEs [10, 12].

4. Numerical experiments

In this section, we solve (*a*) the single NLSE and (*b*) two coupled NLSEs. All calculations were performed on an IBM RISC 6000/530 workstation (14 megaflop performance).

The wavefunction is discretized over the x-interval $[a, b]$ and the time is discretized over the t-interval $[0, T]$. The Laplace operator A is calculated by FFT techniques whereas the function $\varphi(x, t)$ occurring in equations (12) and (17) is discretized. Thus, all discrete space points are simultaneously propagated in time according to the iteration schemes based on S_n.

4.1. Single NLSE

Equation (11) has a single soliton solution,

$$\varphi(x,t) = \mathrm{e}^{-\mathrm{i}(2x-3t+\pi/2)}\,\mathrm{sech}(x-4t). \tag{18}$$

We take as the initial condition

$$\varphi(x,0) = \mathrm{e}^{-\mathrm{i}(2x+\pi/2)}\,\mathrm{sech}(x). \tag{19}$$

We use the following parameters: $a = -20$, $b = 240$, $T = 50$, space points $= 1024$.

In table 1, we report numerical results, for S_2, S_3, S_5, S_7 and S_9, where we have defined the mean L^2 errors as L^2 error $= (\Delta x\sum e_i^2)^{1/2}$, where $e_i = |s^n - s^r|$, s^n is a numerical solution and s^r is an exact solution. The errors in amplitude AMP and phase PHA are compared to the exact solution (equation (18)).

Clearly both S_2 and S_9 are not efficient. S_2 converges too slowly, whereas S_9 costs lots of computation time (CPU) since it has too many exponential operators. We have found similar results for time-independent [16] and time-dependent [17] LSEs.

The results in table 1 show that S_7 is the most efficient iteration scheme. Thus, although S_7 comprises 15 exponentials, the high accuracy (error $\mathrm{O}(\Delta t^7)$) at each iteration step makes this scheme economical for high accuracy.

Table 1. Time integration comparisons for the single soliton solution (19) for $T = 50$.

S_n	Δt	AMP error	PHA error	CPU (s)
S_2	0.0125	0.82E-02	0.22	95
	0.005	0.29E-02	0.90E-01	191
	0.0025	0.15E-02	0.44E-01	355
	0.00125	0.77E-03	0.22E-02	771
S_3	0.025	0.22E-02	0.81E-01	82
	0.0125	0.56E-02	0.21E-01	168
	0.005	0.89E-03	0.32E-02	337
	0.0025	0.22E-03	0.82E-03	656
S_5	0.1	0.31E-0.1	0.24	42
	0.05	0.20E-02	0.73E-02	85
	0.025	0.13E-03	0.46E-03	173
	0.0125	0.79E-05	0.31E-04	351
S_7	0.2	0.23E-01	0.48	43
	0.1	0.43E-03	0.72E-02	83
	0.05	0.57E-05	0.54E-04	164
S_9	0.1	0.15	1.85	169
	0.05	0.97E-04	0.91E-02	333
	0.025	0.39E-06	0.60E-05	650

$-20 \leqslant x \leqslant 240$, number of space points = 1024.

4.2. *Two coupled NLSEs*

Next we consider the coupled equations (1) and first apply the transforms

$$\varphi_{1,2} = \phi_{1,2} \exp[\mathrm{i}v_{1,2}^2 t/4 - \mathrm{i}v_{1,2}x/2] \tag{20}$$

to obtain the simpler expressions

$$\begin{aligned} &\mathrm{i}\phi_{1,t} + \phi_{1,xx} + 2(R_{11}|\phi_1|^2 + R_{12}|\phi_2|^2)\phi_1 = 0 \\ &\mathrm{i}\phi_{2,t} + \phi_{2,xx} + 2(R_{21}|\phi_1|^2 + R_{22}|\phi_2|^2)\phi_2 = 0. \end{aligned} \tag{21}$$

These are coupled nonlinear parabolic partial differential equations to which we apply again the high-order split exponential operator schemes developed above. Setting $R_{12} = R_{21} > 0$ allows us to find stationary solutions of equation (18), among which are stationary non-topological solitons [4].

Exact solutions with the single solitons of equations (18) are given by

$$\varphi_1(x,t) = \frac{1}{(a+\mu^2)^{1/2}} \exp[\mathrm{i}\lambda_1 R_{12} t]^* \operatorname{sech}[R_{12}^{1/2}(x - v_1 t)] \tag{22}$$

$$\varphi_2(x,t) = \frac{\mu}{(a+\mu^2)^{1/2}} \exp[\mathrm{i}\lambda_2 R_{12} t - \mathrm{i}\delta R_{12}^{1/2}(x - v_1 t)]^* \operatorname{sech}[R_{12}^{1/2}(x - v_1 t)] \tag{23}$$

where

$$a = R_{11}/R_{12} \qquad c = R_{22}/R_{12} \qquad \mu^2 = (a-1)/(c-1) \qquad \delta = (v_2 - v_2)/R^{1/2} \tag{24}$$

Table 2. Time integration comparisons of coupled NLSEs for $T = 10$.

S_n	Δt	AMP1 error	PHA1 error	AMP2 error	PHA2 error	CPU (s)
S_2	0.01	0.55E-02	0.71	0.31E-02	1.79	64
	0.005	0.25E-02	0.70	0.14E-02	1.45	125
	0.0025	0.13E-02	0.69	0.72E-03	0.91	235
S_3	0.025	0.38E-02	0.53E-01	0.15E-02	0.53E-01	28
	0.01	0.61E-03	0.88E-02	0.24E-03	0.88E-02	68
	0.005	0.16E-03	0.23E-02	0.59E-04	0.21E-02	138
S_5	0.04	0.14E-03	0.24E-02	0.54E-04	0.24E-02	49
	0.02	0.80E-05	0.14E-03	0.32E-05	0.15E-03	98
	0.01	0.55E-06	0.91E-05	0.21E-06	0.91E-05	198
S_7	0.1	0.11E-02	0.43	0.47E-03	0.39	49
	0.05	0.19E-04	0.22E-02	0.74E-05	0.21E-01	96
	0.025	0.28E-06	0.98E-05	0.11E-06	0.99E-05	185

$-25 \leqslant x \leqslant 120$, number of space points = 1024.

Table 3. Time integration comparisons of coupled NLSEs for $T = 100$.

S_n	Δt	AMP1 error	PHA1 error	AMP2 error	PHA2 error	CPU (s)
S_2	0.01	0.22E-0.1	0.93	0.53E-02	1.01	639
	0.005	0.39E-02	0.78	0.18E-02	0.71	1265
	0.0025	0.16E-02	0.41	0.69E-03	0.40	2486
S_3	0.02	0.23E-01	0.13	0.13E-01	0.12	334
	0.01	0.58E-02	0.31E-01	0.30E-02	0.31E-01	660
	0.005	0.14E-02	0.75E-02	0.75E-02	0.77E-02	1302
S_5	0.04	0.13E-02	0.64E-01	0.69E-03	0.64E-01	497
	0.02	0.83E-04	0.47E-03	0.43E-04	0.49E-03	974
	0.01	0.52E-05	0.29E-04	0.27E-05	0.30E-04	1907
S_7	0.04	0.69	2.93	0.38	2.98	1158
	0.033	0.72E-02	1.13	0.42E-02	1.71	1360
	0.031	0.92E-05	0.67E-04	0.48E-05	0.66E-04	1476
	0.025	0.27E-05	0.18E-04	0.13E-05	0.20E-04	1824

$-25 \leqslant x \leqslant 120$, number of space points = 1024.

and λ_1 and λ_2 satisfy the relation $\upsilon = (\lambda_2 - \delta^2/4)\lambda_1$.

Unlike numerical procedures for solving coupled LSEs [17], the diagonalization of the exponential matrices $\exp[B]$ becomes unnecessary, since the Hamiltonian of coupled NLSEs is simpler than coupled LSEs. One can therefore directly use the newly derived expression (17) for $|\phi_1|^2$ and $|\phi_2|^2$ from the last section, which have the accuracy (Δt^2) to propagate

$$\begin{aligned}\phi_1(t+\Delta t) &= \exp\left[\mathrm{i}\int_t^{t+\Delta t}(\partial^2/\partial x^2 + 2R_{11}|\phi_1|^2 + 2R_{12}|\phi_2|^2)\,\mathrm{d}t\right]\phi_1(t)\\ \phi_2(t+\Delta t) &= \exp\left[\mathrm{i}\int_t^{t+\Delta t}(\partial^2/\partial x^2 + 2R_{21}|\phi_1|^2 + 2R_{22}|\phi_2|^2)\,\mathrm{d}t\right]\phi_2(t).\end{aligned} \tag{25}$$

We take $R_{11} = 2$, $R_{12} = 1$, $R_{22} = 4$, $\upsilon_2 = 2$, $\upsilon_2 = 1$, $\lambda_1 = 1$ and $\upsilon = 1$. First we show results with the total time $T = 10$, $a = -25$, $b = 120$, space points = 1024. In table 2,

Table 4. Time integration comparisons of coupled NLSEs for $T = 1000$.

S_n	Δt	AMP1 error	PHA1 error	AMP2 error	PHA2 error	CPU (s)
S_2	0.01	0.90E-01	0.90	0.38E-01	0.99	45312
	0.005	0.22E-01	0.52	0.98E-02	0.54	91764
S_3	0.01	0.63E-01	0.31	0.27E-01	0.29	59609
	0.005	0.15E-01	0.77E-01	0.66E-02	0.79E-01	116742
S_5	0.04	0.15E-01	0.62	0.64E-02	0.60	43511
	0.02	0.88E-03	0.45E-02	0.38E-03	0.43E-02	86583
S_7	0.05	1.26	0.92	0.72	0.98	83033
	0.025	0.45	0.64	0.34	0.59	163955

$-25 \leqslant x \leqslant 1020$, number of space points = 8192.

we present, for S_2, S_3, S_5, S_7, the L^2 errors for the amplitudes AMP1, AMP2 and the phases PHA1, PHA2 of the solutions ϕ_1, ϕ_2 as functions of the computation time in CPU seconds. The table shows that S_5 and S_7 require fewer CPU seconds and give the best results.

We then extend the total time $T = 10$ to $T = 100$ with the other parameters the same as before in order to see how the errors accumulate. This is reported in table 3 for the total time $T = 100$, again for the schemes S_2, S_3, S_5, S_7. In the accuracy range of 10^{-2} to 10^{-3}, S_5 gives the best results.

We next extend the total time to $T = 1000$ and $a = -25$, $b = 1020$, space points = 8192. Results for S_2, S_3, S_5, S_7 are shown in table 4. For this longer propagation, the numerical efficiency of S_5 is superior to other higher-order iteration schemes. Thus, for long integration times, the higher-order scheme S_7 begins to lose efficiency. This is due to the fact that S_7 involves 15 exponential operators as compared to S_5 with seven exponentials and S_3 only three exponentials [17].

In conclusion, we have shown that the high-order split-step exponential methods (equations (5)–(8)), modified by the high-order estimate of the potential integral (equation (17)), can give new highly efficient algorithms for solving coupled time-dependent NLSEs. We are extending these methods to hyperbolic–parabolic equations such as occur in Maxwell–Schrödinger equations [5–7].

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