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LETTER TO THE EDITOR

Symbolic calculation in development of algorithms: split-step methods for the Gross–Pitaevskii equation

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Abstract

We employ symbolic calculation to perform a systematic study of the accuracy of split-step Fourier transform methods for the time-dependent Gross–Pitaevskii equation (GPE). Provided the most recent approximation for the wavefunction is always used in the nonlinear atom–atom interaction energy, every split-step algorithm we have tried has the same-order time stepping error for the nonlinear GPE and for the linear Schrödinger equation.

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By now, a wealth of empirical and theoretical evidence has accumulated to the effect that the time-dependent and independent versions and multi-component generalizations of the Gross–Pitaevskii equation (GPE) give the basic picture of most phenomena taking place in a weakly interacting dilute-gas atomic Bose–Einstein condensate [1–3]. There are hundreds of journal publications involving direct numerical solutions of the time-dependent and time-independent versions of the GPE, and essentially the same nonlinear Schrödinger equation is a central topic in nonlinear optics [4]. A claim of complete classification of the numerical methods for just the time-dependent problems would be pretentious, but the Crank–Nicholson method and various split-step schemes are common themes. For examples, see [5–8] and the references therein.

Curiously, many research groups have their own numerical methods, the algorithms are often ad hoc, and the convergence properties are not always stated (known?) explicitly. Even at the risk of further proliferation of numerical methods, the purpose of this letter is to point out in the context of the GPE that symbolic calculation, in our case using *Mathematica* [9], is a powerful tool for developing numerical algorithms with known and controlled properties.

Our focus is on the analogues of the classic split-step fast Fourier transform method for the Schrödinger equation [10]. The idea is to split the GPE equation into two parts, one of which only refers to the momentum operator and the other only to the position operator. The wavefunction is then evolved alternatingly in momentum space and in real space. Nonetheless, the original split-operator method [10] is formally based on the algebra of linear operators, and does not directly go over to the nonlinear GPE. Here, we study the accuracy of split-operator

methods for the GPE using power series expansions in the time step. While straightforward in principle, with increasing order such expansions rapidly become unwieldy and are only manageable using symbolic calculation. We directly demonstrate that there is a simple and computationally inexpensive way to include the nonlinearity so that the split-operator method works for the GPE and the favourable properties of the original algorithm [10] that have made it a huge success are preserved.

We first recap the case of the time-dependent Schrödinger equation, for the time being in one spatial dimension. For brevity of the notation we use units such that the mass of the particle and the constant $\hbar$ both equal unity. The problem is to integrate

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = [T+V]\psi(x,t), \qquad T \equiv -\frac{1}{2}\frac{\partial^2}{\partial x^2}, \quad V \equiv V(x). \tag{1}$$

A time step from t to $t+h$ is carried out formally as

$$\psi(x,t+h) = \exp[-\mathrm{i}h(T+V)]\psi(x,t). \tag{2}$$

In position representation $\exp(-\mathrm{i}hV)$ means multiplication by the function $\mathrm{e}^{-\mathrm{i}hV(x)}$. Similarly, in momentum representation, after the Fourier transform $\mathcal{F}[\psi(x,t)] \to \tilde{\psi}(p,t)$, the kinetic-energy exponential multiplies the wavefunction $\tilde{\psi}(p,t)$ by $\mathrm{e}^{-\mathrm{i}hp^2/2}$. However, the operators T and V do not commute, so $\exp[-\mathrm{i}h(T+V)] \neq \exp(-\mathrm{i}hV)\exp(-\mathrm{i}hT)$, and the exponential of the sum of the two operators may be difficult to calculate.

Split-step methods attempt to get past the obstacle of noncommuting operators by approximating

$$\mathrm{e}^{\lambda(A+B)} \simeq \mathrm{e}^{\lambda\beta_n B}\mathrm{e}^{\lambda\alpha_n A}\ldots\mathrm{e}^{\lambda\beta_1 B}\mathrm{e}^{\lambda\alpha_1 A}. \tag{3}$$

In the present discussion it does not matter what the linear operators are, so we refer to generic A and B. We need not be dealing with time stepping, thus we write the scalar parameter as λ. In general, though, we regard λ as small in absolute value. The idea of split-operator methods is to pick the coefficients α_i and β_i so that the right-hand side of the split (3) approximates the left-hand side to as high an order in λ as possible.

We seek split-operator methods using symbolic manipulation on *Mathematica* [9]. We first expand the exponentials. Next, in order to compare the left- and right-hand sides of (3), it is expedient (although in principle unnecessary) to put the operators into a standard order, e.g., all operators B to the left and all operators A to the right. This introduces commutators of the operators, as in $AB = BA + [A,B]$, commutators of A and B with the commutators that are also put in a standard order, and products of commutators that are left in the order in which they originally emerge. Order by order in λ and operator product by operator product we then match the terms on the left- and right-hand sides of (3). This gives multivariate polynomial equations in α_i and β_i that *Mathematica* solves easily and completely, up to a point.

The simplest nontrivial split-operator method found in this way is the original split-operator algorithm [10] with three exponentials. The general operator-algebra argument does not distinguish between the operators A and B, and the choices for the nonzero coefficients $\alpha_1 = \alpha_2 = 1/2, \beta_1 = 1$ and $\beta_1 = \beta_2 = 1/2, \alpha_2 = 1$ will both do. We have, for instance, a split-operator representation

$$\exp\left\{-\mathrm{i}h\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)\right]\right\} = \exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)\exp[-\mathrm{i}hV(x)]\exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right) + \mathrm{O}(h^3). \tag{4}$$

Time stepping as in (2) is implemented using the fast Fourier transformation. This algorithm preserves the norm of the wavefunction, which is an issue when standard PDE solvers are applied to the time-dependent Schrödinger equation. The implementation of the exponential of the kinetic energy is a high-order spectral method, and the exponential with the potential energy is done exactly in principle.

Table 1. Nonzero coefficients for minimal split-step methods with real coefficients for the orders of error $O(\lambda^3)$, $O(\lambda^4)$ and $O(\lambda^5)$. The temporary notations are $\Gamma = \sqrt{\frac{16-48\gamma+45\gamma^2-12\gamma^3}{9-12\gamma}}$, $\xi = \frac{1}{2-\sqrt[3]{2}}$ and γ is a real parameter restricted so that Γ remains real.

	$O(\lambda^3)$	$O(\lambda^4)$	$O(\lambda^5)$
α_1	$\frac{1}{2}$	$1-\frac{3\gamma-4/3\mp\Gamma}{2\gamma(\gamma\mp\Gamma)}$	$\frac{1}{2}\xi$
β_1	1	$\frac{\gamma\mp\Gamma}{2}$	ξ
α_2	$\frac{1}{2}$	$\frac{3-4\gamma}{2(2-3\gamma)}$	$\frac{1-\sqrt[3]{2}}{2}\xi$
β_2		$\frac{\gamma\pm\Gamma}{2}$	$-\sqrt[3]{2}\xi$
α_3		$\frac{4/3-\gamma\pm\Gamma}{2\gamma(\gamma\pm\Gamma)}$	$\frac{1-\sqrt[3]{2}}{2}\xi$
β_3		1-γ	ξ
β_4			$\frac{1}{2}\xi$

A five-exponential split exists with an error $O(\lambda^4)$, but the coefficients α_i and β_i are not real and the algorithm is not absolutely stable. There is a whole family of six-exponential splits with a continuous-valued free parameter that all have an error $O(\lambda^4)$, and the coefficients are real for a range of the values of the free parameter. It takes a seven-exponential split to gain another reduction of the error to $O(\lambda^5)$. Higher order methods may also be found. Here we stop at $O(\lambda^5)$, and list in table 1 the coefficients α_i, β_i for all minimal (smallest possible number of exponentials for the given order) split-operator methods with real coefficient. The first publication known to us that gives these coefficients is [11].

On the other hand, the Gross–Pitaevskii equation (GPE) reads in suitable units

$$\mathrm{i}\frac{\partial}{\partial t}\psi = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi|^2\right]\psi, \tag{5}$$

where g (usually > 0) encapsulates the strength of the (usually repulsive) atom–atom interactions. The GPE is nonlinear and as such does not fit the operator algebra framework we have used to derive split-operator methods, but the square of the wavefunction formally behaves like a potential energy. One is tempted to add it to the potential-energy term in the time stepper, as in

$$\psi(x,t+h) \simeq \exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)\exp\{-\mathrm{i}h[V(x)+g|\psi(x,t)|^2]\}\exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)\psi(x,t). \tag{6}$$

Nonetheless, as the wavefunction evolves in time, it is not clear what to insert for the square of the wavefunction in the exponential. In fact, doing the step as in (6) drops an order in accuracy, and the error turns out to be $O(h^2)$.

In an attempt to find a better method we split the split-operator step explicitly,

$$\begin{aligned} &\psi_0 = \psi(x,t), \qquad \psi_1 = \exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)\psi_0, \\ &\psi_2 = \exp\{-\mathrm{i}h[V(x)+g|c_0\psi_0+c_1\psi_1|^2]\}\psi_1, \qquad \psi(x,t+h) = \exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)\psi_2. \end{aligned} \tag{7}$$

At the stage when the square of the wavefunction is needed, there are already two versions of the wavefunction available. The hope is to pick a linear combination of the two with so far unknown real coefficients c_0 and c_1 to regain the error $O(h^3)$.

In order to produce the 'exact' result for comparisons we write

$$\psi(x,t+h) = \psi(x,t) + \frac{h}{1!}\frac{\partial}{\partial t}\psi(x,t) + \frac{h^2}{2!}\frac{\partial^2}{\partial t^2}\psi(x,t) + \cdots. \tag{8}$$

The nth time derivative of the wavefunction is obtained inductively. The GPE itself amounts to

$$\frac{\partial\psi}{\partial t} = -\mathrm{i}\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi|^2\right]\psi. \tag{9}$$

The second time derivative of ψ is found by taking the time derivative of (9), which after an exchange of the order of spatial and time derivatives gives

$$\frac{\partial^2\psi}{\partial t^2} = -\mathrm{i}\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi|^2\right]\frac{\partial\psi}{\partial t} - \mathrm{i}g\psi\left(\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right). \tag{10}$$

But now, using (9) again, all time derivatives may be eliminated from the right-hand side of (10) in favour of spatial derivatives and multiplicative functions. The second time derivative is thereby expressed in terms of spatial derivatives of ψ with orders ranging from 0 to 4. The third, fourth, etc, time derivatives are found similarly in terms of spatial derivatives only. This procedure is executed with a simple *Mathematica* algorithm, where we treat real and imaginary parts of the wavefunction separately. A mechanical implementation is well advised as the terms multiply rapidly with the order of time derivative; after a complete expansion of the spatial derivatives, the real part of the fourth time derivative already has 168 linearly independent terms.

The split-operator algorithm to be tested is implemented by expanding the exponentials into power series of the operators, e.g.,

$$\exp\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right) = 1 + \frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2} + \frac{1}{2!}\left(\frac{\mathrm{i}h}{4}\frac{\partial^2}{\partial x^2}\right)^2 + \cdots, \tag{11}$$

and acting the series-form operators on the initial wavefunction in the sequence prescribed in (3). Such expansions also become extremely tedious when the order in h increases, but an implementation with *Mathematica* is straightforward.

Finally, we compare the exact result and the split-step result. For each order, and for each linearly independent term in a given order, we find the condition that the results coincide. This again gives multivariate polynomial equations for the unknown coefficients c_i, which *Mathematica* solves easily. Our *Mathematica* programs are small and simple, although the desire to keep the run times short (here, at most a couple of hours) has forced us into a few unexpected implementation tricks.

It turns out that the method (7) gives an error $\mathrm{O}(h^3)$ if and only if the coefficients c_0 and c_1 satisfy $c_0 = 0$, $|c_1| = 1$; in other words, if the most recent available wavefunction is used in $g|\psi|^2$.

We have done a similar analysis for all split-operator methods with the coefficients listed in table 1, starting with both the position step and the momentum step. The result was the same every time: if the most recently available version of the wavefunction is used whenever $g|\psi|^2$ is needed alongside the potential energy, the split-operator method for the GPE has the same order of accuracy in the time step as the corresponding split-operator method for the Schrödinger equation. Whether using the most recent update of the wavefunction is also a necessary condition for the same order of time stepping error in the linear and in the nonlinear problem depends on the split-operator method on hand. For instance, if one starts the three-split method with a position step and writes

$$\begin{aligned}&\psi_0 = \psi(x,t), \quad \psi_1 = \exp\{[-\tfrac{1}{2}\mathrm{i}h[V(x) + g|\psi_0|^2]\}\psi_0, \quad \psi_2 = \exp\left(\frac{\mathrm{i}h}{2}\frac{\partial^2}{\partial x^2}\right)\psi_1,\\ &\psi(x,t+h) = \exp\left\{-\tfrac{1}{2}\mathrm{i}h[V(x) + g|c_0\psi_0 + c_1\psi_2 + c_2\psi_2|^2]\right\}\psi_1,\end{aligned} \tag{12}$$

all choices with $c_2 = \pm 1$ and $c_1 = -c_0$ give an error $\mathrm{O}(h^3)$.

In the seven-step $O(h^5)$ method on the order of 20 000 terms must identically cancel to validate our result, so that clearly it is not an accident. We believe that our observation holds for every minimal split-step method, for arbitrary high orders. Also, so far our examples have been in one spatial dimension. The split-operator algorithms for the Schrödinger equation work for arbitrary operators A and B, and go over unchanged to any number of spatial dimensions. Replacing the second derivative in position with a multidimensional Laplacian should not change anything in the underlying structure of the split-operator method or the exact result in the GPE case either. Our best guess is that the split-operator algorithms for the GPE work the same way in more than one spatial dimension. We have verified this explicitly for the $O(h^3)$ three-exponential splits in two and three spatial dimensions.

Our results undoubtedly originate from some algebraic structure possessed by differential operators. Suzuki [12] has, in fact, classified split-operator methods such as (3), and not only for linear operators but also when $e^{\lambda A}$ stands for a member of a Lie group generated by A. Mapping of the initial state to the final state over a time t in Hamiltonian mechanics serves as an example. The GPE may be derived from a classical Hamiltonian, and as such it fits Suzuki's framework. However, there is a (at least practical) difference from the schemes considered by Suzuki [12] and pursued with symplectic integrators [7] that in the presence of the nonlinearity we do not solve the GPE without the spatial derivatives exactly, which means that we do not construct the corresponding operator $e^{\lambda A}$ exactly. Here this added approximation seems to have no ill effect on the accuracy of higher order split-operator methods. Bandrauk and Shen [13] have presented analytical and numerical considerations closely related to ours, but our findings are more general in some respects: their argument does not apply to the six-exponent $O(h^4)$ methods, we include an external potential $V(\mathbf{x})$, and we demonstrate that, as far as the order of the numerical error is concerned, it is immaterial whether one starts the operator splitting with a position or a momentum step.

At any rate, our point is symbolic calculation as a tool, not to what extent our results may or may not be considered new. Understanding the convergence properties of algorithms, such as the scaling of truncation error with spatial or temporal step size, is an integral part of sound computational practice. Traditionally, such understanding arises from pen-and-paper mathematics and/or numerical experiments. We are demonstrating here another mode, brute-force symbolic calculation. For instance, computationally demanding problems involving sets of coupled GPEs are encountered in multi-component condensates, and in atom–molecule coupling. Integrating the GPE and related equations in imaginary time, a frequently employed method to find the ground state for nonlinearly coupled classical fields invites additional interesting and possibly important related questions. Now, given a specific problem, someone whose expertise and interest lie in physics rather than numerical methods could readily investigate the convergence of an algorithm and develop higher order algorithms symbolically.

In conclusion, we promote the use of symbolic calculation, possibly extensive symbolic calculation, as a tool for developing numerical algorithms. In our specific example we have demonstrated that, by using the most recent update as the wavefunction wherever the square of the wavefunction is needed alongside the potential energy, the split-step Fourier transform method goes over from the Schrödinger equation to the Gross–Pitaevskii equation with all of its favourable properties intact.

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