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Fourier-splitting methods for the dynamics of rotating Bose–Einstein condensates

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ABSTRACT

We present a new method to propagate rotating Bose–Einstein condensates subject to explicitly time-dependent trapping potentials. Using algebraic techniques, we combine Magnus expansions and splitting methods to yield any order methods for the multivariate and nonautonomous quadratic part of the Hamiltonian that can be computed using only Fourier transforms at the cost of solving a small system of polynomial equations. The resulting scheme solves the challenging component of the (nonlinear) Hamiltonian and can be combined with optimized splitting methods to yield efficient algorithms for rotating Bose–Einstein condensates. The method is particularly efficient for potentials that can be regarded as perturbed rotating and trapped condensates, e.g., for small nonlinearities, since it retains the near-integrable structure of the problem. For large nonlinearities, the method remains highly efficient if higher order $p > 2$ is sought. Furthermore, we show how it can be adapted to the presence of dissipation terms. Numerical examples illustrate the performance of the scheme.

1. Introduction

The centerpiece of this work is the construction of an efficient geometric integrator for the two-dimensional harmonically trapped rotational Schrödinger equation in atomic units ($\hbar = m = 1$) subject to periodic boundary conditions

$$i\partial_t \psi(\mathbf{r}, t) = H_A(t)\psi(\mathbf{r}, t), \qquad \psi(\mathbf{r}, 0) = \psi_0 \in L^2([-\pi, \pi]^2), \tag{1}$$

with the explicitly time-dependent Hamiltonian

$$H_A(t) = \tfrac{1}{2}\mathbf{p}^T\mathbf{p} + \tfrac{1}{2}\left(\omega_x(t)^2x^2 + \omega_y(t)^2y^2\right) + \Omega L_z,$$

where $\mathbf{r} = (x, y)^T$, $\mathbf{p} = (p_x, p_y)^T$, $L_z = xp_y - yp_x$ denotes the angular momentum operator and $p_k = -i\partial_k$, $k = x, y$. This includes the case of unbounded domains since the solution vanishes up to round-off at sufficiently large spatial intervals due to the harmonic trapping potential. For simplicity of the presentation, we have chosen a simple form of the Hamiltonian (1), but our methodology also applies to virtually all relevant polynomial Hamiltonians of degree ≤ 2 in any dimension with arbitrary time-dependencies and we will show how to extend the presented techniques for more general quadratic and linear time-dependencies which are used to model collisions of atoms and molecules [1,2]. The generalization to three dimensions is straightforward and will be briefly addressed in Section 2.

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The efficient solution of (1) is of paramount importance to the computation of the dynamics of rotating Bose–Einstein condensates as we will see below, and in contrast to previous efforts [3–12], time-dependent (trapping) potentials and nonlinearities can be treated without tempering the algebraic structure of the problem. The presence of such time-dependencies impedes a simple transformation to a rotating system of coordinates which would eliminate the rotation term L_z for autonomous H_A. We want to stress that this is also the reason why we do not discuss methods that are concerned with ground state computations, such as imaginary time propagation or minimizing the energy functional. Nevertheless, these methods are highly relevant in order to obtain suitable initial conditions for the numerical integration.

At any given time t and for *any order* $p > 1$, we show that, for a sufficiently small time-step h, there exist cheaply computable coefficients $f_j(t,h), g_k(t,h), e_l(t,h) \in i\mathbb{R}$ obeying a small system of polynomial equations such that

$$e^{f_0 x^2} e^{f_1 y^2 + g_1 p_x^2 - e_1 y p_x} e^{f_2 x^2 + g_2 p_y^2 + e_2 x p_y} e^{f_3 y^2 + g_3 p_x^2 - e_3 y p_x} = \varphi_{t,t+h}^{H_A} + \mathcal{O}\left(h^{p+1}\right), \tag{2}$$

where $\varphi_{t,t+h}^{H_A}$ denotes the exact flow of (1) from t to $t+h$. By virtue of this decomposition, named $\Phi_{t,t+h}^{[p]}$, the position and moment coordinates are decoupled and can be diagonalized using Fourier transforms. After discretization, only six (one-dimensional) changes from coordinate to momentum space and vice versa per time-step exponents are required. These changes are performed by Fast Fourier Transforms (FFT) and hence suggest the name *Fourier-splitting*. The approximation preserves *unitarity* (and thus the L_2-norm) and *gauge invariance* of the exact solution and hence, it can be considered a geometric integrator in the sense of Ref. [13]. Furthermore, one can associate a time-dependent Hamiltonian with the decomposition which is exactly solved at each step.

The method is particularly successful for perturbed problems of the form

$$H = H_A(t) + \varepsilon B(t, \mathbf{r}, |\psi|), \qquad \varepsilon \ll 1, \tag{3}$$

with a small parameter ε, and some real-valued function B, which includes the Gross–Pitaevskii equation (GPE) for Bose–Einstein condensates as special case. The (nonlinear) Hamiltonian H with $B = g|\psi|^2 + V$ describes the evolution of a rotating Bose–Einstein condensate (BEC) subject to a harmonic (parabolic) trapping potential plus some perturbation εV. After the first experimental realization of BECs [14–16] and the consequently awarded Nobel prize in 2001, continuous attention of numerical analysts [3–6,8–10,12] has been drawn to the solution of the autonomous version of (1), which is obtained by dropping all time-dependencies in the Hamiltonian.

The flow of the perturbation B can be easily computed since B is diagonal in coordinate space and leaves the modulus $|\psi|$ constant, see Lemma 2.1 for details. Using (2), the exact flow can be approximated by Strang's method to

$$\varphi_{h/2}^{\varepsilon\tilde{B}(t+h)} \circ \Phi_{t,t+h}^{[p]} \circ \varphi_{h/2}^{\varepsilon\tilde{B}(t)} = \varphi_{t,t+h}^{H} + \mathcal{O}\left(\varepsilon h^3 + h^{p+1}\right), \tag{4}$$

where the tildes, $\tilde{B}$, indicate frozen (nonlinear) operators, i.e., $\varphi_h^{\tilde{B}(s)}$ is the flow of $i\dot{u}(t) = B(s)u(t)$. The term proportional to h^{p+1} originates from the error in the approximation of the part H_A by the pth order method $\Phi^{[p]}$ (2). Observe that the outer exponentials of (2) are diagonal in coordinate space and no further FFT is necessary to solve the full problem (4). An alternative approach [4,5] splits the system into simultaneously diagonalizable parts $T_x = \frac{1}{2}p_x^2 - \Omega y p_x$, $T_y = \frac{1}{2}p_y^2 + \Omega x p_y$, $W = \frac{1}{2}\left(\omega_x(t)^2 x^2 + \omega_y(t)^2 y^2\right) + \varepsilon B(t)$ and then

$$\varphi_{h/2}^{\tilde{W}(t+h)} \circ \varphi_{h/2}^{T_x} \circ \varphi_h^{T_y} \circ \varphi_{h/2}^{T_x} \circ \varphi_{h/2}^{\tilde{W}(t)} = \varphi_{t,t+h}^{H} + \mathcal{O}\left(h^3\right), \tag{5}$$

which also requires six FFTs but the small factor ε in the error is lost. If the time is frozen in H_A, Laguerre transforms [6,8–10] or a decomposition similar to (2) [3] can be used to advance H_A *without* recovering the small factor and even lose the property $[B,[B,[B,H_A]]] = 0$ which simplifies the design of highly efficient splitting methods [17].

Eventually, the method will be embedded in such a splitting framework that generalizes (4) and by comparing with (5), it becomes clear that the number of flows φ that have to be treated individually is reduced to two which will enable us to use optimized splitting methods from the literature. In consequence, we will see in the numerical experiments that the new procedure is efficient even for non-perturbed settings

$$H = H_A(t) + \frac{1}{\varepsilon}B(t, \mathbf{r}, |\psi|), \qquad \varepsilon \ll 1.$$

The decomposition is built upon earlier works for rotating but autonomous BEC [3] and explicitly time-dependent one-dimensional harmonic oscillators [18], where Fourier-splittings have been used for simpler Hamiltonians.

In the following section, we give a short introduction to some numerical concepts which will culminate in the derivation of our method. As described, the method addresses the solution of the dominant part in the Hamiltonian, i.e., kinetic energy, trapping and rotation, H_A. Its form is closely related to a splitting method, in fact, if the coefficients f, g, e were taken to be

$$f_0 = 0,\ f_1 = \frac{1}{4}\omega_y(t)^2,\ g_1 = \frac{1}{4},\ e_1 = \frac{1}{2}\Omega,\ f_2 = \frac{1}{2}\omega_x(t)^2,\ g_2 = \frac{1}{2},\ e_2 = \Omega,\ f_3 = f_1,\ g_3 = g_1,\ e_3 = e_1,$$

we would recover a second order Strang splitting. We show how to modify these scalar coefficients in order yield an any-order approximation using the same number of exponentials. Once we have established how to solve this part of the