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A Fast Time Splitting Finite Difference Approach to Gross–Pitaevskii Equations

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Abstract. We propose an idea to solve the Gross–Pitaevskii equation for dark structures inside an infinite constant background density $\rho_\infty = |\psi_\infty|^2$, without the introduction of artificial boundary conditions. We map the unbounded physical domain $\mathbb{R}^3$ into the bounded domain $(-1,1)^3$ and discretize the rescaled equation by equispaced 4th-order finite differences. This results in a free boundary approach, which can be solved in time by the Strang splitting method. The linear part is solved by a new, fast approximation of the action of the matrix exponential at machine precision accuracy, while the nonlinear part can be solved exactly. Numerical results confirm existing ones based on the Fourier pseudospectral method and point out some weaknesses of the latter such as the need of a quite large computational domain, and thus a consequent critical computational effort, in order to provide reliable time evolution of the vortical structures, of their reconnections, and of integral quantities like mass, energy, and momentum. The free boundary approach reproduces them correctly, also in finite subdomains, at low computational cost. We show the versatility of this method by carrying out one- and three-dimensional simulations and by using it also in the case of Bose–Einstein condensates, for which $\psi \to 0$ as the spatial variables tend to infinity.

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1 Introduction

The nonlinear (cubic) Schrödinger equation with external potential

$$\mathrm{i}\frac{\partial\psi}{\partial t}(\boldsymbol{x},t)+a\nabla^2\psi(\boldsymbol{x},t)-V(\boldsymbol{x})\psi(\boldsymbol{x},t)+s|\psi(\boldsymbol{x},t)|^2\psi(\boldsymbol{x},t), \quad \boldsymbol{x}\in\mathbb{R}^3, \tag{1.1}$$

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where ψ is the complex wavefunction, $a>0$ and $s\in\mathbb{R}$, is commonly used as a model for the dynamics of Bose–Einstein condensates (BECs, see [3] for a review of the mathematical theory and numerical methods) and of superfluids (see [6,21] for the derivation of such an equation). In both cases, it is also known as Gross–Pitaevskii equation (GPE). From the mathematical point of view, one of the main differences between BECs and superfluid simulations is in the boundary conditions satisfied by the wavefunction ψ. In the first case they are vanishing, that is $\psi\to 0$ as $|\boldsymbol{x}|\to\infty$, whereas for superfluids the interest is in the dynamics of dark structures, such as solitons, vortex lines, and vortex rings, which are objects with a core of (near) zero density $\rho=|\psi|^2$ inside an infinite constant background density ρ_∞. In order to impose the boundary conditions in the former case, the unbounded domain $\mathbb{R}^3$ is usually truncated and homogeneous Dirichlet or periodic boundary conditions are set. Hence, sine or Fourier pseudospectral discretizations in space can be used. In the latter case, common simple techniques are quite artificial and consist in homogeneous Neumann boundary conditions (see [13]) or periodic boundary conditions, after a proper mirroring of the truncated computational domain (see [13, 17, 23]). Even though the domain has to be doubled in the directions lacking periodicity, the pseudospectral Fourier discretization in space is commonly used because it fits well with the time splitting Fourier pseudospectral (TSFP) method which, in the context of BECs, is the method of choice, due to its simplicity, efficiency (thanks to the Fast Fourier Transform), spectral accuracy in space, and the properties of unconditional stability, time reversibility, gauge invariance, and mass preservation (see [3, § 4.1]). Quite recently, it was proposed in [15] a new simple method, called Modulus Square Dirichlet (MSD), for the treatment of boundary conditions in the form

$$\rho_{|b}=\left|\psi_{|b}\right|^2=B,\quad B>0, \tag{1.2}$$

where $\psi_{|b}$ denotes the restriction of ψ at the boundaries of a *bounded* domain and B is the value of the modulus square which must be constant both in space and time at the boundaries. For this reason, MSD boundary conditions cannot be used for straight vortices as their density $\rho=|\psi|^2$ is not constant at boundaries that intersect their cores. Overall, the method introduced in [15] is a Runge–Kutta finite difference scheme of order four both in space and time. Other approaches to the solution of the Gross–Pitaevskii equation with non-vanishing boundary conditions are based on the far field asymptotic behavior (see [4]), or on the imposition of inhomogeneous Dirichlet boundary conditions in a truncated domain (see [26,27]). In this paper we propose another simple way to treat this type of boundary conditions. We are concerned with superfluid simulations, for which the GPE takes the form

$$\psi_t=\frac{\mathrm{i}}{2}\nabla^2\psi+\frac{\mathrm{i}}{2}\left(1-|\psi|^2\right)\psi. \tag{1.3}$$

It is usually understood to have $\rho=|\psi|^2=1$ at infinity (see [6]), although straight vortices are an exception. First of all, we explicitly compute in Section 2 mass, energy and momentum variations over a bounded domain Ω, taking into account the peculiarity of the boundary conditions. In Section 3 we perform a change of variable $\eta(\boldsymbol{y},t)=\psi(\boldsymbol{x},t)$, so as