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Spectral methods for dissipative nonlinear Schrödinger equations

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Abstract

In this technical report we describe an application of spectral methods to numerically solve some nonlinear Schrödinger equations with dissipative terms and carefully study the problem of vortex formation.

Keywords: Bose–Einstein condensation, dissipation, vortex formation, spectral methods

1 Introduction

A Bose–Einstein condensate (BEC) is a state of matter of a dilute gas of interacting bosons confined in an external potential and cooled to temperatures very near to absolute zero. Under such conditions, a large fraction of the bosons occupies the same quantum state and quantum effects become apparent on a macroscopic scale.

A spectacular quantum phenomenon is the formation of quantized vortices when the condensate is stirred into rotation. The mechanism is not yet completely understood and represents an active research field both in physics and in mathematics.

A BEC trapped in an external potential is usually described by a “macroscopic wave function” Ψ obeying the Gross–Pitaevskii (GP) equation. In the 3D frame rotating with the frequency Ω around the Z axis the GP equation reads

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} + V_{\text{rot}} + g |\Psi|^2 - \Omega L_Z \right) \Psi . \quad (1)$$

Here $g = 4\pi\hbar^2 a/m$ (coupling constant) represents the strength of interactions characterized by the s -wave scattering length $a > 0$ and $L_Z = -i\hbar(X\partial_Y - Y\partial_X)$ the angular momentum. The wave function is normalized by the total particle number. We assume that the external harmonic trapping potential has the form

$$V_{\text{trap}}(X, Y, Z) = \frac{1}{2}m [\omega_{\perp}^2 (X^2 + Y^2) + \omega_Z^2 Z^2] ,$$

and that the potential that drives the rotation is

$$V_{\text{rot}}(X, Y, Z) = \frac{1}{2}m\omega_{\perp}^2 (\varepsilon_X X^2 + \varepsilon_Y Y^2) .$$

with the anisotropy parameters $\varepsilon_X \neq \varepsilon_Y$. Under a proper reduction to 2D and normalization, equation (1) can be rewritten (in the laboratory frame)

$$i \frac{\partial \psi}{\partial t} = \left(-\frac{1}{2} \nabla^2 + V + \theta |\psi|^2 \right) \psi . \quad (2)$$

Here V is the trapping and rotating potential defined by

$$V(x, y, t) = \frac{(1 + \varepsilon_x)}{2} (x \cos \Omega t + y \sin \Omega t)^2 + \frac{(1 + \varepsilon_y)}{2} (-x \sin \Omega t + y \cos \Omega t)^2 .$$

2 GPE with extrinsic dissipation

In order to study the vortex formation by numerical experiments, in [6] the following dissipative generalization of (1) was proposed:

$$(i - \gamma) \frac{\partial \psi}{\partial t} = \left[-\frac{1}{2} \nabla^2 + V + \theta |\psi|^2 - \mu + \gamma(x\partial_y - y\partial_x) \right] \psi . \quad (3)$$

This equation somehow models friction between the condensate and the normal cloud: quoting [6, 11], “*the term with γ introduces the dissipation. Although the detailed mechanism of the dissipation is yet to be understood the observation of the vortex lattices implies the presence of dissipation.*” “*When the condensate is grown from a rotating vapor cloud the growth process itself is dissipative, and in the experiments [...] dissipation can arise by transfer of atoms between the thermal cloud and the condensate. [...] A dissipative term arises from collisions between atoms in the thermal cloud trapped by the same potential as the condensate, in which one of the colliding atoms enters the condensate after the collision.*”

One can see that a pure advection term appears. A difficulty with this equation is that, in order to preserve the total number of particles, it is necessary to introduce the ψ -dependent chemical potential μ . A further problem is to understand whether this picture is valid at zero temperature or not.

Equation (3), rewritten in the rotating frame, has been discretized in space by a spectral method, namely Galerkin’s method applied to the decomposition into Hermite functions (cf. [1, 3, 5]). Hermite functions naturally vanish at infinity and, thus, no artificial boundary condition is imposed as usually done in the literature. For the time discretization, an explicit Runge–Kutta method of order four has been used [5]. Since the chemical potential μ depends on ψ , given the solution ψ at a certain time, μ was computed and kept constant for the next time step. The ground state solution (cf. [4]) of the pure Gross–Pitaevskii Equation (i.e., $\gamma = \mu = 0$) was chosen as initial condition. We note that, if the initial condition satisfies the symmetry condition $\psi_0(x, y) = \psi_0(-x, -y)$, then the same is true for the solution $\psi(x, y, t)$, as it can be shown by substituting x with $-x$ and y with $-y$ in equation (3). According to [6], the values for the parameters were $\varepsilon_x = 0.03$, $\varepsilon_y = 0.09$ and $\Omega = 0.7$. The dissipation constant γ was ranging between 0 and 0.03 and the coupling constant θ between 0 and $500/\sqrt{2}$. From our simulations, we can draw the following conclusions:

- If $\gamma = 0$ and the space discretization is fine enough, i.e., a sufficiently large number N ($N \geq 32$) of Hermite functions is used, no vortex appears during the simulation. On the contrary, if a poor space resolution

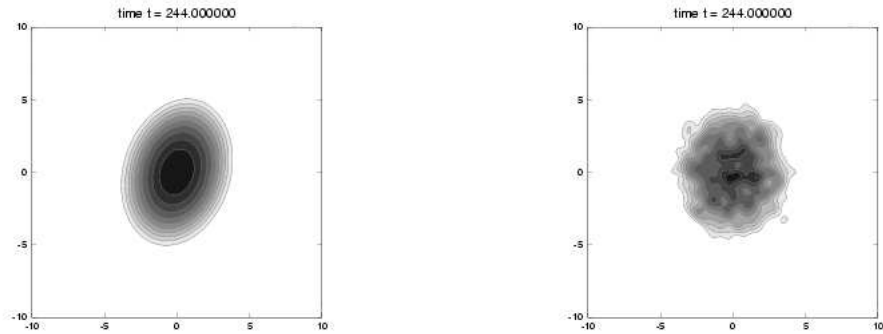


Figure 1: $|\psi|^2$ at time $t = 244$ with $N = 64$ Hermite functions (left) and with $N = 16$ (right).

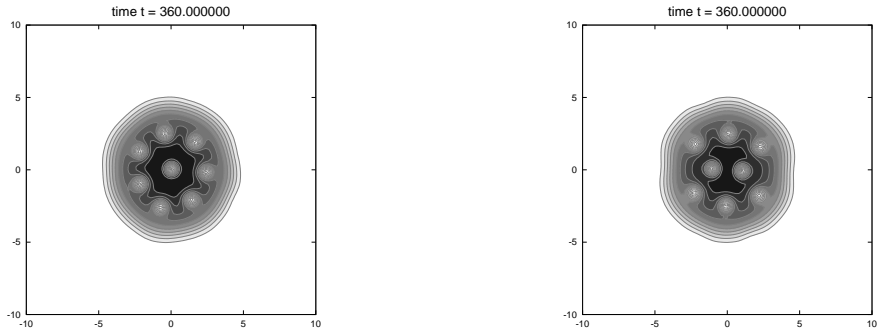


Figure 2: $|\psi|^2$ at time $t = 360$ with the whole set of Hermite basis functions (left) and with only even Hermite basis functions (right).

is used (e.g., $N = 16$), then some artificial (and unstable) vortices appear during the simulation (see Figure 1). This confirms experiments shown in [12].

- If $\theta = 0$ (no cubic term in the equation) no vortex appears during the simulation.
- For $\gamma = 0.03$ and $\theta = 500/\sqrt{2}$ the simulations show results in agreement with those reported in [6], with a final stable lattice of vortices, in which the symmetry $\psi(x, y, t) = \psi(-x, -y, t)$ is broken, due to numerical effects, see Figure 2 (left).
- If only the *even* Hermite functions are used, than the result is a stable and *symmetric* lattice of vortices, see Figure 2 (right), with an energy slightly higher than the energy corresponding to the unsymmetric lattice.

3 Schrödinger equation with vorticity

In this section we consider a new dissipative generalization of the GP equation, recently proposed in [2]:

$$\begin{cases} i \frac{\partial \psi}{\partial t} = \left[\frac{1}{2} (i \nabla + A)^2 + V + \theta |\psi|^2 \right] \psi \\ \frac{\partial A}{\partial t} = \left(b_* - \frac{1}{2} \nabla \right) \times (\nabla \times A) \end{cases} \quad (4)$$

where A is a real vector field, b_* is defined as

$$b_* = \nabla S - A - \frac{1}{2} \nabla \ln \rho ,$$

being S and ρ the phase and the absolute value of ψ , i.e., $\psi = \rho^{\frac{1}{2}} e^{iS}$. If $\theta = 0$, this is the generalization of the Schrödinger equation which arises in Stochastic Quantization with the Stochastic Lagrangian Variational principle as introduced in [7, 9]. Indeed, for $\theta = 0$ and $A = 0$, one gets the usual Schrödinger equation. Moreover, if the Hamiltonian operator $\mathcal{H} = -\frac{1}{2} \nabla^2 + V$ is bounded from below in $L^2(dx)$, then for generic initial data the solution asymptotically relaxes towards a solution where A is equal to zero almost surely with respect to the Lebesgue measure. Thus the set of the solutions to the canonical Schrödinger equation acts as an attracting set. Indeed, denoting by $E(t)$ the energy functional

$$E(t) = \int_{\mathbb{R}^3} \left[\frac{1}{2} |i \nabla \psi + A \psi|^2 + V |\psi|^2 \right] dx$$

the “Energy theorem” proved in [7] claims that, under mild regularity assumptions, the following equality holds

$$\frac{d}{dt} E(t) = -\frac{1}{2} \int_{\mathbb{R}^3} |\nabla \times A|^2 |\psi|^2 dx \leq 0 . \quad (5)$$

If $\theta \neq 0$, equation (4) arises naturally in the stochastic quantization of a system of trapped pair interacting bosons [8]. Notably, the energy theorem still holds in this case, with $E(t)$ replaced by

$$E_\theta(t) = \int_{\mathbb{R}^3} \left[\frac{1}{2} |i \nabla \psi + A \psi|^2 + \frac{\theta}{2} |\psi|^2 + V |\psi|^2 \right] dx$$

while the right side of (5) remains unchanged (see [2]).

Hereafter we assume $\theta = 0$. Since the spectral method based on Hermite functions appeared to be a good candidate for the simulation of vortex dynamics without causing spurious effects at the boundary, we chose to apply it to equation (4). The energy theorem proved in [7, 9] assures that

$$E(t) = \int_{\mathbb{R}^3} \left[\frac{1}{2} |i\nabla\psi + A\psi|^2 + V|\psi|^2 \right] dx < +\infty ,$$

therefore $A\psi = \Gamma \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C})$ and Γ can be naturally expanded into Hermite functions. Equation (4) in the unknowns ψ and Γ reads

$$\left\{ \begin{array}{l} \psi\bar{\psi} \frac{\partial\psi}{\partial t} = -\frac{i}{2}\psi(-\bar{\psi}\nabla^2\psi + |\Gamma|^2 + i\bar{\psi}\nabla \cdot \Gamma + i\bar{\Gamma} \cdot \nabla\psi) - i\psi\bar{\psi}V\psi \\ \psi\bar{\psi} \frac{\partial\Gamma}{\partial t} = -\frac{i}{2}\nabla\bar{\psi} \times (\nabla\psi \times \Gamma) + \frac{1}{2}\nabla \times [\bar{\psi}(\nabla\psi \times \Gamma - \psi\nabla \times \Gamma)] + \\ \bar{\psi} \left[\left(\frac{1}{2}\nabla\psi - \Gamma \right) \times (\nabla \times \Gamma) \right] + \frac{i}{2}(\psi\nabla\bar{\psi} - \bar{\psi}\nabla\psi) \times (\nabla \times \Gamma) + \\ \left[\frac{1}{2}(i-1)\nabla\psi + \Gamma \right] \times (\nabla\psi \times \bar{\Gamma}) + \Gamma\bar{\psi} \frac{\partial\psi}{\partial t} , \end{array} \right. \quad (6)$$

where the first equation was multiplied by $-i\psi$ with the aim of having the same ‘‘mass’’ matrix for both the equations when Galerkin’s method is applied. As in the previous case, we considered the 2D version of the model. Integration by parts was applied to each second order term in the equations. Once the problem was discretized in space, the explicit Runge–Kutta–Fehlberg 4(5) (RKF45) method with variable step size was employed for time integration. It should be noticed that, although the method is explicit, a linear system has to be solved at each stage because of the mass matrix.

If a linear-Gaussian initial condition with radial symmetry, namely

$$\begin{aligned} \psi_0(r) &= \sqrt{\frac{\sigma_0}{\pi}} e^{-\sigma_0 r^2/2} \\ A_0(r) &= -a_0 r \hat{r} + \alpha_0 r \hat{\theta} \end{aligned} \quad (7)$$

is taken for equation (4), then the global solution is still linear-Gaussian with radial symmetry (cf. [10])

$$\begin{aligned} \psi(r, t) &= \sqrt{\frac{\sigma(t)}{\pi}} e^{-\sigma(t)r^2/2} \\ A(r, t) &= -a(t)r\hat{r} + \alpha(t)r\hat{\theta} \end{aligned}$$

where $\sigma(t)$, $a(t)$ and $\alpha(t)$ satisfy

$$\begin{cases} \dot{\sigma}(t) = -2a(t)\sigma(t) & \sigma(0) = \sigma_0 \\ \dot{a}(t) = \sigma^2(t) + \alpha^2(t) - a^2(t) - 1 & a(0) = a_0 \\ \dot{\alpha}(t) = -2(a(t) + \sigma(t))\alpha(t) & \alpha(0) = \alpha_0 \end{cases} \quad (8)$$

and the corresponding energy is

$$E(t) = \frac{1}{2\sigma(t)}(\sigma^2(t) + a^2(t) + \alpha^2(t) + 1) .$$

In order to verify the correct implementation, we chose a linear-Gaussian initial solution (7), with $\Gamma_0(r) = A_0(r)\psi_0(r)$, for the PDEs system (6) and compared the solution with that of the much simpler ODEs system (8). In our first experiments, we successfully reproduced the “breathing” phenomenon [5], i.e., we chose $\sigma_0 = 2$, $a_0 = 0$ and $\alpha_0 = 0$, so that the first equation in system (6) is the linear Schrödinger equation multiplied by $-i\psi\bar{\psi}$ and the second one has the trivial solution $\Gamma(t) \equiv \Gamma_0 = A_0\psi = 0$ for $t \geq 0$. We observed the conservation of the energy and a perfect match between the PDEs and ODEs results. Then we tested a more general linear-Gaussian solution by taking the initial solution (7) with $\sigma_0 = 2$, $a_0 = 1$ and $\alpha_0 = 2$. The

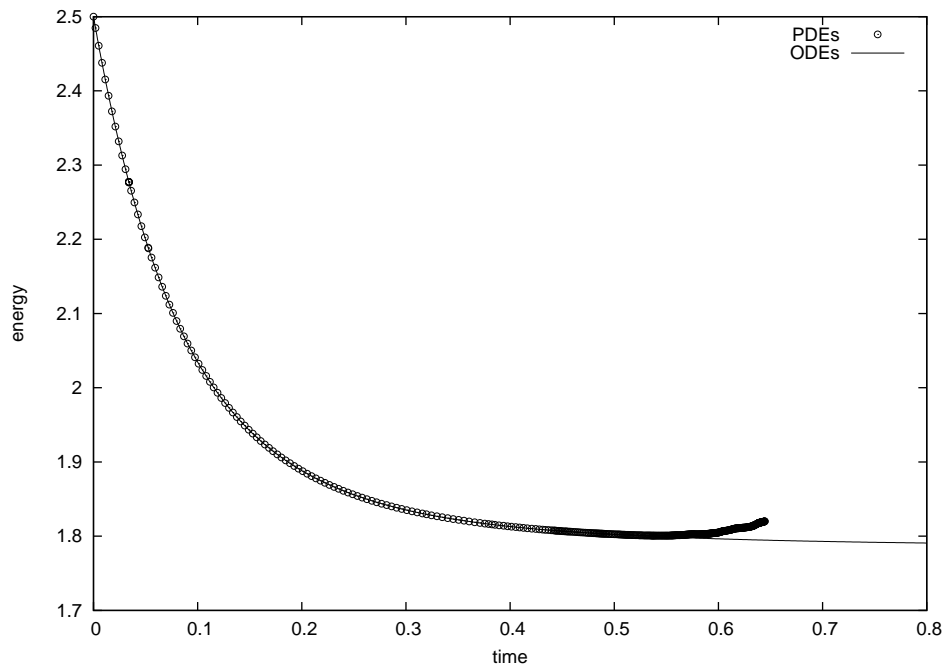


Figure 3: PDEs and ODEs computed energies for $\sigma_0 = 2$, $a_0 = 0$ and $\alpha_0 = 0$

energy comparison is reported in Figure 3. We observe a very good agreement of the computed energies up to about $t = 0.5$. Then, the solution of the PDEs system departs from the correct solution, since the corresponding energy increases instead of decreasing (see (5)). From the numerical point of view, we can see that the RKF45 scheme, in the effort of limiting the error, keeps reducing the time step size, up to useless values. In order to exclude stiffness issues, we also implemented the backward (implicit) Euler method, based on a Newton-like method with a modified Jacobian for the resulting non-linear system, obtaining the same behaviour as for the explicit method. A further investigation of the problem led to the conclusion that the mass matrix is very ill-conditioned (condition numbers of order 10^{22}). However, when $a_0 = \alpha_0 = 0$ and thus $\Gamma(t) \equiv 0$, despite of condition numbers of order 10^{18} , the correct solution is very well captured and maintained in time. This suggests that the errors due to the ill-conditioned mass matrix have a fatal effect only when the second equation plays a non-trivial role in system (6).

Future work may be twofold: either *ad hoc* numerical methods for improving the numerical solution of ill-conditioned systems should be devised, or completely new approaches, such as Monte Carlo methods, should be employed.

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