

NUMERICAL COMPUTATION OF QUANTIZED VORTICES IN THE BOSE-EINSTEIN CONDENSATE

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Abstract. The theoretical analysis of many recent experimental work on a single component Bose-Einstein condensate has been based on the mean-field Gross-Pitaevskii equations. We discuss a few algorithms for solving the Gross-Pitaevskii equations and we use them to compute the quantized vortices in Bose-Einstein condensate.

Key words. vortices, Bose-Einstein condensate, Gross-Pitaevskii equation, numerical schemes, finite element, finite difference, operator-splitting, symplectic and multi-symplectic integration

1. Introduction. Bose-Einstein condensation was first predicted in 1924 by Bose and Einstein. However, the experimental confirmation of Bose-Einstein condensation in atomic gases was only achieved recently in 1995. It was considered as such an important development that the centennial Nobel Prize for Physics has been awarded to the researchers who created this so-called fifth state of matter in the laboratory, Eric Cornell, Wolfgang Ketterle, and Carl Wieman. These researchers were also cited for their early fundamental studies of the properties of the condensates.

One of the early questions asked of BECs were whether they were superfluids. A particularly interesting signature of superfluids is the ability to support quantized circulation. The existence of quantized vortices in the Bose-Einstein condensate has been well documented, see for instance [7, 8, 12, 22, 25, 26, 34, 31, 32, 38]. The vortex cores in the Bose-Einstein condensate are about a thousand times larger than those in the superfluid ^4He so that they can be examined more closely: “*two of the most interesting things in a vortex’s life are its birth and death. Now we can look at both*”, claimed by E. Cornell. In the last few years, there has been a great surge in the studies of quantized vortices in the Bose-Einstein condensate both experimentally and theoretically.

Theoretical studies of vortices in the BEC experiments have often been made in the framework of the nonlinear Gross-Pitaevskii equation, well known for superfluids, but which provides a very good description of Bose-Einstein condensates: it is assumed that the N particles of the gas are condensed in the same state for which the wave function ϕ minimizes the Gross-Pitaevskii energy.

The quantized vortices may be observed in a Bose-Einstein condensate with either optical traps or magnetic traps. For simplicity, we focus on the case of a condensate being placed in a rotating magnetic trap, though much of our discussion can be applied to the case of an optical trap as well. By introducing a rotating frame at the angular velocity $\tilde{\Omega} = \tilde{\Omega}_z$, the trapping potential becomes time independent, and the wave function ϕ minimizes the energy

$$\begin{aligned} \mathcal{E}_{3D}(\phi) = & \int \frac{\hbar^2}{2m} |\nabla \phi|^2 + \frac{m}{2} \sum_{\alpha} \omega_{\alpha}^2 r_{\alpha}^2 |\phi|^2 \\ (1.1) \quad & + \frac{N}{2} g_{3D} |\phi|^4 - \hbar \tilde{\Omega} \cdot (i\phi, \nabla \phi \times \mathbf{x}), \end{aligned}$$

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under the constraint

$$\int |\phi|^2 = 1.$$

Here, for any complex quantities u, v and their complex conjugates $\bar{u}, \bar{v}$, $(u, v) = (u\bar{v} + \bar{u}v)/2$. The terms in the energy correspond to the kinetic energy, the trapping potential energy, the interaction energy and the inertial due to the change of frame.

In the recent works of [3, 4], a rigorous mathematical framework for the study of the energy $\mathcal{E}_{3D}$ and its two dimensional version has been established in the Thomas Fermi limit. The asymptotic energy expansion and limiting behavior of its minimizers are characterized. The study was based on the observation that the Gross-Pitaevskii energy has a striking similarity with the high-kappa, high-field limit of the Ginzburg-Landau free energy used in the modeling of superconductors [10, 16, 19].

Another consequence of this close resemblance is the fact that we were able to construct numerical integration codes for the Gross-Pitaevskii equations by modifying an extensive battery of codes developed over the years for the numerical simulation of vortex dynamics in Ginzburg-Landau models [17, 14, 18, 19].

Similar to [3], we introduce the characteristic length $d = (\hbar/m\omega_x)^{1/2}$ and re-scale the distance by $R = d/\sqrt{\varepsilon}$ where $\varepsilon^2 = \hbar^2/(2Ngm)$. Define the new variable $u(\mathbf{r}) = R\psi(\mathbf{x})$ where $\mathbf{x} = R\mathbf{r}$. Also let $\omega = \omega_x$, $\omega_y = \lambda_y\omega$, $\omega_z = \lambda_z\omega$ with $0 \leq \lambda_y, \lambda_z \leq 1$ and set $\Omega = \tilde{\Omega}/\varepsilon\omega$. The nondimensionalized energy can then be rewritten as:

$$E_0(u) = \int \frac{1}{2} |\nabla u|^2 + \frac{1}{2\varepsilon^2} (x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2) |u|^2 + \frac{1}{4\varepsilon^2} |u|^4 + \Omega \cdot (iu, \nabla u \times \mathbf{r}).$$

Due to the constraint that the integral of $|u|^2$ must equal to 1, it is equivalent to minimize

$$(1.2) \quad E(u) = \int |\nabla u|^2 + 2\Omega \cdot (iu, \nabla u \times \mathbf{r}) + \frac{1}{2\varepsilon^2} |u|^4 - \frac{1}{\varepsilon^2} a(\mathbf{r}) |u|^2$$

where $a(\mathbf{r}) = \alpha - (x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2)$ for some constant α which is chosen so that the integral of $a(\mathbf{r})$ on the ellipsoid $\mathcal{D} = \{a > 0\} = \{x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2 < \alpha\}$ is equal to 1.

Corresponding the physical experiments conducted recently, we may take $\Omega = (0, 0, \Omega)^T$. The form of the energy (1.1) is close to the Ginzburg-Landau free energy functional for superconductors [17] in the high-kappa, high field limit [10, 16]. Indeed, the energy in (1.2) can be rewritten as

$$(1.3) \quad E(u) = \int_{\mathcal{D}} \left\{ |(\nabla - i\mathbf{A})u|^2 + \frac{1}{2\varepsilon^2} (a_\varepsilon(\mathbf{r}) - |u|^2)^2 \right\} + c_\varepsilon$$

where $a_\varepsilon(\mathbf{r}) = a(\mathbf{r}) - \varepsilon^2 \Omega^2 r^2$, $\mathbf{A}$ is a vector potential defined by

$$\mathbf{A} = \begin{pmatrix} y \\ -x \\ 0 \end{pmatrix} \Omega,$$

and the constant c_ε is given by

$$c_\varepsilon = \int_{\mathcal{D}} \left\{ \frac{1}{2\varepsilon^2} (a^2(\mathbf{r}) - a_\varepsilon^2(\mathbf{r})) \right\}.$$

The vector $\mathbf{A}$ may be viewed as a given magnetic vector potential so that the magnetic field plays the role of the angular velocity of the rotation since $\text{curl } \mathbf{A} = 2\Omega$. The trapping potential in the BEC may be linked to the inhomogeneities modeled in the Ginzburg-Landau model to study the pinning mechanism [19].

The unique feature of the Gross-Pitaevskii model is the addition of the constraint on the L^2 norm of u , which would eliminate the trivial state $u = 0$ from consideration. This complication has been worked around in the theoretical analysis developed by [3, 4] in the Thomas-Fermi limit, largely due to the fact that

$$\int_{\mathcal{D}} a(\mathbf{r}) d\mathbf{r} = 1.$$

An interesting signature of the BEC that has attracted a lot of attentions is the nucleation of vortices at high angular velocity. The energy minimizers and critical velocities of vortex nucleation have been studied analytically in [3, 4] in the Thomas-Fermi limit $\varepsilon \rightarrow 0$. The main ingredient of the analysis lies in the decoupling of the energy into three sources: a part coming from the state without vortices, another part from contribution of individual vortices and an additional part produced due to the rotation. In many of the experiments, ε ranges in $10^{-3} \sim 10^{-2}$. We have carried out numerical simulations that produced detailed bifurcation diagrams which confirmed the theoretical analysis for ε in these ranges.

We now present a number of numerical algorithms that are useful in the study of energy minimizers of the Gross-Pitaevskii energy as well as their dynamical properties.

2. The model equations. We begin by describe the differential equations associated with the minimizers of the Gross-Pitaevskii energy as well as the time-dependent G-P equations.

2.1. The steady state equation. The minimizers of the G-P energy satisfies the equation:

$$(2.1) \quad -(\nabla - i\mathbf{A})^2 u + \frac{1}{\varepsilon^2} |u|^2 u - \frac{a_\varepsilon(\mathbf{r})}{\varepsilon^2} u = \mu_\varepsilon(u) u \quad \text{in } \mathcal{D}$$

where $\mu_\varepsilon(u)$ is a constant multiplier corresponding to the constraint

$$\int_{\mathcal{D}} |u|^2 = 1.$$

One may impose the boundary condition $u = 0$ since no particle is allowed to go outside the trap. One may also elect to apply a natural variational boundary condition that will alter very little the behavior of the solution if the computation domain is chosen to be slightly larger than $\mathcal{D}$.

2.2. The time-dependent Gross-Pitaevskii equation. The dynamics of the BEC may be modeled by the time-dependent G-P equation:

$$(2.2) \quad i \frac{\partial u}{\partial t} - (\nabla - i\mathbf{A})^2 u + \frac{1}{\varepsilon^2} |u|^2 u - \frac{a_\varepsilon(\mathbf{r})}{\varepsilon^2} u = 0$$

in $\mathcal{D}$ with initial condition $u(\mathbf{r}, 0) = u_0(\mathbf{r})$ in $\mathcal{D}$ and boundary condition $u = 0$ or $(\nabla - i\mathbf{A})u \cdot \mathbf{n} = 0$ on $\partial\mathcal{D}$. The constraint $\int_{\mathcal{D}} |u|^2 = 1$ is automatically preserved at all time and the energy remains constant as well.

2.3. Evolution in the imaginary time. To numerically compute the minimizers of (1.2), we consider the time-dependent equation in the imaginary time:

$$(2.3) \quad \frac{\partial u}{\partial t} - (\nabla - i\mathbf{A})^2 u + \frac{1}{\varepsilon^2} |u|^2 u - \frac{a_\varepsilon(\mathbf{r})}{\varepsilon^2} u = \mu_\varepsilon(u) u$$

in $\mathcal{D}$ with initial condition $u(\mathbf{r}, 0) = u_0(\mathbf{r})$ in $\mathcal{D}$ and boundary condition $u = 0$ on $\partial\mathcal{D}$. $\mu_\varepsilon(u)$ again denotes the Lagrange multiplier. If u_0 satisfies the constraint $\|u_0\| = 1$, then we may determine $\mu_\varepsilon(u)$ by

$$\mu_\varepsilon(u) = \int_{\mathcal{D}} \left\{ |(\nabla - i\mathbf{A}) u|^2 + \frac{1}{\varepsilon^2} |u|^4 - \frac{a_\varepsilon(\mathbf{r})}{\varepsilon^2} |u|^2 \right\} d\mathcal{D},$$

In [3], discussion on the existence and uniqueness of the weak solution has been given. The long time asymptotic behavior may also be examined using techniques similar to that in [30].

2.4. The Thomas-Fermi regime. In the experimental setting, ε often takes small value, thus, analytical studies of solutions of the Gross-Pitaeskkii equation may be made in the $\varepsilon \rightarrow 0$ limit, that is, in the so-called Thomas-Fermi regime.

As an illustration, for the two dimensional version of the energy, a renormalized energy has been derived in [3] based on the asymptotic behavior as $\varepsilon \rightarrow 0$. It was shown that the energetically favorable locations of the vortices $\{(x_i, y_i)\}$ of a n -vortex minimizer of the energy is determined by minimizing

$$\sum_{i \neq j} \log \left(|x_i - x_j|^2 + \frac{|y_i - y_j|^2}{\lambda^2} \right) - \alpha \sum_i (x_i^2 + y_i^2).$$

where α is a given positive constant and λ is the aspect ratio of two dimensionall harmonic magnetic trap.

Away from the Thomas-Fermi regime, most of the existing studies rely on some results of numerical simulations. It is thus of great interests to discuss various types of numerical schemes applicable to the solution of the Gross-Pitaevskii equations.

3. Numerical schemes. There are various ways to solve the time-dependent Gross-Pitaevskii equations, see for example [8] or [22]. Here, we outline several possible numerical schemes.

To solve the steady state equation and to integrate the time dependent equation in imaginary time, we take the advantage of the similarity with the solution of the high-kappa high-field time-dependent Ginzburg-Landau equations [16], and adapt a code developed in [16, 17, 18, 19]. For integration in real time, the Hamiltonian structure of the G-P equation can be utilized.

3.1. Spatial discretization. For spatial discretization, there are several possibilities, including finite element approximation [17, 19], gauge invariant difference approximation [15] and finite volume approximations [20].

For instance, for the gauge invariant difference approximation, let h be the spatial mesh size, j, k be the grid indices in the $x - y$ plane, one may introduce the **link variables** $\Phi_{j+1/2, k} = \exp(-i\mathbf{A}_{j+1/2, k}^1 h)$, $\Phi_{j, k+1/2} = \exp(-i\mathbf{A}_{j+1/2, k}^2 h)$. Then, we may use the approximation

$$(\nabla - i\mathbf{A})^2 u_{jkl} \approx \bar{\Phi}_{j-1/2, j} \frac{u_{(j-1)kl} - u_{jkl}}{h^2} + \Phi_{j+1/2, k} \frac{u_{(j+1)kl} - u_{jkl}}{h^2}$$

$$\begin{aligned}
& + \bar{\Phi}_{j,k-1/2} \frac{u_{j(k-1)l} - u_{jkl}}{h^2} + \Phi_{j+1/2,k} \frac{u_{j(k+1)l} - u_{jkl}}{h^2} \\
& + \frac{u_{jk(l+1)} + u_{jk(l-1)} - 2u_{jkl}}{h^2}.
\end{aligned}$$

Such a spatial difference scheme conveniently preserves the symmetry of the resulting discrete operator. Based on this, one may easily get a semi-discrete in space scheme for both the steady state and the time-dependent G-P equation.

For unstructured triangular grids, a finite volume method can be obtained as a generalization of the above technique [20].

3.2. Solving the equation in imaginary time. For time-discretization, it is important to get asymptotically stable schemes for large time which in general requiring the use of implicit schemes with no limitations on the time step size.

Let $\{u_n\}$ be approximate solutions of $\{u(t_n)\}$ at discrete time $\{t_n\}$ with time-step $\Delta t_n = t_n - t_{n-1}$. In [3], two time-discretization schemes have been introduced:

A first order backward-Euler in time discretization:. Given u_{n-1} , we solve for u^* :

$$\begin{aligned}
(3.1) \quad & \frac{u^* - u_{n-1}}{\Delta t_n} - (\nabla - i\mathbf{A})^2 u^* - \mu(u_{n-1})u^* \\
& + \frac{1}{\varepsilon^2} |u^*|^2 u^* - \frac{1}{\varepsilon^2} a_\varepsilon u^* = 0
\end{aligned}$$

Then, we apply the projection $u_n = u^* / \|u^*\|$. Both the backward Euler step and the projection step gives only first order in time accuracy.

A norm-preserving, energy-decreasing second order scheme. For any u, v , let $f(u, v) = (|u|^2 + |v|^2)(u + v)/2$. Given u_{n-1} , we first solve for u^* :

$$\begin{aligned}
(3.2) \quad & \frac{2(u^* - u_{n-1})}{\Delta t_n} - (\nabla - i\mathbf{A})^2 u^* - \nu(u^*)u^* \\
& + \frac{1}{\varepsilon^2} f(2u^* - u_{n-1}, u_{n-1}) - \frac{1}{\varepsilon^2} a_\varepsilon u^* = 0
\end{aligned}$$

where $\nu(u^*)$ is given by

$$\begin{aligned}
\nu(u^*) \int_{\mathcal{D}} |u^*|^2 &= \int_{\mathcal{D}} \left\{ |(\nabla - i\mathbf{A}) u^*|^2 \right\} \\
&+ \int \left\{ \frac{1}{\varepsilon^2} f(2u^* - u_{n-1}, u_{n-1}) \bar{u}^* - \frac{a_\varepsilon}{\varepsilon^2} |u^*|^2 \right\}.
\end{aligned}$$

Then, $u_n = 2u^* - u_{n-1}$.

During the discrete time evolution, the energy decreases while the norm is preserved. This discrete scheme is second order in time and unconditionally stable. It captures some essential features of the continuous dynamic system, making it suitable for long time integration and for studies of meta-stabilities of the solutions.

3.3. Solving the equation in real time. When one is interested in the dynamics of vortices in real time, the time-dependent Gross-Pitaevskii equation needs to be solved efficiently and accurately in time. We now present two general approaches: one that uses time-splitting (operator splitting) techniques and one that preserves certain intrinsic properties of the equation.

3.4. Time-splitting scheme. Similar to the study on many evolutionary equations that include the time dependent Schrodinger equations, one can adopt a time or operator-splitting scheme that has been discussed by many authors [29]:

Given u_{n-1} , one may proceed by alternating solve the following subproblems:

1. For each position $\mathbf{r}$, solve the ODE:

$$iu_t = (a_\varepsilon(\mathbf{r}) - |u|^2)u.$$

2. For each (x, y) , solve the linear equation in time and z :

$$iu_t = \partial_{zz}u \quad \text{in} \quad [t, t + \lambda_2] .$$

3. For each z , solve the linear equation in time and x, y :

$$iu_t = (\nabla - i\mathbf{A})^2 u , \quad \text{in} \quad [t, t + \lambda_3] .$$

Here, λ_i 's may be viewed as fractional time-steps. The three subproblems may be solved alternatingly and repeatedly.

Note that an explicit solution of the ODE systems in the step 1 is given by

$$u(\mathbf{r}, t + \lambda_1) = u(\mathbf{r}, t) \exp \left(i\lambda_1(|u(\mathbf{r}, t)|^2 - a_\varepsilon(\mathbf{r}))/\varepsilon^2 \right) .$$

Steps 2 and 3 can be further discretized using an Euler or other time integration schemes to preserve some properties of the original equation and to ensure better stability. For instance, a Crank-Nicolson scheme for steps 2 and 3 would preserve the L^2 norm of the solution which is a property enjoyed by the time-dependent G-P equation.

The differential operators involved in those two steps commute with each other, a key property to allow construction of high order approximation schemes. Due to the linearity of the problems involved in those two steps, fast solvers may be applied. We refer to [5, 28, 36] for further discussions on the operator splitting strategies as well as applications to time-dependent Schrodinger equations.

3.5. Symplectic and multi-symplectic scheme. The time-dependent Gross-Pitaevskii equation is a Hamiltonian system which enjoys both the symplectic and multi-symplectic properties. Thus, it is desirable to use discrete schemes that preserve the symplectic [11] and multi-symplectic structures [6, 11, 33].

Symplectic integrator. : one may use a standard practice to rewrite the time-dependent G-P equation as a Hamiltonian system. Let $u = p + iq$ where p, q are the real and imaginary part of u , and let $E(p, q)$ denote $E(u)$ as in the equation (1.2), then we have

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = J \begin{pmatrix} \partial/\partial p \\ \partial/\partial q \end{pmatrix} E(p, q) \quad \text{where} \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} .$$

For $Z_t = J\nabla_Z E(Z)$, the following second order symplectic schemes may be applied [11]:

$$Z_n - Z_{n-1} = \Delta t J \nabla_Z E \left(\frac{Z_n + Z_{n-1}}{2} \right) ,$$

and a fourth order R-K symplectic integrator is given by

$$\begin{aligned} K_1 &= Z_{n-1} + \frac{\Delta t}{12} J \left(3\nabla_Z E(K_1) + (3 - 2\sqrt{3})E(K_2) \right) , \\ K_2 &= Z_{n-1} + \frac{\Delta t}{12} J \left((3 + 2\sqrt{3})\nabla_Z E(K_1) + 3E(K_2) \right) , \end{aligned}$$

with

$$Z_n - Z_{n-1} = \frac{\Delta t}{2} J (\nabla_Z E(K_1) + \nabla_Z E(K_2)) .$$

Multi-symplectic integrator. : More recently, multi-symplectic schemes for integrating Hamiltonian systems of nonlinear PDEs have received much attention [6, 11, 33]. The time-dependent G-P equation also possesses a multi-symplectic structure, namely, let $Z = (p, q, \mathbf{v}, \mathbf{w})$ with $\mathbf{v} = \nabla p - \mathbf{A}q$, $\mathbf{w} = \nabla q + \mathbf{A}p$, and

$$S(Z) = \frac{1}{2}(|\mathbf{v}|^2 + |\mathbf{w}|^2) + \mathbf{A} \cdot \mathbf{v}q - \mathbf{A} \cdot \mathbf{w}p + \frac{1}{4}(a(\mathbf{r}) - |p|^2 - |q|^2)^2 .$$

then, the G-P equation can be rewritten as a multi-symplectic Hamiltonian system:

$$(3.3) \quad M \frac{\partial}{\partial t} Z + K_1 \frac{\partial}{\partial x} Z + K_2 \frac{\partial}{\partial y} Z + K_3 \frac{\partial}{\partial z} Z = \nabla_Z S(Z) ,$$

where $\nabla_Z S(Z)$ denotes the gradient of the function $S = S(Z)$ with respect to the variable Z and

$$M = \begin{pmatrix} J & \mathbf{O} \\ \mathbf{O} & \mathbf{O}_{6 \times 6} \end{pmatrix} ,$$

$$K_1 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} ,$$

$$K_2 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} ,$$

and

$$K_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} .$$

The system (3.3) has a multi-symplectic conservation law:

$$\frac{\partial}{\partial t}(-dp \wedge dq) + \nabla \cdot (dp \wedge d\mathbf{v} + dq \wedge d\mathbf{w}) = 0 ,$$

as well as the local energy conservation law:

$$\frac{\partial}{\partial t} \left[S - \frac{1}{2} (ZK_1Z_x + ZK_2Z_y + ZK_3Z_z) \right] + \nabla \cdot Z \left(\sum_{j=1}^3 K_j \right) Z_t = 0 .$$

Giving a uniform Cartesian grid, let Z_c denote the center average of the Z on the eight vertices, Z_{fx+} and Z_{fx-} be the averages of Z on the four vertices in each face in the x -direction. $Z_{fy\pm}$ and $Z_{fz\pm}$ follow similar convention. Let $Z^{n+1/2}$ be the averages of Z^n and Z^{n+1} at two consecutive time steps. Then based on the approach used in [27], the following difference scheme preserves the multi-symplectic property in the discrete sense:

$$\begin{aligned} M \frac{Z_c^{n+1} - Z_c^n}{\Delta t} + K_1 \frac{Z_{fx+}^{n+1/2} - Z_{fx-}^{n+1/2}}{\Delta x} + K_2 \frac{Z_{fy+}^{n+1/2} - Z_{fy-}^{n+1/2}}{\Delta y} \\ + K_3 \frac{Z_{fz+}^{n+1/2} - Z_{fz-}^{n+1/2}}{\Delta y} = \nabla_Z S(Z_c^{n+1/2}) . \end{aligned}$$

Developing efficient iterative schemes for the solution of the above difference approximation will be an immediate need to make the multi-symplectic integrator effective for multi-dimensional PDEs. For instance, it has been suggested in [11, 27] that if the nonlinear terms on the right hand side is completely lagged behind, the resulting linear systems at each iteration would share the same coefficient matrix for all iteration and all time steps. The coefficient matrix is sparse, but not symmetric. Direct calculation of the inverse has been used in problems with only one spatial dimension, though in higher dimensional case, memory requirement will constrain such a strategy. Still, an efficient fast solver may be feasible in higher space dimensions.

One may similarly develop spectral or pseudospectral spatial discretization in settings where a periodic boundary condition is applicable.

3.6. Some numerical examples. The recent experimental works have produced vortices ranging from a few to a few hundred. In figure 1, a two-dimensional simulation of a minimizer of the G-P energy was given along with an experimental picture produced by the MIT group (http://cua.mit.edu/ketterle_group/home.htm). Here, $\varepsilon = 10^{-2}$ and we have used a symmetric trap, i.e., a trap with $\lambda_y = 1$, the angular velocity was taken to be $\Omega = 150$. The initial condition is given to be a vortex free state which exhibits a parabolic profile.

Other numerical solutions including those for anisotropic traps have been reported in [3]. One of the important issues remain to be studied further is related to spontaneous nucleation of the vortices and the dynamic and thermodynamic stability of the vortex solution. This can be facilitated by rigorous mathematical analysis as well as extensive numerical simulations.

4. Conclusion. We have presented some numerical integration schemes for the solution of the Gross-Pitaevskii equations. They are applicable to various forms of the equations, thus allow us to numerical investigate many model equations closely related to physical experiments that are currently underway. The numerical simulations will

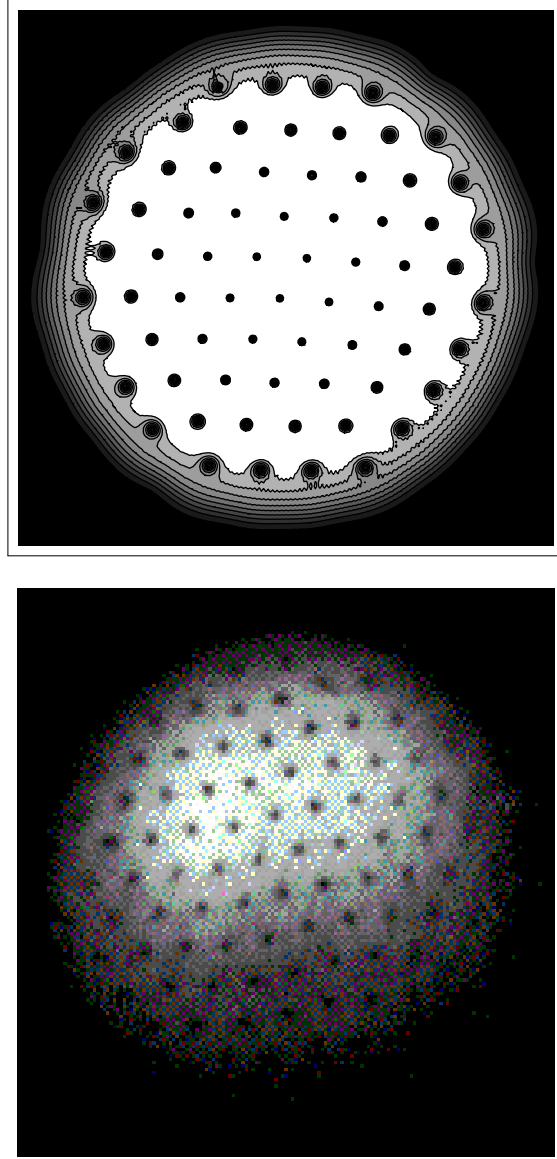


FIG. 3.1. *Vortex solutions. Top: contour plots of $|u|$ at $\Omega = 155$. Bottom: MIT experiments*

be conducted in cooperation with physicists so to gain further insight on the properties of the Bose-Einstein condensate. We expect to report more of our findings in future publications.

One naturally looks beyond the recent exciting scientific understanding of the Bose-Einstein to seek for technological application. We end the paper by quoting the press release of the Royal Swedish Academy of Sciences: “*It is interesting to speculate on areas for the application of BEC. The new control of matter which this technology involves is going to bring revolutionary applications in such fields as precision mea-*

surement and nanotechnology". No doubt that numerical simulation will be becoming a useful tool in the future development.

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