

Timecrystalline vorticity and anyonic exchange in a cold atom Bose-Einstein condensate

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Quantum vortices are the principal excitations in many macroscopic quantum systems, including superfluids and cold atom Bose-Einstein condensates. They are characterized by a quantized phase circulation of the wave function around a vortex core. Here we employ the Gross-Pitaevskii equation to investigate the structure of minimum energy vortices in cold atom Bose-Einstein condensates, in a nonrotating axially symmetric harmonic trap. For a generic value of the angular momentum along the symmetry axis, the energy minima are eccentric vortices. We find that the vortices precess around the center of the trap uniformly, in a timecrystalline fashion. Furthermore, we demonstrate that when two identical vortices exchange their position, the wave function acquires a phase with an anyonic character. Our results reveal that quantum vortices have an unexpectedly rich phenomenology, suggestive of applications to emerging subjects from quantum computation to simulation and information processing.

Bose-Einstein condensate is a widely investigated realization of a coherent macroscopic quantum state. In particular, dilute condensates of trapped ultra-cold atoms have unique quantum features that facilitate a high level of experimental control [1–3]. Various realizations are studied vigorously, both in earth-bound and in earth-orbiting laboratories [4]. Among the goals is the development of ultra-sensitive sensors and detectors [5], and the properties of cold atom condensates are also employed as a platform for quantum computation and simulation [6].

Quantum vortices are the principal topological excitations in a cold atom Bose-Einstein condensate [7–10]. A vortex is characterized by an integer valued circulation

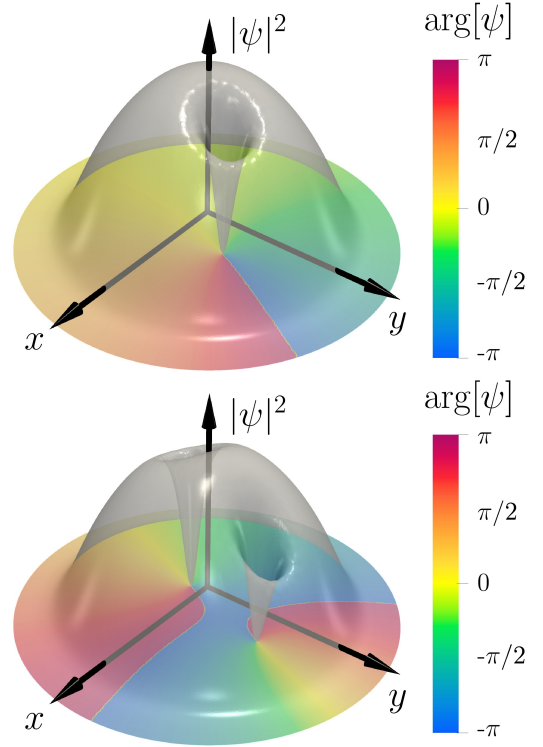


Figure 1. Examples of asymmetric vortex configurations of a Bose-Einstein condensate in an axially symmetric harmonic trap. The elevation of the semitransparent surface stems from the condensate density $|\psi|^2$, while the coloring projected onto the xy -plane indicates the value of the phase $\arg[\psi]$ of the macroscopic wave function. The examples shown are minima of the two dimensional Gross-Pitaevskii free energy (4), with non-integer values of the angular momentum (1) $L_z = 0.80$ (top panel) and $L_z = 1.48$ (bottom panel). The vortices precess around the trap center in accordance with the time dependent Gross-Pitaevskii equation (3).

of the macroscopic wave function $\psi(\mathbf{x})$

$$\frac{1}{2\pi} \oint d\ell \cdot \nabla \arg[\psi] \in \mathbb{Z}$$

around its core. The time-dependent Gross-Pitaevskii equation [11, 12] governs the dynamics of the macroscopic wave function, at the level of the mean field theory. This is a nonlinear Schrödinger equation with quartic nonlinearity that accounts for interactions between the atoms

[13–17]. Vortices that appear in rotating cold atom Bose-Einstein condensates have been extensively studied, both experimentally and theoretically [16, 18, 19]. At the level of the Gross-Pitaevskii equation these vortices are commonly modelled as stationary solutions in a co-rotating frame [13–17, 20–22]. The rotating condensate accommodates growing angular velocity by forming vortices. This goes with a discontinuous increase in angular momentum. Hence a rotating condensate cannot support an arbitrary value of the angular momentum [20]. However, here we show that condensates with an arbitrary angular momentum do exist as minimum energy solutions of a time dependent Gross-Pitaevskii equation. These solutions are eccentric vortices that precess around the center of a non-rotating axially symmetric trap, as illustrated in Fig. 1.

We consider a two dimensional Gross-Pitaevskii equation on the xy -plane with an axially symmetric harmonic trap. This approximates for example an anisotropic three dimensional trap, resulting in an oblate condensate. The macroscopic angular momentum along the z -axis

$$L_z \equiv \int d^2x \psi^* (-i\hbar \mathbf{x} \wedge \nabla) \psi \cdot \mathbf{e}_z \quad (1)$$

and the number of atoms

$$N \equiv \int d^2x \psi^* \psi \quad (2)$$

are conserved. Typically, in a Bose-Einstein condensate of ultra-cold alkali atoms $N \sim 10^4 - 10^6$. In a mean field theory the condensate is described by the time-dependent Gross-Pitaevskii equation, which in dimensionless units (with $\hbar = N = 1$ [17]) amounts to

$$i\partial_t \psi = -\frac{1}{2} \nabla^2 \psi + \frac{|\mathbf{x}|^2}{2} \psi + g|\psi|^2 \psi \equiv \frac{\delta F}{\delta \psi^*}. \quad (3)$$

Here g is a dimensionless coupling that accounts for the interactions between the atoms with typical values $10^1 - 10^3$, and F is the free energy

$$F = \int d^2x \left\{ \frac{1}{2} |\nabla \psi|^2 + \frac{|\mathbf{x}|^2}{2} |\psi|^2 + \frac{g}{2} |\psi|^4 \right\}. \quad (4)$$

The Lagrange multiplier theorem [23] states that with fixed angular momentum (1) and fixed number of particles (2) the minimum of F is also a critical point of

$$F_\lambda = F + \lambda_z (L_z - l_z) + \lambda_N (N - 1), \quad (5)$$

where λ_z , λ_N are the Lagrange multipliers that enforce the values $L_z = l_z$ and $N = 1$, respectively. The critical points of F_λ obey

$$-\frac{1}{2} \nabla^2 \psi + \frac{|\mathbf{x}|^2}{2} \psi + g|\psi|^2 \psi = -\lambda_N \psi + i\lambda_z \mathbf{x} \wedge \nabla \psi \cdot \mathbf{e}_z, \quad (6)$$

together with the conditions (1) and (2).

Let $\psi_{min}(\mathbf{x})$ be a solution of (6) and let λ_N^{min} and λ_z^{min} denote the corresponding values of the Lagrange multipliers. Hence $\psi_{min}(\mathbf{x})$ is a critical point of F_λ and it is also a minimum of the free energy (4) that simultaneously satisfies the conditions $N = 1$ and $L_z = l_z$. But whenever the Lagrange multipliers do not vanish, $\psi_{min}(\mathbf{x})$ cannot be a critical point of F . Its time evolution obeys

$$i\partial_t \psi = -\lambda_N^{min} \psi + i\lambda_z^{min} \mathbf{x} \wedge \nabla \psi \cdot \mathbf{e}_z \quad (7)$$

with $\psi(\mathbf{x}, t = 0) = \psi_{min}(\mathbf{x})$, and both λ_N^{min} and λ_z^{min} are time independent [24]. As described in [24], if there is no minimum energy solution with vanishing Lagrange multipliers the time evolution is that of a Hamiltonian time crystal [25, 26]. Indeed, both L_z and N are conserved Noether charges, and the minimum energy wave function $\psi_{min}(\mathbf{x})$ spontaneously breaks the ensuing symmetries. The time evolution equation (7) is a symmetry transformation of $\psi_{min}(\mathbf{x})$ that is generated by a definite linear combination of the two conserved Noether charges. This is the essence of spontaneous symmetry breaking, now realized in a time dependent context, that defines a Hamiltonian time crystal [24].

To search for minimum energy solutions of the time-dependent Gross-Pitaevskii equation, we numerically minimize the free energy (4) subject to the conditions $L_z = l_z$ and $N = 1$. The problem is discretized within a finite-element framework [27], and the constrained minimization problem is then solved using the Augmented Lagrangian Method [28]. Minimal energy states for angular momentum values $l_z \in (0, 2]$ with $N = 1$, and for three representative values of the interaction coupling $g = 5$, $g = 100$ and $g = 400$ are displayed in Figure 2; see also [28].

For non-vanishing values of the angular momentum $0 < l_z < 1$ the minimum energy configuration $\psi_{min}(\mathbf{x})$ is an eccentric vortex (see regime A). As l_z increases the vortex core approaches the trap center. Similar eccentric vortices have been previously described theoretically in [20, 29], and apparently observed experimentally in [30]. As shown in regime B, when $l_z = 1$, the core position coincides with the center of the trap, and the Lagrange multipliers feature a discontinuity. This is the single vortex solution that has been described extensively in the literature [13–17, 21, 22]. When l_z becomes larger than one, a second vortex appears, and there are two qualitatively different two-vortex configurations. As l_z increases, these are sequentially asymmetric (regime C) and then symmetric (regime D) with respect to the trap center. Because it depends on g , there is no universal value of l_z that separates these two regimes. At higher values of angular momentum, $l_z \approx 1.8$ with the exact value depending on g , additional vortices start entering the condensate; this is the regime E in Fig. 2. Remark that for $g = 100$ and $g = 400$ a third vortex moves towards the trap center as l_z increases, while for $g = 5$ a pair of vortices enters. Further increase of the angular momentum introduces additional vortices in the conden-

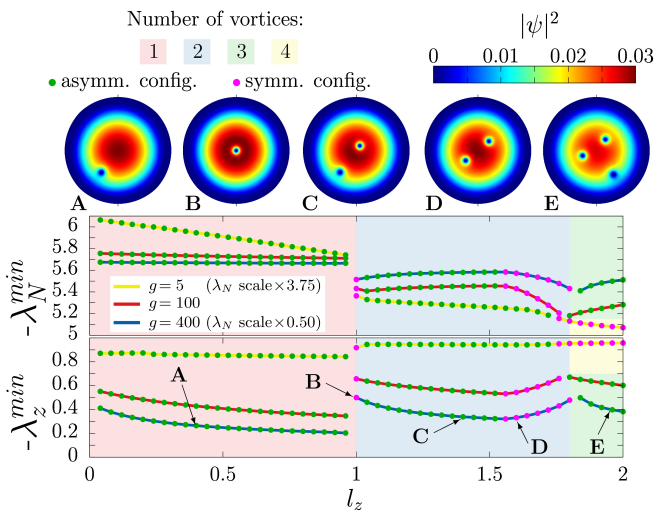


Figure 2. Minimum energy states for angular momenta $l_z \in (0, 2]$. The bottom row shows the dependence of the multipliers λ_N^{min} and λ_z^{min} on the angular momentum l_z for $g = 5, 100$ and 400 . The panels on the top row display the density of the condensate $|\psi|^2$ for qualitatively different solutions with $g = 400$, obtained for different values of l_z (zoomed to relevant data while the actual numerical domain is larger). At the vortex core the density $|\psi|^2$ vanishes and the phase circulation is 2π . The five regimes A – E are detailed in the text.

sate (not shown).

The case $l_z = 1$, denoted by B in Fig. 2, is a particular case. The core of the vortex coincides with the center of the trap. The corresponding $\psi_{min}(\mathbf{x})$ is an angular momentum eigenstate with eigenvalue $l_z \equiv m = 1$, and the solution of the time-dependent Gross-Pitaevskii equation (7) is simply an overall phase rotation with no change in the core position,

$$\psi(\mathbf{x}, t) = \exp\{i(\lambda_q^{min} + m\lambda_z^{min})t\} \psi_{min}(\mathbf{x}). \quad (8)$$

More generally, whenever $\psi_{min}(\mathbf{x})$ is an angular momentum eigenstate the time evolution amounts to a multiplication by a phase factor (8). However, for generic l_z the minimum energy configuration $\psi_{min}(\mathbf{x})$ is not an eigenstate of the angular momentum and thus its time evolution is more elaborate than mere multiplication by a time dependent phase.

We simulate the time evolution (3) of the minimum energy configuration $\psi_{min}(\mathbf{x})$ using a Crank-Nicolson algorithm. Simulation details together with animation of the time evolution can be found in the Supplementary material [28]. For all values of l_z the vortex configuration rotates uniformly around the trap center. This uniform rotation is a consequence of the equation (7) which determines the time evolution in terms of the two conserved charges. As an example, in Figure 3 we analyze the time evolution of a symmetric vortex pair in regime D of Figure 2, with $g = 5$. The vortex pair rotates around the trap center at a constant distance, with an angular

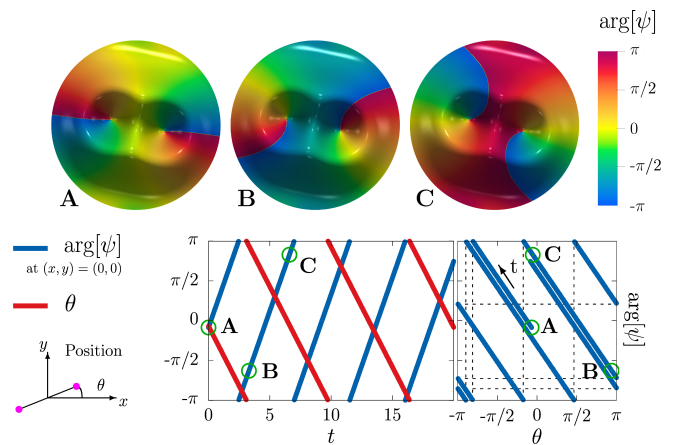


Figure 3. The evolution of a minimum energy configuration $\psi_{min}(\mathbf{x})$, in the case of a symmetric vortex pair (with $g = 5$) in region D of Figure 2. The bottom panels show the evolution of θ , the rotation angle of the pair, and of the value of the phase $\arg[\psi]$ measured at the center of the trap. The three panels A–C on the top row are snapshots displaying the phase $\arg[\psi]$ after rotations $\theta = \theta_0$, $\theta = \theta_0 + \pi$ and $\theta = \theta_0 + 2\pi$ respectively. Since the Lagrange multipliers λ_N^{min} and λ_z^{min} are not commensurate, $\arg[\psi](t)$ and $\theta(t)$ feature different periodicities. As a result after π rotations of the pair the phase profile is not simply an overall phase multiplication. This stresses the anyonic nature of such an exchange.

velocity specified by λ_z^{min} . At the same time the phase of the wave function evolves with a rate that depends on λ_N^{min} . In short, the value λ_N^{min} is the rate of change in the phase $\arg[\psi](t)$, as measured at the center of the trap. Similarly, the rate of change of $\theta(t)$ that measures the rotation of the pair, equals λ_z^{min} . Since the two Lagrange multipliers are in general not commensurate, $\theta(t)$ and $\arg[\psi](t)$ have different periodicities. It follows that when the vortices exchange their positions, the change in the phase of the wave function is not by an integer multiple of π . Such a change in the phase of a wave function is the hallmark of anyonic exchange statistics [31, 32].

In summary, we have investigated the static properties and the time evolution of minimum energy vortex configurations of the two dimensional Gross-Pitaevskii free energy, as function of the angular momentum. This models a Bose-Einstein condensate of ultra-cold alkali atoms in an axially symmetric harmonic oscillator trap. There are two Noether charges, which correspond to the number of atoms and to the axial component of the macroscopic angular momentum. For generic values of the angular momentum, the minimum energy configurations are eccentric vortices. They precess uniformly around the center of the trap, in a timecrystalline fashion. Whenever the time evolution exchanges the positions of two vortices, the phase of the wave function changes nontrivially, in a way that is consistent with anyonic exchange statistics. These properties could become relevant for example in the development of future quantum technologies.

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- [28] see Supplementary Materials in Appendix for technical details and additional informations. Animations can be found in *ancillary files* on arXiv server. See also animations at <http://www.theophys.kth.se/~garaud/time-crystal-bec.html>.
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Appendix A: Description of the supplementary animations (see ancillary files)

There are three animations that illustrate the results of presented in the manuscript. The supplementary animations display the following:

- **movie-1.mp4**: shows the minimal energy configurations that simultaneously satisfy $N = \int |\psi|^2 = 1$ and $l_z \in [0, 2)$. Here, the interaction coupling is $g = 400$. The left panel shows the density $|\psi|^2$ while the right panel displays the phase $\arg[\psi]$ of the condensate. The elevation of the semitransparent surface stems for the condensate density $|\psi|^2$, while the coloring of the surface (also projected onto the xy -plane) indicates the values of the density $|\psi|^2$ and of the phase $\arg[\psi]$ of the macroscopic wave function.
- **movie-2.mp4**: shows the time-crystalline evolution of a single eccentric vortex. The starting configuration is the minimum energy configuration $\psi_{min}(\mathbf{x})$ for an angular momentum $l_z = 0.8$. Here the interaction coupling is $g = 5$. On the left panel, the elevation of the surface and the coloring stem for the condensate density $|\psi|^2$. The right panel displays the phase $\arg[\psi]$ of the condensate.
- **movie-3.mp4**: shows the time-crystalline evolution of a symmetric pair of vortices. The starting configuration is the minimum energy configuration $\psi_{min}(\mathbf{x})$ for an angular momentum $l_z = 1.7$. Here the interaction coupling is $g = 5$. On the left panel, the elevation of the surface and the coloring stem for the condensate density $|\psi|^2$. The right panel displays the phase $\arg[\psi]$ of the condensate.

Appendix B: Details of the numerical methods

In the numerical investigations in the main body of the paper, we use Finite-Element Methods (FEM) (see e.g. [33, 34]) both for the minimization and for the time-evolution. In practice we use the finite-element framework provided by the FreeFEM library [27]. Within the finite-element framework, the constrained minimization is addressed using an Augmented Lagrangian Method together within a non-linear conjugate gradient algorithm. The time-dependent Gross-Pitaevskii equation, is integrated using a Crank-Nicolson algorithm with a forward extrapolation of the nonlinear term.

1. Finite-element formulation

We consider the domain Ω which a bounded open subset of \mathbb{R}^2 and denote $\partial\Omega$ its boundary. $H(\Omega)$ stands for the Hilbert space, such that a function belonging to $H(\Omega)$, and its weak derivatives have a finite L^2 -norm. Furthermore, $\mathcal{H}(\Omega) = \{u + iv \mid u, v \in H(\Omega)\}$ denotes the Hilbert spaces of complex-valued functions. The Hilbert spaces of real- and complex-valued functions are equipped with the inner products $\langle \cdot, \cdot \rangle$, defined as:

$$\langle u, v \rangle = \int_{\Omega} uv, \text{ for } u, v \in H(\Omega), \quad \text{and} \quad \langle u, v \rangle = \int_{\Omega} u^*v, \text{ for } u, v \in \mathcal{H}(\Omega). \quad (\text{B1})$$

The spatial domain Ω is discretized as a mesh of triangles using for the Delaunay-Voronoi algorithm, and the regular partition \mathcal{T}_h of Ω refers to the family of the triangles that compose the mesh. Given a spatial discretization, the

functions are approximated to belong to a *finite-element space* whose properties correspond to the details of the Hilbert spaces to which the functions belong. We define $P_h^{(2)}$ as the 2-nd order Lagrange finite-element subspace of $H(\Omega)$, and correspondingly $\mathcal{P}_h^{(2)}$ for $\mathcal{H}(\Omega)$. Now, the physical degrees of freedom can be discretized in their finite element subspaces. And we define the finite-element description of the degrees of freedom as $\psi \mapsto \psi^{(h)} \in P_h^{(2)}$. This describes a linear vector space of finite dimension, for which a basis can be found. The canonical basis consists of the shape functions $\phi_k(\mathbf{x})$, and thus

$$V_h(\mathcal{T}_h, P^{(2)}) = \left\{ w(\mathbf{x}) = \sum_{k=1}^M w_k \phi_k(\mathbf{x}), \phi_k(\mathbf{x}) \in P_h^{(2)} \right\}. \quad (\text{B2})$$

Here M is the dimension of V_h (the number of vertices), the w_k are called the degrees of freedom of w and M the number of the degrees of freedom. To summarize, a given function is approximated as its decomposition: $w(\mathbf{x}) = \sum_{k=1}^M w_k \phi_k(\mathbf{x})$, on a given basis of shape functions $\phi_k(\mathbf{x})$ of the polynomial functions $P^{(2)}$ for the triangle T_{i_k} . The finite element space $V_h(\mathcal{T}_h, P^{(2)})$ hence denotes the space of continuous, piecewise quadratic functions of x, y on each triangle of \mathcal{T}_h .

2. Constrained minimization: Augmented Lagrangian Method

In the main body of the paper, we aim to minimize the free energy while enforcing a set of two conditions. Such problems, referred to as *constrained optimization* are studied in great details, see for example textbooks [35–38]. Here we describe the numerical algorithms that were used in the main body of the paper, to solve the constrained optimization problem. The Augmented Lagrangian Method (ALM) used to solve the constrained optimization is based on the following. In terms of the original energy functional to be minimized F , and the set of conditions C_i , the augmented Lagrangian F^{aug} is defined as

$$F^{\text{aug}} := F + \frac{\mu}{2} \left(\sum_j C_j^2 \right) + \sum_j \lambda_j C_j. \quad (\text{B3})$$

Here μ is a penalty parameter and λ_j are the Lagrange multipliers associated with the conditions C_j . In the Augmented Lagrangian Method, the augmented Lagrangian is minimized, and the penalty μ is iteratively increased while the multipliers $\lambda_j \leftarrow \lambda_j + \mu C_j$ until all conditions are satisfied with a specified accuracy. The ALM algorithm has the property to converge in a finite number of iterations. Our choice for the minimization algorithm within each ALM iteration is a non-linear conjugate gradient algorithm [39–41].

In this work, the minimized functional F is the dimensionless Gross-Pitaevskii free energy [17]

$$F = \int d^2x \left\{ \frac{1}{2} |\nabla \psi|^2 + V(\mathbf{x}) |\psi|^2 + \frac{g}{2} |\psi|^4 \right\}, \quad (\text{B4})$$

where g is the dimensionless coupling that accounts for the interatomic interactions, and $V(\mathbf{x})$ is the trapping potential. In the main body we considered an harmonic oscillator trapping potential $V(\mathbf{x}) = |\mathbf{x}|^2/2$. Since the derivations here do not depend on the specific form of the potential, we keep in general in the following. The two conditions specifying the particle number $N = 1$ and the value l_z of the angular momentum are

$$C_N = N - 1 \equiv \int d^2x |\psi|^2 - 1 \quad \text{and} \quad C_z = L_z - l_z \equiv \int d^2x \psi^* [\mathbf{e}_z \cdot (-i\mathbf{x} \wedge \nabla)] \psi - l_z. \quad (\text{B5})$$

Hence, the variations of the augmented Lagrangian with respect to ψ^* and λ_i give the set of equations

$$-\frac{1}{2} \nabla^2 \psi + [V(\mathbf{x}) + g|\psi|^2] \psi + \tilde{\lambda}_N \psi + \tilde{\lambda}_z \mathcal{L}_z \psi = 0, \quad \text{where } \tilde{\lambda}_i = (\mu C_i + \lambda_i) \quad (\text{B6a})$$

$$C_i = 0, \quad \text{and } i = N, z, \quad (\text{B6b})$$

where the angular momentum operator is $\mathcal{L}_z = \mathbf{e}_z \cdot (-i\mathbf{x} \wedge \nabla)$. The associated weak form, is obtained by multiplying the equation (B6a) by test functions $\psi_w \in \mathcal{H}(\Omega)$, integrating over Ω and integrating by parts the Laplace operator. Alternatively the weak form is calculated as the Fréchet derivative of the augmented Lagrangian as (B3). In terms of the inner products (B1), we find

$$[\psi_w] \cdot F'(\psi) = \frac{1}{2} \langle \nabla \psi_w, \nabla \psi \rangle + \langle \psi_w, [V(\mathbf{x}) + g|\psi|^2] \psi \rangle + \tilde{\lambda}_N \langle \psi_w, \psi \rangle + \tilde{\lambda}_z \langle \psi_w, \mathcal{L}_z \psi \rangle. \quad (\text{B7})$$

This formulation, hence corresponds to the variations of the Lagrangian with respect to all degrees of freedom. It can be seen as the gradient of a function to be minimized. To do so we choose a nonlinear conjugate gradient algorithm.

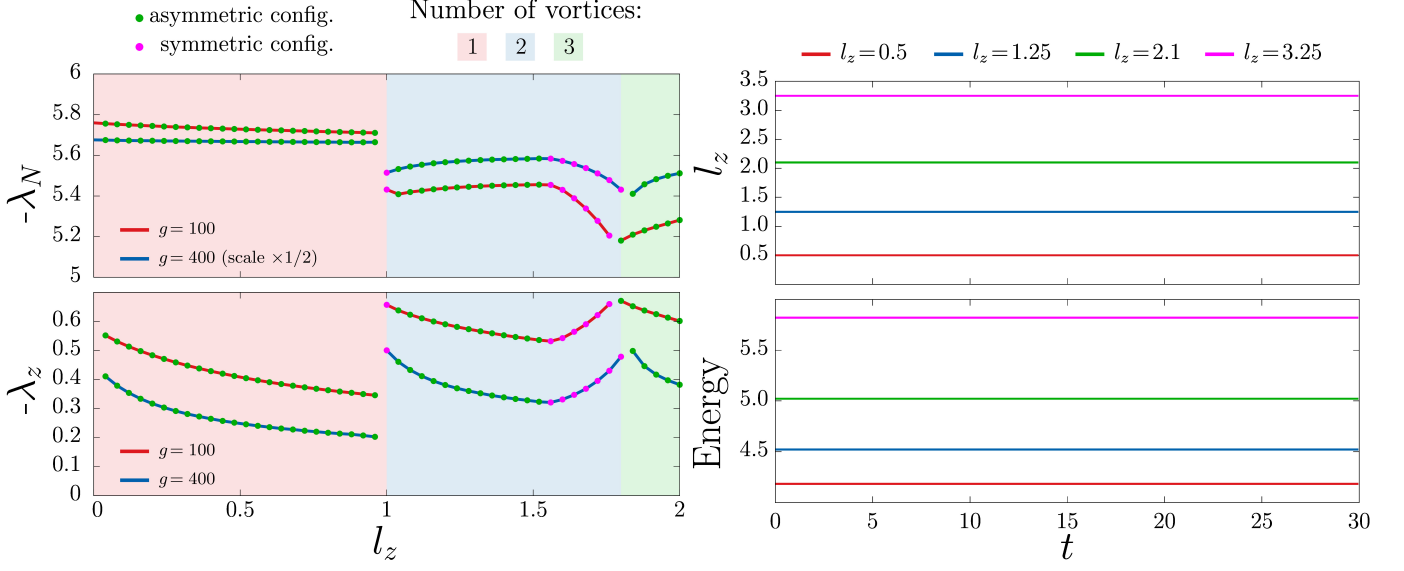


Figure 4. Details of the results of simulations where the particle number is $N = 1$. The dependence of the Lagrange multipliers on the constrained angular momentum l_z are displayed on the leftmost panel. The right panels illustrate that the time-evolution algorithm (B15) used here indeed preserves the energy (bottom), the angular momentum (top) and the particle number (not shown).

Error estimates

To estimate the quality of the solution, a global error can be derived by multiplying (B6a) by ψ^* and integrating over the domain Ω (and again integrating by part the Laplace operator). The error is alternatively obtained by replacing the test functions ψ_w by ψ in (B7):

$$\int \frac{1}{2} |\nabla \psi|^2 + [V(\mathbf{x}) + g|\psi|^2] |\psi|^2 + \tilde{\lambda}_q \int |\psi|^2 + \tilde{\lambda}_z \int \psi^* \mathcal{L}_z \psi = 0 \quad (\text{B8a})$$

$$F + \frac{g}{2} \int |\psi|^4 + \tilde{\lambda}_N (C_N + 1) + \tilde{\lambda}_z (C_z + l_z) = 0 \quad (\text{B8b})$$

$$1 + \frac{\sum_i \tilde{\lambda}_i (C_i - l_i)}{F + \frac{g}{2} \int |\psi|^4} = \text{err}. \quad (\text{B8c})$$

In practice during our constrained minimization simulations, we obtain the typical values for the relative error to be around 10^{-5} .

Numerical minimization of the weak formulation (B7) of the augmented Lagrangian (B3) gives the minimal energy states under the specified values of the constraints (B5). In all generality we consider unit particle number $N = 1$ for various values of the angular momentum l_z . The corresponding values of the Lagrange multipliers are displayed in Fig. 4.

3. Time evolution: forward extrapolated Crank-Nicolson algorithm

To address the question of the time-dependent Gross-Pitaevskii equation, the strategy is to use a Crank-Nicolson algorithm [42] to iterate the time series. More precisely, for efficient calculations, we write a semi-implicit scheme where the nonlinear part is linearized using a forward Richardson extrapolation. The time-dependent Gross-Pitaevskii reads as:

$$i\partial_t \psi = -\frac{1}{2} \nabla^2 \psi + [V(\mathbf{x}) + g|\psi|^2] \psi. \quad (\text{B9})$$

The weak form, obtained by multiplying by test functions $\psi_w \in \mathcal{H}(\Omega)$ and integrating by parts reads as, in terms of the inner products (B1),

$$\langle \psi_w, i\partial_t \psi \rangle = \frac{1}{2} \langle \nabla \psi_w, \nabla \psi \rangle + \langle \psi_w, [V(\mathbf{x}) + g|\psi|^2] \psi \rangle. \quad (\text{B10})$$

The discretization of the time turns the continuous evolution into a recursive series over the uniform partition $\{t\}_{n=0}^N$ of the time variable. The time variable is discretized as $t = n\Delta t$ and the wave function at the step n is $\psi_n := \psi(n\Delta t)$. The Crank-Nicolson scheme, uses (Forward-)Euler definition of the time derivative, while the r.h.s of Eq. (B10) is evaluated at the averaged times. Introducing the notations

$$\partial_t \psi := \delta_t \psi_n = \frac{\psi_{n+1} - \psi_n}{\Delta t}, \quad \text{and} \quad \bar{\psi}_n = \frac{\psi_{n+1} + \psi_n}{2}, \quad (\text{B11})$$

the Crank-Nicolson scheme for the time-dependent Gross-Pitaevskii equation (B10) reads as:

$$\langle \psi_w, i\delta_t \psi_n \rangle = \frac{1}{2} \langle \nabla \psi_w, \nabla \bar{\psi}_n \rangle + \langle \psi_w, V(\mathbf{x}) \bar{\psi}_n \rangle + \langle \psi_w, g|\bar{\psi}_n|^2 \bar{\psi}_n \rangle. \quad (\text{B12})$$

This fully implicit scheme results in a nonlinear algebraic system which is very demanding to solve. The alternative to solving the nonlinear algebraic problem is to approximate the nonlinear part in terms of values at previous time steps. Very schematically, the idea of the modified algorithm is to approximate the fields in the nonlinear term by using an extrapolation of the previous time steps, that retains the same order of truncation error as the rest of time series. Thus, using the forward extrapolation the averaged wave function in the non-linear term becomes $\bar{\psi}_n \approx (3\psi_n - \psi_{n-1})/2$. Next, defining the time-discretized operators:

$$\mathcal{O}_1 \psi = \left\langle \psi_w, \frac{i\psi}{\Delta t} \right\rangle - \left\langle \nabla \psi_w, \frac{1}{4} \nabla \psi \right\rangle - \left\langle \psi_w, \frac{1}{2} V(\mathbf{x}) \psi \right\rangle, \quad (\text{B13a})$$

$$\mathcal{O}_2 \psi = \left\langle \psi_w, \frac{i\psi}{\Delta t} \right\rangle + \left\langle \nabla \psi_w, \frac{1}{4} \nabla \psi \right\rangle + \left\langle \psi_w, \frac{1}{2} V(\mathbf{x}) \psi \right\rangle, \quad (\text{B13b})$$

$$\mathcal{U}_n \psi = \left\langle \psi_w, \frac{g}{8} |3\psi_n - \psi_{n-1}|^2 \psi \right\rangle, \quad (\text{B13c})$$

allows to rewrite Eq. (B12) in the compact form

$$\mathcal{O}_1 \psi_{n+1} = \mathcal{O}_2 \psi_n + \mathcal{U}_n (3\psi_n - \psi_{n-1}). \quad (\text{B14})$$

Hence the time-evolution is formally given by the recursion

$$\psi_{n+1} = \mathcal{O}_1^{-1} [\mathcal{O}_2 \psi_n + \mathcal{U}_n (3\psi_n - \psi_{n-1})]. \quad (\text{B15})$$

The spatial discretization is achieved by replacing the wave function ψ by its finite-element space representation $\psi^{(h)} \in V_h(\mathcal{T}_h, \mathcal{P}^{(2)})$ in the time-dependent Gross-Pitaevskii equation (B15). The test functions ψ_w now take values in the same discrete space as $\psi^{(h)}$. Denoting the matrix representation of the time-discretized evolution operators (B13), as:

$$\mathcal{O}_1 \mapsto \mathbf{M}_\psi, \quad \mathcal{O}_2 \mapsto \mathbf{N}_\psi, \quad \text{and} \quad \mathcal{U}_n (3\psi_n - \psi_{n-1}) \mapsto \mathbf{L}_\psi, \quad (\text{B16})$$

the recursion Eq. (B15) reduce to a linear system that read as:

$$[\mathbf{M}_\psi] \left[\psi_{n+1}^{(h)} \right] - [\mathbf{N}_\psi] \left[\psi_n^{(h)} \right] = [\mathbf{L}_\psi]. \quad (\text{B17})$$

The vector \mathbf{L}_ψ which is a function of $\psi_n^{(h)}$ and $\psi_{n-1}^{(h)}$, has to be recalculated at each step. The matrices \mathbf{M}_ψ and \mathbf{N}_ψ , on the other hand, are constant matrices to be allocated just once and are in principle easily preconditioned. Finally the recursion is thus given by

$$\left[\psi_{n+1}^{(h)} \right] = [\mathbf{M}_\psi]^{-1} \left([\mathbf{N}_\psi] \left[\psi_n^{(h)} \right] + [\mathbf{L}_\psi] \right), \quad (\text{B18})$$

which requires recalculating the vectors \mathbf{L}_ψ at each step and then multiplying by the inverse matrices.

The numerical simulations of the time-evolution algorithm (B18) representing the discretized evolution scheme (B15) accurately reproduces the intrinsic physical properties of the time-dependent Gross-Pitaevskii equation. Namely it preserves the conserved quantities like the energy, the angular momentum, and the particle number. A consistency check, as displayed on Fig. 4, shows that these are indeed (exactly) conserved during the time-evolution.