Deflation-based Identification of Nonlinear Excitations of the 3D Gross–Pitaevskii equation

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We present previously unknown solutions to the 3D Gross–Pitaevskii equation describing atomic Bose-Einstein condensates. This model supports elaborate patterns, including excited states bearing vorticity. The discovered coherent structures exhibit striking topological features, involving combinations of vortex rings and multiple, possibly bent vortex lines. Although unstable, many of them persist for long times in dynamical simulations. These solutions were identified by a state-of-the-art numerical technique called deflation, which is expected to be applicable to many problems from other areas of physics.

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Introduction. The nonlinear Schrödinger (NLS) or Gross–Pitaevskii (GP) equation [1–6] is a fundamental partial differential equation that combines dispersion and nonlinearity. It has been central to a variety of areas of mathematical physics for several decades. The NLS/GP model has facilitated a universal description of a wide range of phenomena, including electric fields in optical fibers [7], Langmuir waves in plasmas [8], freak waves in the ocean [9], and Bose-Einstein condensates (BECs). In the past 25 years since the experimental realization of atomic BECs, the NLS/GP model has enabled the theoretical identification and experimental observation of a wide range of coherent structures, including (but not limited to) dark [10] and bright [11] solitary waves, two-dimensional vortical patterns and lattices [12, 13] as well as vortex lines and rings [14].

The examination of three-dimensional (3D) systems has been a key frontier of recent studies in BECs. Recent theoretical advances have enabled the capturing of a number of such states [15]. Some, especially topological ones such as skyrmions, monopoles and Alice rings [16, 17] have been of particular interest since the early exploration of BECs, while others such as knots [18] have been studied more recently. In this manuscript, we apply a powerful numerical technique called deflation [19–21] to identify multiple solutions of the 3D NLS/GP equation.

Many of the solutions obtained by this process are identifiable as nonlinear extensions of solutions of the (analytically tractable) linear limit of the problem, or as bifurcations therefrom. Yet other solutions are highly unexpected and are not previously known, to the best of our knowledge. Without deflation, it would be very difficult to identify these complex (literally and figuratively) topological stationary points of the infinite-dimensional energy landscape. In fact, as we increase the atom number of the system, we observe this complexity to be substantially enhanced and lead to states which, while stationary, are not straightforwardly decomposable into simpler linear or nonlinear building blocks (see Fig. 5). This showcases, in our view, the utility and potential impact of the deflation method to complex 3D physical problems. This seems worth exploring further, not only within atomic BECs but also more broadly.

To further investigate the nature of the identified solutions, we compute their spectral linearization (so-called Bogoliubov-de Gennes, abbreviated BdG hereafter) modes, and conduct transient simulations of prototypical unstable states to explore the dynamical behavior of their instabilities.

Theoretical and Numerical Setup. The 3D NLS/GP model of interest is of the form [4–6]:

\[
i \psi_t = -\frac{1}{2} \nabla^2 \psi + |\psi|^2 \psi + V(\mathbf{r})\psi,
\]

(1)

subject to homogeneous Dirichlet conditions on the boundary of the domain \(D = [-6,6]^3\). Here, \(\psi\) plays the role of the suitably normalized (see [6] for details) wavefunction, while \(V\) is the external confining potential of the form \(V(\mathbf{r}) = \frac{1}{2} \Omega^2 |\mathbf{r}|^2\), a spherically symmetric trap of strength \(\Omega\), which we fix to \(\Omega = 1\). The boundary conditions do not affect the solutions for this choice of the trap strength since the domain is chosen large enough so that the solutions vanish well before reaching the boundary. Using the standard standing wave decomposition \(\psi = e^{-i\mu t} \phi\) (where \(\mu > 0\) is the chemical potential), we obtain the stationary NLS/GP elliptic problem of the form:

\[
F(\phi) = -\frac{1}{2} \nabla^2 \phi + |\phi|^2 \phi + V(\mathbf{r})\phi - \mu \phi = 0.
\]

(2)

This equation is discretized using piecewise cubic Lagrange finite elements on a structured hexahedral grid using the Firedrake finite element library [22]. Multiple solutions to the discretized problem are sought using deflation, which we briefly describe here.
Suppose that Newton’s method has discovered an isolated root $\phi_1$ of $F$. Deflation constructs a new problem $G$ via

$$G(\phi) = \left( \frac{1}{\| \phi - \phi_1 \|^2 + 1} \right) F(\phi),$$

(3)

where $\| \cdot \|$ is a suitable norm, in this case the $H^1$ norm. The essential idea is that $\| \phi - \phi_1 \|^2$ approaches 0 faster than $F(\phi)$ does as $\phi \to \phi_1$, hence avoiding the convergence to $\phi_1$ of a Newton iteration applied to $G$. The addition of 1 ensures that $G(\phi) \approx F(\phi)$ far from $\phi_1$. By applying Newton’s method to $G$, an additional root $\phi_2 \neq \phi_1$ can be found, and the process repeated (by premultiplying with additional factors) until Newton’s method fails to converge from the available initial guesses.

Previous applications of deflation to the study of BECs in 2D interleaved with continuation in $\mu$, capturing solutions as they bifurcate from known ones [20, 21]. This strategy is too expensive in 3D and so a different approach is taken here. We fix $\mu = 6$ and exploit the linear (low-density, i.e. $|\phi|^2 \to 0$) limit states to furnish a large number of initial guesses for Newton’s method. The algorithm proceeds as follows. Given an initial guess, the inner loop applies Newton’s method and deflation until no more solutions are found. The outer loop iterates over the available initial guesses. The outer loop terminates when no guess yields any solutions. We emphasize that at each application of Newton’s method, all previously computed solutions are deflated, to avoid their rediscovery.

The initial guesses used were the eigenstates of the linear limit in Cartesian, cylindrical and spherical coordinates. The Cartesian eigenstates are given by

$$|k, m, n\rangle \equiv H_k(\sqrt{\Omega}x)H_m(\sqrt{\Omega}y)H_n(\sqrt{\Omega}z)e^{-\Omega r^2}/2,$$

(4)

with associated energy (i.e. chemical potential) $E_{k,m,n} = (k + m + n + 3/2)\Omega$. The $H_{k,m,n}$ in (4) stand for the Hermite polynomials and $k, m$ and $n$ are nonnegative integers. The cylindrical eigenstates are given by

$$|K, l, n\rangle_{cyl} \equiv q_K,l(R) e^{il\theta} H_n(\sqrt{\Omega}z)e^{-\Omega(R^2+z^2)/2},$$

(5)

with $E_{K,l,n} = (2K + |l| + n + 3/2)\Omega$ where $K, n$ are nonnegative integers, and $l = 0, \pm 1, \pm 2, \ldots$. The radial profile $q_{K,l}$ in (5) is given by $q_{K,l} \sim r^l E_K^l(\Omega R^2)e^{-\Omega R^2}/2\Omega$ where $E_K^l$ are the associated Laguerre polynomials in $R = \sqrt{x^2+y^2}$.

Finally, the spherical eigenstates are given by

$$|K, l, m\rangle_{sph},$$

where the radial part is similar but now in the spherical variable $r = \sqrt{x^2+y^2+z^2}$, and the angular part is described by the spherical harmonics $Y_{l,m}(\theta, \phi)$ with $E_{K,l,m} = (2K + l + 3/2)\Omega$. The quantum numbers $K$ and $l$ are nonnegative integers and $m = 0, \pm 1, \ldots, \pm l$. All these states with $E \leq \mu = 6$ were used in the process described above.

Once a solution has been discovered, the next step is the consideration of the spectral stability of the solutions via the well-established [4–6] BdG analysis. More specifically, we assume the following perturbation ansatz around a stationary solution $\phi^0(x, y, z)$:

$$\tilde{\psi}(x, y, z, t) = e^{-i\mu t} \left\{ \phi^0 + \epsilon [ae^{i\omega t} + b^* e^{-i\omega t}] \right\},$$

(6)

where $\epsilon$ is a (formal) small perturbation parameter. This results in an operator eigenvalue problem that depends on the stationary state $\phi^0$. Upon solving the relevant problem for the eigenfrequencies $\omega$ and eigenvectors $(a, b)^T$ (see the Supplemental Material), we obtain stability information, i.e., real $\omega$ implies stability (vibrations), while complex $\omega$ is associated with instability. The eigenvalues are calculated using a Krylov–Schur method [23] implemented in SLEPc [24]. For the unstable solutions, we explore their dynamical evolution via transient numerical simulations of (1), using a Crank-Nicolson time-stepping scheme that conserves the atom number and energy of the solutions [25]. We now turn to discussing the solutions obtained through the application of these numerical methods for the 3D NLS/GP problem.

![FIG. 1: Some solutions obtained by deflation that emanate from the second eigenvalue of the linear spectrum at $\mu = 7/2$. The colors represent the argument of the solutions, ranging from $-\pi$ to $\pi$ (blue and red represent a phase of 0 and $\pm \pi$, respectively). The states in panels (a)-(d) and (f) are real, while (e) is complex.](image)

**Numerical Results.** We briefly describe the physical meaning of the quantum numbers for the Cartesian, cylindrical and spherical states, as they are useful in what follows. In the case of the Cartesian eigenfunctions, the quantum numbers $k, m,$ and $n$ are simply the numbers of cuts along the $x$-, $y$-, and $z$-axes respectively. For instance, in Fig. 1, panel (a) represents a $|0, 0, 2\rangle$ Cartesian state with 2 cuts along the $z$-axis (and $\pi$ phase differences across them), while panel (b) is $|1, 1, 0\rangle$, bearing one planar cut along the $x$-axis, and one along the $y$-axis. Combinations of states are also possible, such as...
the one in panel (c) of \(|2,0,0\rangle + r |0,2,0\rangle + |0,0,2\rangle\) (in the particular example of this panel \(r \approx 3.39\)), which forms a 2D ring along the \(y\)- and \(z\)-axes embedded in 3D space.

Vortical structures and rings can be identified in the cylindrical system of coordinates. Here, \(K\) denotes the number of cylindrical (nodal) surfaces, \(l\) the topological charge of the configuration and \(n\) the number of planar cuts along the \(z\)-axis. For example, panel (d) is a so-called ring dark soliton state (extended in 3D) \(|1,0,0\rangle_{\text{cyl}}\) that has been recently considered in [26], and panel (e) is \(|0,2,0\rangle_{\text{cyl}}\) i.e., a vortex line, piercing through the BEC with topological charge \(l = 2\).

Finally, in the spherical representation, \(K\) denotes the number of spherical (nodal) shells within the solution, \(l - m\) denotes the number of planar cuts along the \(z\)-axis, and \(m\) denotes the topological charge of vortical lines. Panel (f) is \(|1,0,0\rangle_{\text{sph}}\), a spherical shell dark solitary wave, which is also connected with recent work [27].

The ground state of the system (starting at \(\mu = 3/2\)) is known to always be spectrally and nonlinearly stable [4, 5]. The case of the first excited states (e.g. dipolar states and single vortex lines) emanating from \(\mu = 5/2\) is interesting but reasonably well understood on the basis of corresponding 2D studies [6], since no fundamentally novel states appear to emerge in 3D, as observed in Fig. 1 of the Supplemental Material. We there focus our discussion on states emanating from the second excited state of the linear problem at \(\mu = 7/2\); see also the relevant bifurcation diagram in Fig. 2 of the Supplemental Material. The states here are sufficiently complex to feature the emergence of unexpected patterns, yet it will still be possible to connect them to fundamental building blocks of topological patterns such as vortex lines and rings [14].

Examples of these solutions are shown in Fig. 2. In this figure, we observe that deflation enables us to converge to states with multiple coherent structures present such as the one of panel (a) consisting of a vortex line and a planar dark soliton. The linear state corresponding to such a nonlinear waveform is \(|0,1,1\rangle_{\text{cyl}}\). However, more complex multi-vortex topological states can progressively be identified as well. Panel (b) represents a pair of vortex lines: at the linear limit such a state can be formulated as the linear combination \(|1,1,0\rangle + i |0,2,0\rangle\), in line with what is known about vortex dipole bifurcations [6]. Panel (c) represents what was termed a vortex star in [28], arising at the linear limit via the linear combination \(|2,0,0\rangle - |0,2,0\rangle + i |2,0,0\rangle - |0,0,2\rangle\). Panel (d) shows a generalization of the well-known 2D vortex quadrupole [29] with 4 alternating topological charge bent vortex lines.

The solutions in Fig. 2(a)-(d) either allow for a direct tracing of their linear limit or have been previously identified. However, deflation allows us to go well beyond these. Important examples of this arise in panels (e) and (f) of Fig. 2. Panel (e) consists of a vortex ring combined with 2 (oppositely charged) vortex line “handles”. This state, too, can be identified at the linear limit through a more complex topologically charged combination, as \(|2,0,0\rangle + |0,2,0\rangle + i |1,0,1\rangle\). Such a state exhibiting a vortex ring with multiple vortex lines attached to it has not been previously reported, to the best of our knowledge. Even more complex is the state in panel (f), which does not bear a linear analogue. This state involves 2 vortex rings, both of which are bent; i.e. instead of having two “perpendicular” vortex rings (e.g., in the \(xy\)- and \(yz\)-planes), it is as if the top half of the one has connected itself with the right half of the other and the bottom half of one with the left half of the other. This configuration was discovered by deflation at \(\mu = 6\) but the branch terminates by \(\mu = 5.7\) without ever reaching the linear limit of \(\mu = 7/2\). In other words, this appears to be a purely nonlinear state not derivable by some suitable combination of linear eigenstates.

We now explore the BdG spectral stability of selected solutions. In fact, some of the identified waveforms are dynamically robust for an interval within their existence range; see also the Supplemental Material. An example of this form is the spherical shell dark soliton of Fig. 1(f) with its spectrum presented in Fig. 3(a). However, most are indeed dynamically unstable, as expected; see, e.g., the case of the vortex star in Fig. 3(b). Interestingly, our BdG computations reveal that it is not the case that the most complex states are also the most unstable ones (see Fig. 3 and the Supplemental Material). An example of this type can be found in the vortex ring-double vortex line state of Fig. 2(e) with spectrum presented in Fig. 3(c). While the solution is highly complex, it only bears a single unstable mode for a wide parametric interval, and at most bears two over the interval studied.

We complement the stability analysis of these states with transient numerical simulations using the Crank–Nicolson method to observe the dynamical implications.
of their instabilities. We perturb the relevant stationary state along its most unstable eigendirection. In the case of Fig. 2(e), we observe in the snapshots of the evolution of Fig. 4 that the vortex ring and two vortex lines break up into two vortex lines which are strongly bent (in fact, they are somewhat reminiscent of the U-shaped vortex lines of [30]). Over time, the configuration is characterized by splittings and reconnections (including ones re-formulating the original configuration). We have performed similar computations for other complex, topological states such as that shown in Fig. 2(f), showcasing in some such cases more radical dynamical breakups, i.e., the eventual persistence of a single, strongly excited vortex line; see relevant snapshots and the movies in the Supplemental Material.

FIG. 4: Snapshots of the vortex ring-double vortex line state obtained by solving the time-dependent NLS equation with the Crank-Nicolson time-stepping scheme. The steady-state solution of panel (e) in Fig. 2 is initially perturbed along its dominant unstable eigenmode.

We close our presentation of the numerical results of deflation by offering a glimpse into the capabilities of the method for discovering higher excited states, i.e., ones that are initiated not from the 2nd (as up to now), but rather from the 3rd and 4th excited states at $\mu = 9/2$ and $\mu = 11/2$, respectively. Some of the relevant nonlinear states discovered with deflation can be found in Fig. 5. The first examples, such as those of panels (a) and (b) can be identified straightforwardly: panel (a) represents a nonlinear configuration bearing 9 vortex lines in a generalization of the star-shaped configuration of Fig. 2(c) and [28]. Fig. 5(b) appears to be a configuration bearing two perpendicular vortex rings (now joined—cf. panel Fig. 2(f)), along with 5 vortex lines: 4 of these are tangent, similar to the ones of Fig. 2(e), while one is piercing through the planes of the two rings. Going beyond these, however, the states become highly complex. Fig. 5(c) shows what appears to be a combination of an S-shaped and 2 U-shaped vortex lines (in the terminology of [30]) along with a clearly discernible vortex ring. Labyrinthine patterns of conjoined vortex rings and vortex lines appear; at the moment we do not have any immediate classification. Fig. 5(d) displays an apparent lattice of vortex rings, while panel Fig. 5(e) is reminiscent of the vortex ring cages that appear in the dynamical instabilities of other states such as the spherical dark shell solitary wave of Fig. 1(f) [27]. Fig. 5(f) displays a conglomeration of bent vortex lines. Once again, all of these solutions have not been previously identified as stationary states of the 3D NLS/GP model, to the best of our knowledge.

Conclusions & Future Challenges. Deflation reveals unknown and intriguing dynamical states of a fundamental model for 3D Bose-Einstein condensates. By building a priori knowledge of the linear eigenstates into the deflation procedure, we are able to identify a wide range of solutions. Many of the solutions found can be characterized using these underlying linear limits. However, deflation can also discover numerous unexpected topological nonlinear states such as the vortex ring with 2 vortex lines, or the coupled bent vortex rings of Fig. 2. Despite their complexity, such states may only be weakly unstable (thus potentially tractable experimentally) and feature long-time dynamics consisting of splittings and recombinations towards the original state. As the nonlinearity of the model is increased, so is the complexity of the available topological states; yet the numerical methods discussed here appear to remain efficient in this regime. They reveal not only solutions that are generalizations of previous ones, but also vortex ring lattices, cages, bent-connected-multivortex ring and line patterns, and more. These warrant further study, topological classification and deeper physical understanding. We believe that this technique paves the way for a wide range of future exciting explorations in this and related fields.

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ranging from the first excited state at \( \mu = 5/2 \). Fig. 6(a) shows a \([1, 0, 0]\) Cartesian state with one cut along the \( x \)-axis. Fig. 6(b) shows \([0, 1, 0]_cyl\) corresponding to a single vortex line with topological charge \( l = 1 \). The rotations of these solutions along the \( x, y, \) and \( z \) axes such as the \([0, 1, 0]\) and \([0, 0, 1]\) Cartesian states are also obtained by deflation but are not reported.

**Supplemental Material**

**Solutions emanating from the 1st excited state.** Deflation identified three solutions emanating from the first excited state at \( \mu = 5/2 \). Fig. 6(a) shows a \([1, 0, 0]\) Cartesian state with one cut along the \( x \)-axis. Fig. 6(b) shows \([0, 1, 0]_cyl\) corresponding to a single vortex line with topological charge \( l = 1 \). The rotations of these solutions along the \( x, y, \) and \( z \) axes such as the \([0, 1, 0]\) and \([0, 0, 1]\) Cartesian states are also obtained by deflation but are not reported.

![Images](image1.png)

**Fig. 6:** Solutions emanating from the first excited state \( \mu = 5/2 \). Panels (a) and (b) show a dipole and single vortex line solution. The colours represent the argument of the solutions, ranging from \(-\pi\) to \(\pi\) (blue and red represent a phase of 0 and \(\pm\pi\), respectively). Panel (c) corresponds to the density isosurfaces of the Chladni soliton at densities 0.30 and 0.35.

**Bifurcation diagram of the 2nd excited states.** As discussed in the paper, the steady-state solutions to the nonlinear Schrödinger equation are identified by the deflation method at \( \mu = 6 \). The branches are then continued backward in \( \mu \) down to the linear limit by a standard zero-order continuation method [31, §4.2]. A typical example of a relevant solution is shown in Fig. 6(c) and represents a so-called Chladni soliton, previously identified in cylindrical geometry in [15, 32]. We present the bifurcation diagram of the solutions emanating from the second excited state in Fig. 7. Our diagnostic functional is the total number of atoms (or squared \( L^2 \) norm):

\[
N = \int_D |\psi|^2 \, dx.
\]

The inset panel in the top-left corner of Fig. 7 uses the atom number difference \( \Delta N \) between the branches 2(a) and 2(a)* to illustrate a bifurcation in the diagram. The latter branch bifurcates from the former around \( \mu = 5.84 \) and is shown in Fig. 8.

**Bogoliubov-de Gennes stability analysis.** The stability of a stationary solution \( \phi^0 \) to the NLS equation is determined by perturbing it with the following ansatz:

\[
\tilde{\psi}(x, y, z, t) = e^{-i\mu t} \left\{ \phi^0 + \epsilon [a e^{i\omega t} + b^* e^{-i\omega^* t}] \right\},
\]

where \( \epsilon \) is a small perturbation parameter, \( \omega \) is the eigenfrequency, and \( (a, b)^\top \) the corresponding eigenvector. After substituting (8) into the time-dependent NLS equation:

\[
i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \nabla^2 \psi + V(r)\psi + |\psi|^2 \psi,
\]

we obtain the following complex eigenvalue problem

\[
\begin{pmatrix}
A_{11} & A_{12} \\
A_{12}^* & -A_{11}
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix}
= \rho
\begin{pmatrix}
a \\
b
\end{pmatrix},
\]

where \( \rho = -\omega \) is the eigenvalue and the matrix elements are given by

\[
A_{11} = -\frac{1}{2} \nabla^2 + 2|\phi^0|^2 + V(x, y, z) - \mu,
\]

\[
A_{12} = (\phi^0)^2 - (\phi^0_c)^2 + 2i\phi^0_c\phi^0.
\]

We decompose the eigenvector \( (a, b)^\top \) into real and imaginary components as \( a = a_r + ia_c, b = b_r + ib_c, \rho = \rho_r + i\rho_c \) and rewrite (10) as

\[
\begin{pmatrix}
A_{11} & 0 & B_1 & -B_2 \\
0 & A_{11} & B_2 & B_1 \\
-B_1 & -B_2 & -A_{11} & 0 \\
B_2 & -B_1 & 0 & -A_{11}
\end{pmatrix}
\begin{pmatrix}
a_r \\
a_c \\
b_r \\
b_c
\end{pmatrix}
= \rho
\begin{pmatrix}
a_r \\
a_c \\
b_r \\
b_c
\end{pmatrix},
\]

where \( B_1 = (\phi^0)^2 - (\phi^0_c)^2 \) and \( B_2 = 2\phi^0\phi^0_c \). The eigenvalues of the matrix on the right-hand side of (12) are \( \rho_r \pm i\rho_c \) (with multiplicity two). Therefore, solving a real eigenvalue problem with the left-hand matrix of (12) yields the same eigenvalues and eigenvectors as the complex eigenvalue problem (10). We use a Krylov–Schur algorithm with a shift-and-invert spectral transformation [23], implemented in the SLEPc library [24], to solve
FIG. 7: Bifurcation diagram of the solutions emanating from the 2nd excited state at $\mu = 7/2$. The labels indicate the solutions represented in the different panels of Figs. 1 and 2 of the paper. The main panel corresponds to the total number of atoms $N$ as a function of $\mu$, while the top-left inset shows the atom number difference $\Delta N$ between the branch 2(a) and 2(a)*, coloured in red.

FIG. 8: Left: argument of the solution 2(a)* at $\mu = 6$. This branch bifurcates from branch 2(a) at $\mu = 5.84$ (see Fig. 7). Right: density isosurfaces of the state at densities 0.30 and 0.35. The parent branch 2(a) is plotted in Fig. 2(a) of the paper.

The following eigenvalue problem:

$$
\begin{bmatrix}
A_{11} & 0 & B_1 \\
0 & A_{11} & B_2 \\
-B_1 & -B_2 & A_{11}
\end{bmatrix}
\begin{bmatrix}
ar \\
ac \\
b_a
\end{bmatrix}
= \rho
\begin{bmatrix}
ar \\
ac \\
b_a
\end{bmatrix},
$$

(13)

where the matrices are real and $\rho = \rho_r \pm i\rho_c$ is complex. This problem is discretized with the same piecewise cubic finite element method used to find multiple solutions with deflation. The spectra of the solutions emanating from the 2nd excited states, presented in Figs. 1 and 2 of the paper, are respectively displayed in the different panels of Figs. 9 and 10. It is interesting to observe that some of the states such as the doubly charged vortex line of Fig. 1(e) can be dynamically stable for large values of the chemical potential $\mu$, while others such as the anisotropic ring of Fig. 1(f) can be stable for sufficiently low $\mu$.

Dynamics. The NLS equation (9) is integrated in time until $t = 50$ using the following perturbed stationary solution $\psi$ as initial state:

$$
\psi(x, y, z, t = 0) = \phi^0 + \epsilon[a + b^*],
$$

(14)

where $\phi^0$ is a stationary solution discovered by deflation and $(a, b)^\dagger$ is its most unstable eigendirection. The eigenvector $(a, b)^\dagger$ is normalized so that

$$
\int_D |a|^2 + |b|^2 \, dx = 1,
$$

(15)

and the perturbation parameter $\epsilon$ is chosen to be 0.1. We use a modified Crank-Nicolson method in time [25], which preserves to machine precision the square of the $L^2$ norm (i.e., atom number) and the energy of the solutions

$$
E(\psi) = \int_D \frac{1}{4} |\nabla \psi|^2 + \frac{1}{2} V(r)|\psi|^2 + \frac{1}{4} |\psi|^4 \, dx,
$$

(16)
FIG. 9: Spectra of the solutions presented in Fig. 1 of the paper (e.g., the panel (a) corresponds to the branch 1(a), illustrated in the panel (a) of Fig. 1). The real and imaginary parts of the corresponding eigenfrequencies $\omega$ are respectively depicted in the top and bottom panels.

and piecewise cubic finite elements in space. Given the solution $\psi_n$ at time $t_n = n\Delta t$, $\psi_{n+1}$ is obtained by solving the following nonlinear PDE:

$$i\frac{\psi_{n+1} - \psi_n}{\Delta t} = \left( -\frac{1}{2} \nabla^2 + V(r) + \frac{1}{2} (|\psi_{n+1}|^2 + |\psi_n|^2) \right) \frac{\psi_{n+1} + \psi_n}{2},$$

where $\Delta t = 5 \times 10^{-2}$ is the time step used in the numerical simulations. The nonlinear problem is solved with Newton’s method. We present different snapshots of the two vortex rings solution (see Fig. 2(f) of the paper) in Fig. 11. We observe that the original two rings collapse around $t = 30$ to form a single vortex line (see also the relevant movie in the Supplemental Material).

FIG. 10: Spectra of the solutions presented in Fig. 2 (a)-(e) of the paper.

FIG. 11: Snapshots of the two vortex rings state of Fig. 2(f) of the paper, obtained by solving the time-dependent NLS equation with the modified Crank-Nicolson time-stepping scheme.