Quasi-stable quantum vortex knots and links in anisotropic harmonically trapped Bose-Einstein condensates

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Long-time existence of topologically nontrivial configurations of quantum vortices in the form of torus knots and links in trapped Bose-Einstein condensates is demonstrated numerically within the three-dimensional Gross-Pitaevskii equation with external anisotropic parabolic potential. We find out parametric domains near the trap anisotropy – axial over planar frequency trapping ratio \( \lambda \approx 1.5 \sim 1.6 \) where the lifetime of such quasi-stationary rotating vortex structures is many hundreds of typical rotation times. This suggests the potential experimental observability of the structures. We quantify the relevant lifetimes as a function of the model parameters (e.g. \( \lambda \)) and initial condition parameters of the knot profile.

I. INTRODUCTION

Topological structures holding vorticity have been long recognized as objects of high interest in hydrodynamics, optics, and condensed-matter physics [1–3]. Within the particular theme of atomic gases in the realm of Bose-Einstein condensates [4–6], a pristine setting has been identified for the exploration of the properties of such structures. More specifically, the static and dynamical properties of quantized vortices have played a crucial role in a wide range of associated theoretical, numerical and experimental studies; as only a small ensemble of relevant examples, we mention the reviews [7–12].

A focal theme of interest within this nexus of topological charge, nonlinearity and spatial confinement has been the study of vortex rings and simple filaments [13–31] whose interaction dynamics and even leapfrogging [32–34] have been considered. An even more demanding 3D territory that has been less explored (especially so experimentally) has been that of vortex knot structures. These have been examined mainly for a uniform density, thus destroying the structure. In particular, they may not only “untie” as they do in the homogeneous setting, but rather portions of the know may exit the region (confinement induced) around 1.5-1.6. They also revealed that in the trapped setting, distinct destabilization pathways may arise for the knots. In particular, they may not only “untie” as they do in the homogeneous setting, but rather portions of the know may exit the region (confinement induced) of non-vanishing density, thus destroying the structure.

Very recently in Ref. [46], based on the hydrodynamic approximation (with potential perturbations neglected), simple vortex knots were theoretically considered in trapped axisymmetric condensates characterized by an equilibrium density profile \( \rho(z,r) \). In particular, stability of torus vortex knots under suitable conditions was predicted. Its preliminary numerical verification was undertaken very recently by one of the present authors (V.P.R. [47]) within the Gross-Pitaevskii (GP) equation, with the latter representing a suitable three-dimensional (3D) model for a rarefied Bose gas at zero temperature. For a few sets of system parameters, long lifetimes for torus vortex knots, unknots, and links were indeed observed. On the other hand, it is important to highlight that the earlier systematic work of [41] (involving thousands of relevant simulations) predicted instability of all the examined types of knots in the homogeneous condensate cases considered therein.

In light of the above results, there is an important open question remaining. Can knot (or link) structures become dynamically robust in the presence of trapping? Here, we examine this question in the context of variation of model parameters and initial condition parameters. The former are represented by the parametric exploration as a result, e.g., of the trap anisotropy, while the latter are induced by the variation of the vortical pattern initial locations. Given the generic rotation exhibited by knot patterns, we do not seek these as exact stationary solutions. Rather, we consider a large range of dynamical simulations where a perturbed initial configuration is evolved and the outcome of the evolution is assessed, attempting in this way to offer a systematic view of the knot lifetime problem. The relevant extensive numerical simulations suggested, among other things, a definite optimization (maximization) of the vortex knot lifetimes for values of \( \lambda \) (the axial vs. planar trapping strength) around 1.5-1.6. They also revealed that in the trapped setting, distinct destabilization pathways may arise for the knots. In particular, they may not only “untie” as they do in the homogeneous setting, but rather portions of the know may exit the region (confinement induced) of non-vanishing density, thus destroying the structure. We now turn to the relevant theoretical setup and the corresponding detailed numerical findings.
II. THEORETICAL SETUP AND NUMERICAL METHOD

The 3D Gross-Pitaevskii equation in trap units takes the form

\[ i\partial_t \psi = \left[ -\frac{1}{2} \Delta + \frac{1}{2} (r^2 + \lambda^2 z^2) + g|\psi|^2 - \mu \right] \psi, \quad (1) \]

where \( r^2 = x^2 + y^2 \). The principal parameters here are the trap anisotropy \( \lambda \) (the ratio between axial and planar trapping strengths) and the interaction strength: \( g = 4\pi N a/l \), (however, appropriate re-scaling of \( \psi \) is able to give \( g = 1 \)). Here \( \alpha \) is the s-wave scattering length, \( l_r \) is the oscillator length: \( \sqrt{\hbar/m\omega_r} \), \( m \) is the atomic mass, and \( \omega_r \) is the planar trap frequency. The chemical potential \( \mu \) is assumed sufficiently large (here we typically use \( \mu \sim 30\hbar \omega \) unless indicated otherwise), in order to ensure the hydrodynamic – referred to also as Thomas-Fermi – regime. As a result of this regime, the equilibrium condensate density can be well described by the expression:

\[ \rho(z, r) \propto |\mu - (r^2 + \lambda^2 z^2)/2| \]

Thus, the ellipsoid \( r^2 + \lambda^2 z^2 = 2\mu \), with transverse size \( R_\perp = \sqrt{2\mu/\lambda} \), is an effective boundary of the condensate at equilibrium, i.e., its density vanishes outside of this ellipsoid. Following Ref. [40], in the deep Thomas-Fermi limit \( \mu \gg 1 \) quasi-stationary vortex torus knots and links \( T_{p,q} \) are possible. We have knots when \( p \) and \( q \) are co-prime integers (including the case \( p = 1 \) and/or \( q = 1 \) of trivial knots that can be unfolded to a ring – “unknots”), and we have links when \( p = np', q = nq' \), with \( n \geq 2 \) (\( n \) knots or rings that are linked together). For example, the well-known trefoil knot is \( T_{2,3} \), while the Hopf link is \( T_{2,2} \). All such structures were theoretically found in Ref. [40] to have equilibrium toroidal radius \( R_\ast (\mu) = \sqrt{2\mu/3} \), and the healing length at that radius is \( \xi_\ast = \sqrt{3/(2\mu)} \).

The initial (condition for the) position of the vortex core in our studies is assumed to be a distorted torus knot (links are constructed in a similar manner)

\[ r(\varphi) + iz(\varphi) = r_0 + r_1 e^{i\varphi} + \sum_m A_m e^{i(m\varphi + \gamma_m)}, \quad (2) \]

where \( w = q/p \) is the winding number, \( r_0 (r_1) \) is the toroidal (poloidal) radius, \( A_m \) and \( \gamma_m \) are real amplitudes and phases of perturbations. The latter are needed to break the symmetry of the knot and thus introduce “seeds” for the development of possible instabilities. Two variants of vortex shape are studied in our numerical experiments:

(S1) we use \( r_0 = 4.0, r_1 = 0.7 \) and for a single \( m \) we take \( A_m = r_1/20 \) and \( \gamma_m = 0 \), while all the remaining amplitudes are set to zero;

(S2) the sum in Eq. (2) is taken over a finite range \( (q - 10) \leq m \leq (q + 10) \), with all-equal \( A_m \)’s from the set \{0.001, 0.005, 0.010\} \( R_\ast \), and with quasi-random \( \gamma_m \)’s uniformly distributed on interval \([0 : 2\pi]\).

In case S2 a typical value of the sum is about 5\( A_m \) which should be compared to \( r_1 \sim 0.20 R_\ast \). So, \( A_m = 0.001 R_\ast \) gives a nearly perfect torus knot, while \( A_m = 0.01 R_\ast \) results in significant distortions.

Now to construct the full 3D initial condition we need to specify all of the vortex cores in the \((r, z)\) plane for a given \( \phi \) where there are \( p \) vortices, here \( r > 0 \). We are able to construct the phase of the wave function with the superposition of the phase from each vortex:

\[ \Psi(\phi, r, z)/\sqrt{\rho} = \prod_j \psi_{2D}(r - r_j, z - z_j) \quad (3) \]

where \( r_j, z_j \) is the position of the \( j \)-th vortex core and \( \psi_{2D}(r, z) = e^{i\theta} \) with \( \theta = \tan 2(r, z) \) where \( r \) and \( z \) are the distance to a vortex. Thus, the total phase is simply the product of all the vortex core phases.

Additionally, we use a multi-step algorithm to find the “ground” state of the relevant system. More specifically:

(i) We imprint the phase of the ground state as found from Eq. (3).

(ii) We temporarily introduce an additional pinning potential defined by the sum \( V(\phi, r, z) = U \sum_j e^{-B r_j} \), where \( B_j = (z - z_j)^2 + (r - r_j)^2 \), \( U \) and \( B \) are suitable coefficients. We concentrate mainly on the following two choices: (V1) a relatively smooth pinning with \( U = 50, B = 15 \); (V2) a sharp pinning with \( U = 600, B = 240 \).

(iii) We have a short, but heavily damped imaginary time propagation corresponding to a dissipative regime. This step allows a relaxation of wave function in the trap that eliminates large-scale sound-mode perturbations [47].

It should be noted however that despite the pinning, the vortex core still retains some small deviation from the prescribed shape during the dissipative stage. Mainly it is a small increase of \( r_1 \). But with our \( U \) and \( B \), the deviation is less than vortex core width. Another important point is that the relatively smooth pinning (V1) potential results in a “fat” vortex core at the end of stage (iii). As conservative evolution starts, the core returns quickly to its normal width, thus producing some short-scale non-stationary ripples on the density background. The ripples act then as additional perturbations and reduce the vortex lifetime comparatively to more clean backgrounds corresponding to the sharper pinning potential (V2). However, further sharpening of the pinning potential is not efficient as it is unable to trap the vortex.

The time propagation of Eq. (1) takes place with a third-order operator splitting Fourier spectral method, with time step sizes of \( 5 \times 10^{-4} \), with a numerical grid of \( 256^3 \), and with a spacing of \( 0.07 A_\ast \). This method preserves energy at the 8th decimal place for all simulations.

Having provided the setup of our numerical experiments, we now turn to a summary of our extensive numerical investigations.

III. RESULTS

The behavior of a knot in free space has been studied, in particular, in Refs. [37, 11]. The basic motion of a
The trefoil is that the knot rolls over in a regular motion. Eventually the knot will untie as perturbations grow and the regular rolling motion ends. We will now examine the behavior of a knot in various geometries, starting with \( \lambda = 0, 0.85, \) and then looking at 1.6 and 1.8. We present results for trefoil knots with a single-\( m \) perturbation \( S_1 \) and smooth pinning \( V_1 \).

In Figure 1 we show the evolution of a \( T_{23} \) knot in a trap with \( \lambda = 0 \). This is just a tube scenario, involving no confinement in the \( z \) direction. The red line is the 3D vortex, i.e., it represents the position of the vortex core. The vortex positions are extracted by finding the phase singularity on the computational grid \([50]\). We further refine these vortex positions via method used in Ref. \([29]\). Additionally, both the BEC’s density (thin black lines) and the extracted cores are projected (bold black) onto the back planes: \((x,y)\), \((x,z)\), and \((y,z)\). One can discern that early on during the evolution for this scenario the knot gets distorted due to undulations (the so-called Kelvin waves \([6, 22]\)). As a result, already at times earlier than 40 in our dimensionless units, the knot has broken into individual undulating filaments, losing its coherence as a trefoil structure.

The above unconfined along the \( z \)-direction scenario can be compared/contrasted with the trapped case along the \( z \)-direction. In Fig. 2, we show a system with \( \lambda = 0.85 \). This is a tube scenario, involving no confinement in the \( z \) direction. The red line is the 3D vortex, i.e., it represents the position of the vortex core. The vortex positions are extracted by finding the phase singularity on the computational grid \([50]\). We further refine these vortex positions via method used in Ref. \([29]\). Additionally, both the BEC’s density (thin black lines) and the extracted cores are projected (bold black) onto the back planes: \((x,y)\), \((x,z)\), and \((y,z)\). One can discern that early on during the evolution for this scenario the knot gets distorted due to undulations (the so-called Kelvin waves \([6, 22]\)). As a result, already at times earlier than 40 in our dimensionless units, the knot has broken into individual undulating filaments, losing its coherence as a trefoil structure.

To illustrate the main point of our work, namely the dramatic impact of judiciously chosen anisotropy on the lifetimes of the vortex knots, we now turn to a case involving \( \lambda = 1.6 \). In Figure 3, we show the evolution of a \( T_{23} \) knot in a trap with this \( \lambda \). The knot lives over 1100 trap units of time before it unties. Just after the knot unties, it is shown in (c), and then the knot evolves
Figure 3: For $\lambda = 1.8$ snapshots are shown along the demise of the trefoil knot inside the BEC. (a) $t = 202$ initial distortions appear; (b) $t = 263$ growth of undulations appears. (c) At $t = 303$ further growth of undulations is shown, while (d) shows the eventual breakup around at $t = 324$ when a portion of the knot leaves the BEC’s volume. The axes are in oscillator units, $\sqrt{\hbar/m\omega_r}$.

Figure 4: For $\lambda = 1.6$ snapshots showing the decay of the vortex knot. At (a) $t = 500$ and (b) $t = 1000$ the emergence of non-trivial undulations can be observed but these remain small. (c) At $t = 1130$ the knot has untied into a link, while (d) at $t = 1153$ a portion of the link is leaving the volume. The axes are in oscillator units, $\sqrt{\hbar/m\omega_r}$.

Figure 5: For $\lambda = 1.8$ (a) $r_c$ and (b) $z_c$ as a function of $\phi$ are shown at different times 0 (black dash-dot) and 296 (blue). Also see Fig. 3(a) where the same data is displayed in 3D space. From these data we extract $r_0$, $r_1$, and $z$. (c) The radial position of each vortex at $\phi = 0$ as a function of time. (d) The average $r_0$ as a function of time. The y axes are in oscillator units, $\sqrt{\hbar/m\omega_r}$.

and eventually a portion of the structure leaves the volume in (d). Remarkably, under similar initialization as in the cases considered above, we observe a lifetime about 4 times larger than in Fig. 3 and nearly 30 times longer than for the case of Fig. 1. It is then clear that a suitable tuning of the anisotropy can endow a knot structure with very long life times, conceivably enabling its observability in already available, state-of-the-art experimental BEC setups.

To measure the lifetimes of the knot structures, we analyze the extracted core positions within the (approximate Thomas-Fermi) region $0.9R_J$. (The 0.9 prefactor is used to avoid ghost vortices from disrupting the knot analysis.) Then, we order the core positions so that they are a continuous function in $\phi$ spanning the interval from 0 to $2\pi$; see Fig. 5(a) for $r$ (b) $z$ of the
extracted vortex core positions.

When the separation of two points anywhere along the knot exceeds a cutoff distance (larger than the grid spacing) the knot is considered to be broken. This works also for reconnection events as a knot unites. To further the analysis we can extract the toroidal \( r_0(t) \); poloidal \( r_1(t) \); and \( z \), labeled \( z_0(t) \) positions of the vortex in the knot. Using these quantities, we define \( (z) \) by taking the average of the \( z_0 \) coordinate over the entire knot: 

\[ (z) = \frac{1}{N_c} \sum_{i=1}^{N_c} z_i \]

where \( N_c \) is the number of vortex core positions found on our grid; \( r_0 = \langle r \rangle \) is found in the same fashion. To obtain \( r_1 \) at a given time we take 

\[ r_1^2 = \frac{1}{N_c} \sum_{i=1}^{N_c} (z_i - \langle z \rangle)^2 + (r_i - \langle r \rangle)^2. \]

In Fig. 5(c) we show the radial position of the two vortex cores in a knot for \( \phi = 0 \) as a function of time. The position of one core is red while the other is black. We can see their regular motion as they tumble over each other. We can see \( r_0 \) is the average radial position of the knot and \( r_1 \) as the distance the two vortices traverse in their rotation about each other. In Fig. 5(d) we show the extracted \( r_0 \), note the vertical scale difference of (c) and (d).

We contrast the typical evolution of \( r_0, r_1 \) and \( z_0 \) for different \( \lambda \)'s in Fig. 6. In (a) and (b) we show the extracted \( r_0 \) (top panel), \( z_0 \) (middle panel) and \( r_1 \) (bottom panel) for many different geometries. In (a) we show the shorter evolution of \( \lambda = 0.85 \) (red), 2.5 (lack), and 1.8 (blue). Then in (b) we compare the long evolution of \( \lambda = 1.6 \) (green) and 1.8 (blue). The main observation here, corroborating the snapshots presented earlier in Figs. 4, 5 is that we have a huge variation in the lifetime of trapped knots. In particular, while for prolate or highly oblate condensates the knots are highly unstable [see the black and red curves for \( \lambda = 0.85 \) and \( \lambda = 2.5 \) in (a)], it is possible to expand their lifetimes by over a factor of 10, by judiciously tuning the anisotropy towards somewhat oblate condensates, most notably in the case of \( \lambda = 1.6 \), green curve in (b). We observe nearly 100 rotations of the knot in the \( \lambda = 1.6 \) case. Interestingly (but also perhaps somewhat intuitively) this also reflects the corresponding earlier observations for the stability in the case of vortex rings which can be thought of partial constituents of vortex knots. See, e.g., the theoretical analysis of [23], as well as the recent numerical confirmation of [31].

The oscillations in these quantities \( (r_0, r_1, z_0) \) are related to the excitations of the knot, but also correspond to the knot completing a rotation, see Fig. 6. Additionally, it is relevant to note within Fig. 6 that there is a certain “universality” in the way that the knot structure manifests its demise in these diagnostics. For most cases we have looked at (except the \( \lambda = 0 \)), the knot breaks in a fashion where the poloidal (effective) coordinate \( r_1 \) seems to diverge as a portion of the knot leaves the volume or unites.

Besides that, to more precisely determine the domains of maximal lifetime within the parameter space, we performed several series of simulations with initial states prepared using sharp pinning \( V_2 \) and multiple-mode perturbations \( S_2 \) for \( A_m = 0.001R^* \). Similarly, we have varied the knot initial conditions to identify the lifetime dependence on initial conditions, as well as the one on the chemical potential. In these simulations, the lifetime was measured till the moment of first reconnection. The results are shown in the top panel of Fig. 7 as lifetime dependencies over the initial poloidal torus radius \( r_1 \) with a fixed, nearly optimal value of the anisotropy parameter \( \lambda \), and with a fixed, nearly optimal value of the toroidal radius \( r_0 \) (it should be noted here that optimal \( r_0 \) has been empirically found as approximately \( 0.9R^* \) at moderately large \( \mu \sim 30 \), slightly different from the theoretical limit \( 1.0R^* \)). In the bottom panel of Fig. 7 the lifetimes are plotted versus the anisotropy parameter \( \lambda \) for fixed initial \( r_1 \) and \( r_0 \). For comparison, analogous results for

![Figure 6](image-url)

Figure 6: The extracted effective coordinates \( r_0 \) (top panel), \( z_0 \) (middle panel), and \( r_1 \) (b) are shown for different \( \lambda \)'s. In (a) \( \lambda = 0.85 \) (black), 1.8 (blue), and 2.5 (red) are shown. In (b) \( \lambda = 1.6 \) (green), 1.8 (blue) are shown. It is important to note the disparity in the time scales of the breakup of the different anisotropy knot structures. The same initial knot and chemical potential were used. When the knots are no longer complete (untie), the curves are set to zero. The y axes are in oscillator units, \( \sqrt{\hbar/m\omega} \).
smooth pinning V1 and single-\(m\) perturbation S1 are also shown there. Indeed distinct parametric intervals can be identified where simple vortex knots, unknots, and links survive over many hundreds of their revolutions. Prototypical examples of each class are offered in Fig. 7. For instance, for \(1.4 < \lambda < 1.8\), we observe the significant increase of the structure lifetimes (bottom panel). A similar feature arises for \(0.65 < r_1 < 0.8\), as a function of the initial condition parameter \(r_1\), for fixed \(\lambda\).

Here it should be mentioned that a control simulation with large perturbation corresponding to \(A_m = 0.01R_s\) demonstrated decrease of the lifetime in the quasi-stable domain by a factor of roughly ten (not shown). Moderate perturbation with \(A_m = 0.005R_s\) resulted in roughly two times shorter lifetime which is still quite long. Thus, even “less accurately prepared” vortex knots are able to exist for a long time in suitable parametric regimes, as revealed by our study.

Finally, in Fig. 8 we compare trefoil lifetimes as functions of the ratio \(r_1/R_s\), for different values of chemical potential \(\mu\). In this case it is convenient to normalize the results to \(R_s^2(\mu)\) in order to separate the overall tendency \(T_{\text{life}} \sim \mu\). Thus, the normalized lifetime provides a general impression (up to a factor of order 1) about the number of knot rotations before its destruction. We can observe an evident tendency towards an enhanced lifetime for larger values of the chemical potential \(\mu\). This result is intuitively natural since a larger \(\mu\) implies a weaker coupling of the vortical pattern to sound modes.

### IV. CONCLUSIONS

In this work, we have explored the effects of initial condition preparation (through variations of the poloidal coordinate \(r_1\)), trap anisotropy (by tuning the confinement ratio \(\lambda\)) and background density/nonlinearity (varying the chemical potential \(\mu\)) to the lifetime of knot structures in confined atomic Bose-Einstein condensates. Arguably, our most significant finding is that anisotropic traps with (trapping ratios) \(\lambda \approx 1.6\) can essentially stabilize (i.e., lead to enhanced lifetimes by over an order of magnitude) torus vortex knots and links in Bose-Einstein condensates with moderate values of the local induction parameter \(\Lambda = \hbar(R_s/\xi_s) \lesssim 3\). We similarly identified optimal values of \(r_1\) and illustrated the enhanced lifetime for larger chemical potentials \(\mu\).

We observed that the dynamics leading to the eventual demise of the most-long-lived knots and links involves the sound generation by the rotating vortex structures. This process gradually increases the parameter \(r_1\) “pushing it out” of a quasi-stable interval. After that Kelvin waves are produced progressively distorting the knots/links and ultimately leading to their destruction (via either untying or leaving the Thomas-Fermi region). For comparison, recent results based on the Biot-Savart approximation indicate that for vortex knots and links of the same relative sizes in spatially uniform condensates the mechanism of knot destruction is an intrinsic linear instability without stable zones [42, 43].

These results offer, in our view, a systematic understanding of the viability of observation of torus knots in confined atomic condensates. They show how initial condition, trapping and nonlinear features of the underlying problem may enhance the relevant lifetimes rendering them accessible in current state-of-the-art experiments. Moreover, they offer some intuition of the relevant opti-
nality of slightly oblate condensates in connection with corresponding results for vortex rings. Among the important open tasks still remaining are of course the experimental realization of such structures via phase (or perhaps density) engineering, but also a realization of these knots as exact solutions of the system from a computational/numerical perspective. In particular, their rotation suggests that they may be exact periodic orbits of the system, hence computationally demanding periodic orbit identification tools may be used to find such exact solutions and to assess their stability via, e.g., Floquet theory. Relevant possibilities will be explored in future studies.

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