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Vortex-ring solutions of the Gross–Pitaevskii equation for an axisymmtrically trapped Bose–Einstein condensate

C-H Hsueh[1], S-C Gou[1], T-L Horng[2] and Y-M Kao[1]

[1] Department of Physics, National Changhua University of Education, Changhua 50058, Taiwan
[2] Department of Applied Mathematics, Feng Chia University, Taichung 40074, Taiwan

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Abstract

We propose a numerical scheme for obtaining the stationary vortex-ring solutions of the Gross–Pitaevskii (GP) equation for an axisymmetrically trapped Bose–Einstein condensate (BEC). The effective energy functional and the associated GP equation are derived by assuming a trial phase profile for the wavefunction that is subject to the condition of circulation quantization on the rz plane. The wavefunction of the vortex ring is determined by solving the ground state of the effective GP equation numerically. Application of our method to the formation of a three-dimensional Skyrmion in a trapped two-component BEC is demonstrated.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Vortices are hydrodynamic phenomena characterized by the whirling motion of fluid around a centre. A simple and intriguing vortical configuration is the vortex ring, which is a ring-shaped mass of moving fluid rotating around an axis disposed in a circular form. A well-known example is the smoke ring. In fact, vortex rings are frequently observed in a wide range of scales in nature due to their fluid entrainment and slow dissipation. Owing to their compact and persistent nature, vortex rings have been the subject of numerous experimental and theoretical studies in classical fluid mechanics [1].

Other than in classical fluids, vortex rings can also be created in quantum fluids. Virtually, vortex rings can be formed by imparting linear momentum to the fluid with axial symmetry. Accordingly, quantized vortex rings with cores of angstrom size had been observed by accelerating charged particles through a superfluid ^{4}He [2]. Recently, due to the experimental achievements of quantized vortices in trapped dilute alkali gases [3–5], the possibility of realizing vortex rings in atomic Bose–Einstein condensates (BEC) has been intensively studied. Several schemes aiming at this goal have been put forward [6–8]. In particular, Feder *et al*

[8] have proposed using dynamical instabilities in the condensate to make a dark soliton decay into vortex rings. Based on this idea, vortex rings in a trapped BEC were first realized experimentally by Anderson *et al* [9].

In addition to the mechanism of creating vortex rings in atomic BEC, the dynamics of vortex rings in a trapped BEC have also been studied by several authors [10–13]. In this work, we present a numerical scheme that enables one to determine the vortex-ring solutions of the Gross–Pitaevskii (GP) equation for an axisymmetrically trapped Bose–Einstein condensate. Although this problem has been investigated previously, we revisit this subject from a more fundamental perspective, such that no assumptions on the superfluid velocity field are needed.

We start by noting that the kinematics of an infinitely thin circular quantized vortex ring in a homogeneous superfluid is different from that in a trapped BEC. In the former, a vortex ring translates with a constant velocity with its shape and size unchanged, while in the latter, a vortex ring can move back and forth in the trapped condensate, with its size varying in the locomotion [6, 13]. This peculiar feature is resulted from the competition between the effect of the trapping potential and that of the self-induced velocity from the vortex ring's own local curvature. When these two effects are exactly cancelled out, the vortex ring becomes immovable. As a consequence, this equilibrium vortex-ring state is treated as a stationary solution of the GP equation. It is also important to note that the existence of a vortex ring leads to the emergence of a toroidal-like hole in the condensate, around which the atoms rotate with velocities subject to the condition of circulation quantization.

To obtain the vortex-ring solution for a condensate confined in an axially symmetric trap, Guilleumas *et al* [11] have used the line-source approximation to describe the vorticity of the vortex ring and hence to construct the energy functional of the vortex ring. In addition to the main subject (the line-source approximation), the authors have incidentally proposed, in the same paper, a numerical scheme for finding the vortex-ring solutions of GP equation. In this secondary scheme, the authors proposed to include a constraining term $\omega_\phi \langle \hat{L}_\phi \rangle$ in the energy functional [11], where ω_ϕ and $\hat{L}_\phi$ denote the angular velocity and angular momentum about the azimuthal direction (the $\mathbf{e}_\phi$ axis in the cylindrical coordinate), respectively, and the bracket $\langle \cdots \rangle$ indicates the average taken on the stationary configuration of the condensate. The constraining energy, $\omega_\phi \langle \hat{L}_\phi \rangle$, is introduced to account for the nucleation of a vortex on the rz plane. As a consequence, a generalized GP equation can be obtained by minimizing the energy functional, and the stationary solution can be determined numerically.

Although the scheme mentioned above permits a way to determine the vortex-ring solutions of the GP equation without any presumptions, we find that the physical signification of the term $\omega_\phi \langle \hat{L}_\phi \rangle$ is ambiguous and further expositions on its availability are requested. In [11], $\omega_\phi \langle \hat{L}_\phi \rangle$ is considered as the energy needed to support the rotation of the condensate around the core as viewed from the laboratory frame. The angular velocity ω_ϕ is interpreted as the Lagrange multiplier associated with the conservation of $\hat{L}_\phi$ and is treated as a constant. The authors claimed that the vortex-ring solutions can be obtained by solving the GP equation when ω_ϕ is specified. We note that while $\hat{L}_\phi$ is a locally conserved quantity, the associated Lagrange multiplier cannot be a constant everywhere. This suggests that ω_ϕ is essentially a function of position, and thus the constraining energy should be expressed by $\langle \omega_\phi(\mathbf{r}) \hat{L}_\phi \rangle$ rather than $\omega_\phi \langle \hat{L}_\phi \rangle$. Besides, from the irrotational nature of the superfluid, the magnitude of the superfluid velocity at the position $\mathbf{r}$ falls off like $|\mathbf{r} - \mathbf{r}_0|^{-1}$ far from the vortex due to constant circulation, where $\mathbf{r}_0$ is the position of the vortex core. This implies that the angular velocity of the rotating superflow would fall off like $|\mathbf{r} - \mathbf{r}_0|^{-2}$ which is obviously position dependent. All these ambiguities need to be clarified before constructing a correct vortex-ring solution of the GP equation. In fact, it is the inherent constraint such as the

circulation quantization, rather than a fictitious external force, that sets the coherent structure of a quantized vortex. Therefore, in determining the vortex-ring states of a trapped BEC, it is more crucial to resort to the intrinsic restriction on the wavefunction rather than to devise the external constraint in the energy functional, and we address this issue in the present work.

2. Theory

At extremely low temperatures, the dynamics of a trapped scalar Bose–Einstein condensate is described by the time-dependent GP equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\left[-\frac{\hbar^2\nabla^2}{2m}+V_{\mathrm{ext}}(\mathbf{r})+g|\Psi(\mathbf{r},t)|^2\right]\Psi(\mathbf{r},t), \tag{1}$$

where m is the mass of the atom and $g=4\pi\hbar^2a/m$ is the coupling strength (a is the s-wave scattering length). The GP equation (equation (1)) takes a simple form in the case of stationary solutions in which the condensate wavefunction, or the order parameter, evolves according to the law $\Psi(\mathbf{r},t)=\Psi(\mathbf{r})\exp(-\mathrm{i}\mu t/\hbar)$, where μ is the chemical potential. Consequently, the time-dependent GP equation reduces to

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V_{\mathrm{ext}}(\mathbf{r})+g|\Psi(\mathbf{r})|^2\right]\Psi(\mathbf{r})=\mu\Psi(\mathbf{r}). \tag{2}$$

The condensate wavefunction $\Psi(\mathbf{r})$ is normalized by $\int|\Psi(\mathbf{r})|^2\,\mathrm{d}\mathbf{r}=N$, where N is the total number of atoms in the condensate. To be specific, we shall consider the axisymmetric potential $V_{\mathrm{ext}}(\mathbf{r})=(m/2)\left(\omega_\perp^2r^2+\omega_z^2z^2\right)$ in the cylindrical coordinates (r,ϕ,z), and define the aspect ratio $\lambda=\omega_z/\omega_\perp$. In the Thomas–Fermi (TF) regime, $Na/a_\perp\gg1$, the chemical potential is fixed by $\mu=(\hbar\omega_\perp/2)(15\lambda Na/a_\perp)^{2/5}$ [14], where $l_{ho}=(\hbar/m\omega_\perp)^{1/2}$ is the oscillator length in the radial direction. Accordingly, the spatial extensions of the atomic cloud in the radial and axial directions are given by $R_{\mathrm{TF}}=\left(2\mu/m\omega_\perp^2\right)^{1/2}$, $Z_{\mathrm{TF}}=R_{\mathrm{TF}}/\lambda$.

In the quantum hydrodynamic approach, the wavefunction of the condensate can be expressed in the Madelung form $\Psi(\mathbf{r})=\sqrt{\rho(\mathbf{r})}\exp[\mathrm{i}S(\mathbf{r})]$, where $\rho(\mathbf{r})$ and $S(\mathbf{r})$ are respectively the density and the phase of the condensate. It is easily verified that the velocity of the superflow is determined by $\mathbf{v}_{\mathrm{s}}(\mathbf{r})=(\hbar/m)\nabla S(\mathbf{r})$. However, $\mathbf{v}_{\mathrm{s}}(\mathbf{r})$ is not strictly irrotational ($\nabla\times\mathbf{v}_{\mathrm{s}}=0$). In the presence of vortices, the circulation of $\mathbf{v}_{\mathrm{s}}$ is quantized in units of $2\pi\hbar/m$ [15]. Thus,

$$\oint_\Gamma\mathbf{v}_{\mathrm{s}}\cdot\mathrm{d}\mathbf{l}=\kappa\frac{2\pi\hbar}{m}, \tag{3}$$

where κ is an integer and Γ indicates a closed contour around the vortex line. Equation (3) implies that S is a multi-valued function. For example, we can choose $S(\mathbf{r})=\kappa\phi$ for a straight vortex line residing in the z axis in an axisymmetric condensate. Suppose a stationary circular vortex ring, which is axisymmetrically orientated, has formed in the trapped condensate. Assuming that the core centre is located at $(r,z)=(R,Z)$, we can then define the core-centred polar coordinates, i.e.,

$$\zeta(r,z)=\sqrt{(r-R)^2+(z-Z)^2} \tag{4}$$

$$\theta(r,z)=\tan^{-1}\left(\frac{z-Z}{r-R}\right). \tag{5}$$

Accordingly, we write $\Psi(\mathbf{r})=|\Psi(\zeta,\theta)|\exp[\mathrm{i}S(\zeta,\theta)]$, and require that the superfluid velocity associated with $S(\zeta,\theta)$ satisfies equation (3) on the $\zeta\theta$ 'plane'. To assure the multi-valued

character of $S(\zeta,\theta)$, the simplest and most natural choice is to let$S(\zeta,\theta) = \pm\kappa\theta$, in analogy with the case of a central vortex line on the z axis [16]. Specifically, we shall choose $S(\zeta,\theta) = -\kappa\theta$, such that the condensate particles always swirl in a clockwise sense when viewed in the direction of the azimuthal axis $\mathbf{e}_\phi$ ($\mathbf{e}_\phi$ is stipulated to point into the page). Consequently, the phase function, $-\kappa\theta$, creates a swirling superflow described by $\mathbf{v}_s^{(0)}(\zeta,\theta) = v_s^{(0)}(\zeta)\,\mathbf{e}_\theta$, where $v_s^{(0)}(\zeta)$ is a function of ζ only and $v_s^{(0)}(\zeta) \sim 1/\zeta$ provided that ζ is much larger than ξ, the healing length of the condensate. Yet in the current problem, the function $-\kappa\theta$ does not faithfully describe the behaviour of the superflow near the symmetric axis. For an axisymmetrically oriented vortex ring, the radial velocity component of the superflow must vanish on the z axis so that the axial symmetry of the flow pattern can be retained. The velocity field constituted by the term $-\kappa\theta$ thus needs to be modified on the z axis. To overcome this shortcoming, we introduce a compensation velocity field $\delta\mathbf{v}_s = (\hbar/m)\nabla S_1(\zeta,\theta)$ such that the actual velocity is given by $\mathbf{v}_s = \mathbf{v}_s^{(0)} + \delta\mathbf{v}_s$, and correspondingly, $S(\zeta,\theta) = S_0(\theta) + S_1(\zeta,\theta)$, where$S_0(\theta) = -\kappa\theta$ and $S_1(\zeta,\theta)$ is a real, continuous and single-valued function. Since the vortical properties of the superfluid is chiefly determined by the velocity profile $\mathbf{v}_s^{(0)}$, we expect that $\delta\mathbf{v}_s$ produces merely local corrections to $\mathbf{v}_s^{(0)}$ and leaves the global circulation around the vortex core unchanged, that is, $\oint_\Gamma \delta\mathbf{v}_s\cdot\mathrm{d}\mathbf{l} = 0$. The order parameter is then expressed in the following form:

$$\Psi(r,z) = \psi(r,z)\exp[-\mathrm{i}\kappa\theta(r,z)], \tag{6}$$

where $\psi(r,z) = |\Psi(\mathbf{r})|\exp[\mathrm{i}S_1(r,z)]$. Substituting equation (6) into equation (1) and scaling the lengths and energies in units of $a_\perp, \hbar\omega_\perp$, respectively, we obtain the GP equation for $\psi(r,z)$:

$$\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}\right)+\frac{r^2+\lambda^2z^2}{2}+g\,|\psi|^2+\frac{\kappa^2}{2\zeta^2}\right.$$
$$\left.-\frac{\mathrm{i}\kappa}{\zeta^2}\left[(z-Z)\frac{\partial}{\partial r}-(r-R)\frac{\partial}{\partial z}+\frac{z-Z}{2r}\right]\right\}\psi = \mu'\psi. \tag{7}$$

Here, μ' is the chemical potential in the presence of a vortex ring.

It is interesting to point out that the term enclosed in the square bracket in equation (7) is exactly the angular momentum operator $\hat{L}_\phi$ introduced in [11], i.e.,

$$\begin{aligned}\hat{L}_\phi &= \frac{\mathbf{e}_\phi\cdot\hat{\mathbf{L}}+\hat{\mathbf{L}}\cdot\mathbf{e}_\phi}{2}\\ &= \frac{\mathbf{e}_\phi\cdot(\mathbf{r}-\mathbf{r}_0)\times\hat{\mathbf{p}}+(\mathbf{r}-\mathbf{r}_0)\times\hat{\mathbf{p}}\cdot\mathbf{e}_\phi}{2}\\ &= \frac{1}{\mathrm{i}}\left[(z-Z)\left(\frac{\partial}{\partial r}+\frac{1}{2r}\right)-(r-R)\frac{\partial}{\partial z}\right]\end{aligned} \tag{8}$$

where $\hat{\mathbf{p}} = -\mathrm{i}\nabla$ is the linear momentum operator and $\mathbf{r}_0 = R\mathbf{e}_r + Z\mathbf{e}_z$ is the position vector of the core centre[3]. Furthermore, by the dimensional consideration, it is evident that $\tilde{\omega}_\phi(r,z) = \kappa/\zeta^2(r,z)$ is equivalent to the local angular velocity. Thus equation (7) can be written as

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}\right)+\frac{r^2+\lambda^2z^2}{2}+g\,|\psi|^2+\frac{\kappa^2}{2\zeta^2}+\tilde{\omega}_\phi\hat{L}_\phi\right]\psi = \mu'\psi. \tag{9}$$

[3] In [11] the angular momentum was given by $\hat{L}_\phi = [\mathbf{e}_\phi\cdot\mathbf{r}\times\hat{\mathbf{p}}+r\times\hat{\mathbf{p}}\cdot\mathbf{e}_\phi]/2$, which is inexact because the rotation centre is at $\mathbf{r}_0$ rather than at the origin of the trap.

The last equation can be derived from the stationary condition $\delta E'[\psi, \psi^*]/\delta\psi^* = 0$, where $E'[\psi, \psi^*] = E[\psi, \psi^*] - \mu' N$ with the energy functional $E[\psi, \psi^*]$ given by

$$E[\psi, \psi^*] = \int \mathrm{d}\mathbf{r} \left[\frac{1}{2} |\nabla\psi|^2 + \frac{r^2 + \lambda^2 z^2}{2} |\psi|^2 + \frac{\kappa^2}{2\zeta^2} |\psi|^2 + \frac{g}{2} |\psi|^4 \right] + \int \mathrm{d}\mathbf{r}\, \psi^* \tilde{\omega}_\phi \hat{L}_\phi \psi. \quad (10)$$

Comparing our derivation to the expression of the energy functional given in [11], namely,

$$E[\Psi, \Psi^*] = \int \mathrm{d}\mathbf{r} \left[\frac{1}{2} |\nabla\Psi|^2 + \frac{r^2 + \lambda^2 z^2}{2} |\Psi|^2 + \frac{g}{2} |\Psi|^4 \right] + \omega_\phi \int \mathrm{d}\mathbf{r}\, \Psi^* \hat{L}_\phi \Psi, \quad (11)$$

we see that the term $\langle \tilde{\omega}_\phi \hat{L}_\phi \rangle$ appears in equation (10), where the average is taken over the partitioned wavefunction $\psi(r, z)$ rather than the total wavefunction $\Psi(r, z)$. Moreover, the centrifugal potential, $\kappa^2/2\zeta^2$, is included in our expression. We therefore expect that the desired wavefunction vanishes spontaneously at the core centre for $\kappa \neq 0$, since $\kappa^2/2\zeta^2$ diverges at $(r, z) = (R, Z)$. This ensures the formation of a toroidal-like empty region inside the condensate. Finally, it is important to note that although the introduction of $\hat{L}_\phi$ seemingly implies divergence on the z axis ($r = 0$), the wavefunction ψ does not necessarily vanish there. Recalling that the operator ∇^2 contains the term $(1/r)\partial/\partial r$, thus if ψ satisfies the equation $\partial\psi/\partial r + \mathrm{i}\kappa\zeta^{-2}(z - Z)\psi = 0$ at $r = 0$, the divergence can be removed without assuming $\psi = 0$ on the z axis. The required condition for the above equation to hold is that ψ must be a complex function, and this is verified in the following numerical computations.

Before proceeding to solve the equation numerically, here we remark briefly on the difference between the present scheme and the previous one. In the preceding studies, a particular irrotational velocity profile must be presumed (see [10, equation (17)] and [11, equation (11)]) in order to determine the vortex-ring solution. The specified velocity profile yields a distribution of rotational energy, and is treated as an additional external potential. The vortex-ring solution is then obtained by solving the effective GP equation with the method of imaginary time propagation. Nevertheless, the vortex-ring solution so obtained is not exact in general, as the calculated superfluid velocity profile, which is obtained by taking the gradient of the phase of the total wavefunction, is not always consistent with the prescribed one. Besides, treating the rotational energy as an external potential may cause an overestimate in the vortex nucleation energy (see the discussions in [11]). We see that these difficulties can be completely avoided in our scheme. Although the assumption of the trial phase function, S_0, seemingly implies a velocity field, this prescribed velocity profile is not complete as S_0 represents only a partial phase of the total wavefunction and the remaining phase inscribed in ψ is yet to be determined by solving equation (9). Therefore no inconsistency between the true velocity profile and the trial one given by S_0 will be brought about. In addition, since the effective GP equation, equation (9), is derived by substituting the separated wavefunction equation (6) into the usual GP equation, these two equations are equivalent representations and thus no misestimate of vortex energy will be introduced. As a result, the consistency of the vortex-ring solution is ensured in the present scheme.

The effective GP equation (equation (9)), that can be obtained from the extremization of equation (10) with respect to ψ, plays a central role in locating the vortex-ring solution. Since the vortex rings are dynamically stable in the absence of dissipation [10], we expect that the lowest energy solution of equation (9) will minimize the energy functional. This can be further established if we rewrite equation (9) in the form

$$\left[\frac{-1}{2} (\nabla - \mathrm{i}\mathbf{A})^2 + \frac{r^2 + \lambda^2 z^2}{2} + g |\psi|^2 \right] \psi = \mu' \psi, \quad (12)$$

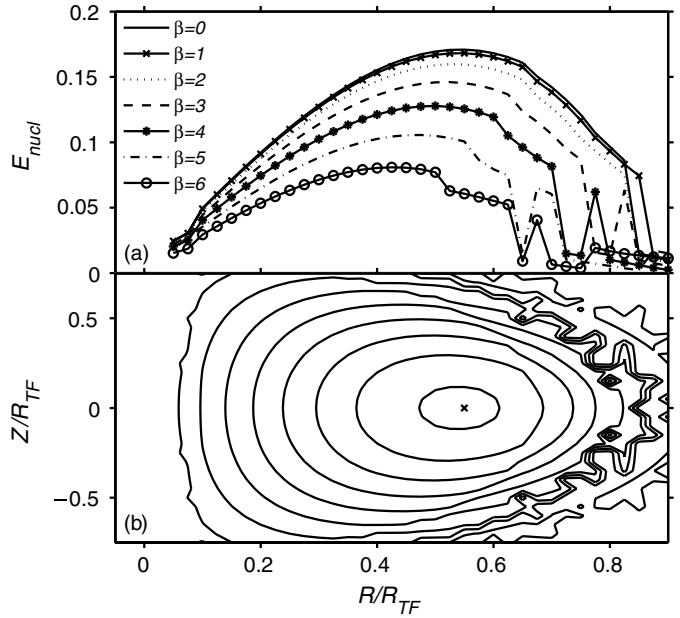

Figure 1. (a) The nucleation energy of the vortex ring as a function of R for various values of $\beta = |Z|/R_{\rm TF}$ in a spherical condensate with $R_{\rm TF} = 10$. (b) The corresponding energy surface of figure 2(a), in which the contours of constant energy are plotted per 0.02 energy unit between 0.171 and 0.

where the gauge potential $\mathbf{A}$ is given by $\mathbf{A} = -(\kappa/\zeta)\,\mathbf{e}_\theta$. The last equation is familiar as it describes the static vortex state in a superfluid. We therefore consider the lowest energy solution of equation (9) as the corresponding vortex-ring solution. The major difference is that this lowest energy solution ψ can only be complex to account for the marginal effects on the velocity field near the z axis.

3. Results and discussion

Since $\psi(r, z)$ satisfies equation (9) and gives the lowest energy eigenvalue, it can be solved numerically by the method of imaginary time propagation on a discretized (r, z) mesh. Now, with specified values for R and Z, the wavefunction $\psi_{R,Z}(r, z)$ minimizing the energy functional $E[\psi, \psi^*]$ can be determined. Obviously, the corresponding energy value E depends on R and Z. In figure 1(a), the nucleation energy of the vortex ring, $E_{\rm nucl}(R, Z) = E(R, Z) - E_0$, as a function of R for various values of Z is shown for a spherical condensate with $\kappa = 1$ and $R_{\rm TF} = 10$, where E_0 is the ground state energy of the condensate in the absence of vortex ring. Basically, the energy of the vortex ring depends on the condensate density ρ, the ring radius R and the vortex-core size ξ, as revealed by the theoretical studies in [17], in which $E = (2\pi^2\hbar^2/m)\rho R \ln(1.59R/\xi)$ is concluded for a large vortex ring ($R \gg \xi$) in a homogeneous condensate. We note that R, ρ and ξ in the last expression are independent parameters, and the energy of the vortex ring is an increasing function of R and ρ but a decreasing one of ξ. Although the situation becomes more complicated for a trapped condensate, in which the atomic density varies with position and hence ρ and ξ are dependent on R, the above energy formula may still provide a useful clue to explore the behaviour of

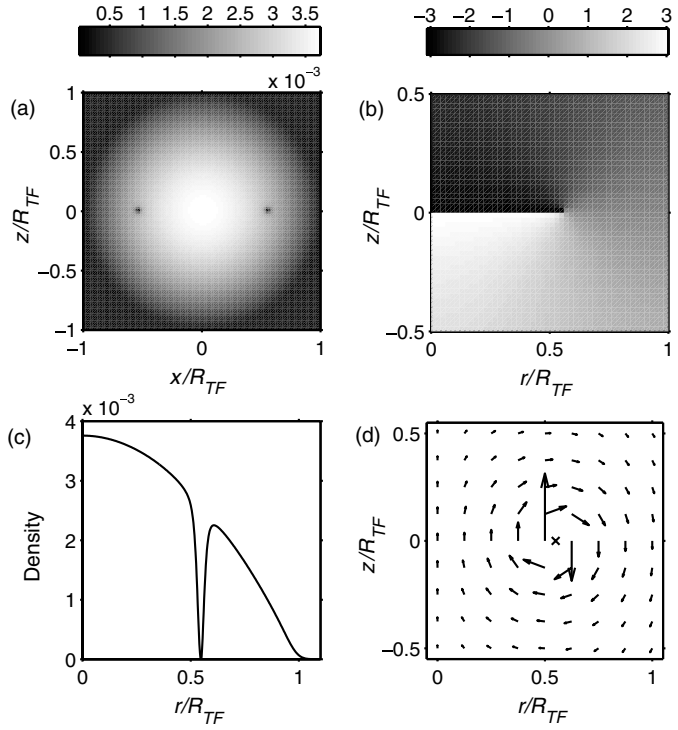

Figure 2. (a) The grey-scale density plot of a singly quantized vortex ring ($\kappa = 1$) in a spherical condensate with $R_{\rm TF} = 10$. The tiny black dots (the vortex cores) reveal the cross-sections of a toroidal-hole in the condensate. (b) The phase variation of the condensate wavefunction around the core of the vortex ring. (c) The radial part of the normalized density profile $N^{-1}|\Psi|^2$ of the condensate at $z = 0$ in the presence of the vortex ring. (d) The corresponding current density field $\mathbf{j}(r, z)$ of the vortex-ring state. The length of the arrow is proportional to the magnitude of $\mathbf{j}(r, z)$ (in arbitrary units).

the energy curves in figure 1(a). As most atoms are concentrated in the central region of the trapped cloud, the atomic density thereabouts varies slowly and thus the energy increases with increasing R in the inner part of the condensate. In contrast, the energy of the vortex ring decreases with increasing R in the outer part of the condensate, as the atomic density decreases rapidly and the vortex core becomes wider in that region. This explains why the energy curves in figure 1(a) all have the shape of a cap. Furthermore, it has already been pointed out in previous studies [10, 11, 13] that vortex ring generally precesses inside the condensate unless a particular ring radius is chosen. Therefore the stationary vortex-ring state corresponds to an unstable equilibrium of motion achieved when $E(R, Z)$ is maximal. For the vortex ring in figure 1(a), the maximum of $E(R, Z)$ or $E_{\rm nucl}(R, Z)$ occurs at $R = 0.550R_{\rm TF}$, $Z = 0$. Here $Z = 0$ is expected as the condensate possesses the reflection symmetry about the xy plane. The energy contours of $E_{\rm nucl}(R, Z)$ are shown in figure 1(b) at equal spacing. Note that $E_{\rm nucl}(R, Z)$ drops rapidly to a very low value on the outer edge of the atomic cloud, suggesting that the vortex ring is not stable thereabout. This might be understood by the idea that the density in that region is not large enough to sustain a vortex.

From figure 2(a), it is evident that a thin toroidal-like hole is formed in the condensate. The phase variation of the condensate wavefunction around the vortex core is shown in

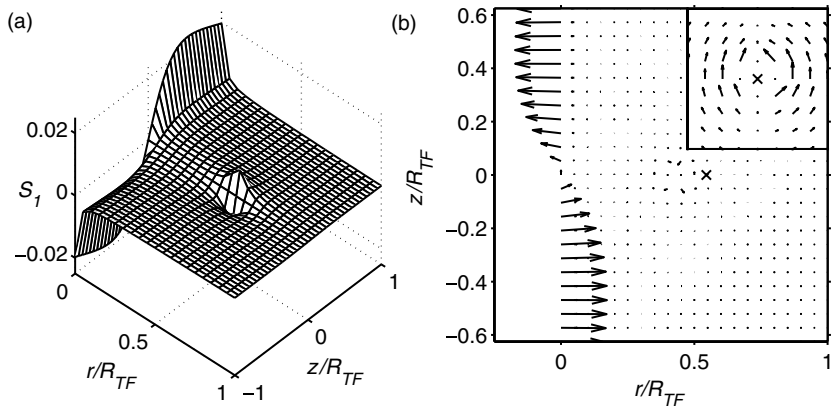

Figure 3. (a) The phase S_1 as a function of r and z. (b) The velocity field $\delta\mathbf{v}_s$ as a function of r and z, where the length of the arrow is proportional to the magnitude of $\delta\mathbf{v}_s$ (in arbitrary units). In the inset, the velocity field in the vicinity of the vortex core (marked by the cross) is shown for $|r/R_{TF} - 0.55| \leqslant 0.01$ and $|z/Z_{TF}| \leqslant 0.01$. In order to be recognizable, the velocity vector at the location of the core is not plotted, as its magnitude overwhelms those at the neighbouring locations.

figure 2(b). Apparently, a 2π phase jump occurs around the singularity residing right at the core centre. Moreover, by direct numerical integration for various closed contours enclosing the core, we have also verified that, within the numerical accuracy, the value of the circulation integral equation (3) is 2π (in oscillator units) which is exactly one quantum of circulation. The corresponding radial density profile of the vortex ring on the xy plane is shown in figure 2(c). In figure 2(d), the current field $\mathbf{j}(\mathbf{r}) = (\Psi^*\nabla\Psi - \Psi\nabla\Psi^*)/2\mathrm{i}$ on the rz plane is shown, in which the rotational behaviour of the flow around the core is well captured. The compensation phase S_1 and the velocity $\delta\mathbf{v}_s$ for the vortex ring in figure 1 are plotted in figures 3(a) and 3(b) respectively as functions of r and z. We find that $S_1(r, z)$ is an odd function of z, i.e., $S_1(r, -z) = -S_1(r, z)$ whose magnitude is generally small and varies slowly in the region of the z axis. In the vicinity of the z axis, the rapid variation of $S_1(r, z)$ gives rise to a shear layer in which the appreciable inward (outward) radial components of $\delta\mathbf{v}_s$ along the positive (negative) z axis force the velocity strictly z directional right at the z axis due to axial symmetry as shown in figure 3(b). Note that there is a small dip-bump structure around the core as shown in figure 3(a), suggesting that the cross-section of the vortex core is non-circular. Further numerical computations reveal that this non-circular character is caused by the density gradient across the vortex core (from the inner side to the outer side of the core centre). Apparently, this non-circular character becomes more noticeable for a smaller condensate, but disappears when the size of the condensate is sufficiently large.

It is important to point out that the above results are consistent with those obtained previously in [10, 13], in which an infinitely thin vortex ring resting on the xy plane will have a radius of $R = R_{TF}/\sqrt{3} = 0.577R_{TF}$ irrespective of the aspect ratio λ. In figure 4(a), the radii of the stationary vortex ring with various R_{TF} are illustrated. We see that with increasing R_{TF}, R increases monotonically yet the ratio R/R_{TF} converges to a limiting value rather slowly in TF regime (figure 4(b)). Extrapolation on the curve of $\ln(R/R_{TF})$ versus $1/R_{TF}$ suggests that $R/R_{TF} \to 0.582$ when $R_{TF} \to \infty$. This estimated limiting value of R/R_{TF} agrees with $1/\sqrt{3}$ with an relative error being less than 1%.

In addition to the case of a single-vortex ring, the present scheme can be employed to construct the equilibrium state of a more complicated vortical configuration with a prescribed

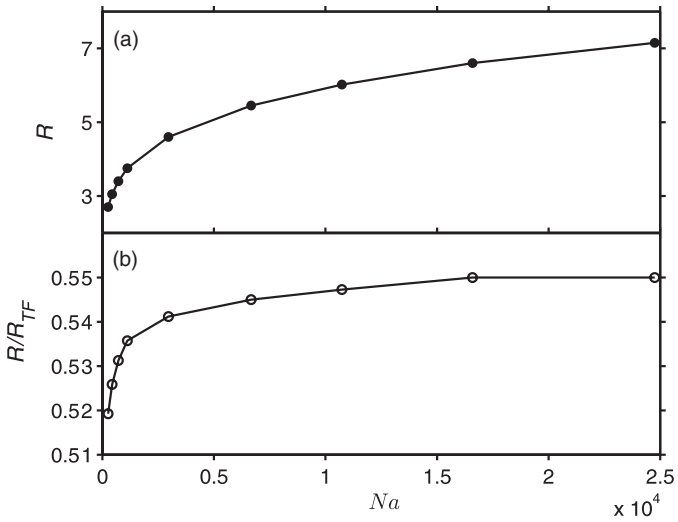

Figure 4. (a) The equilibrium ring radius R as a function of Na for a spherical condensate. (b) The ratio $R/R_{\rm TF}$, as a function of Na for a spherical condensate.

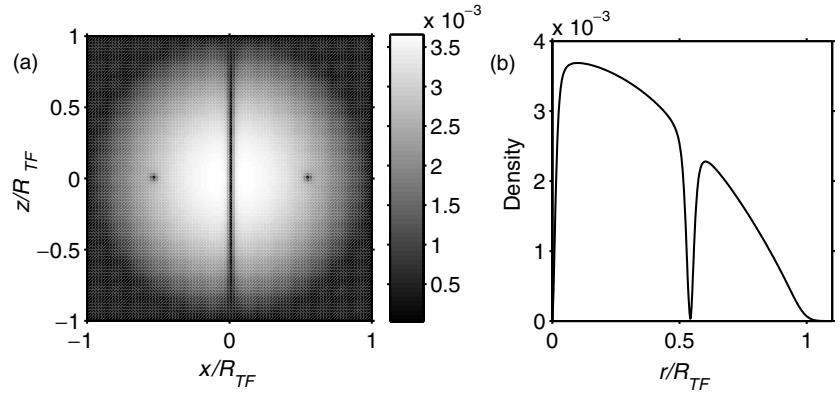

Figure 5. (a) The grey-scale density plot of the vortex complex consisting of a vortex ring ($\kappa = 1$) lying on the xy plane with a single-straight vortex line ($n = 1$) residing in the z axis. (b) The radial part of the normalized density profile $N^{-1}|\Psi|^2$ at $z = 0$ of the vortex complex in figure 5(a).

$\Psi(\mathbf{r})$. For example, by choosing $\Psi(\mathbf{r}) = \psi(r, z)\exp(\mathrm{i}n\phi)\exp[-\mathrm{i}\kappa\theta(r, z)]$, we obtain the wavefunction of a vortex complex consisting of a vortex ring lying on the xy plane with the ring axis coinciding with the z axis and a straight vortex line residing right at the z axis. The corresponding density profiles of such a composite structure with $\kappa = n = 1$ are shown in figure 5.

This vortex complex can be further applied in the phase separation regime of a two-component BEC to mimic the structure of a topological defect known as the Skyrmion. In this theoretical model, one component of the binary mixture is concentrated in the core region of the vortex ring formed by the other, and flows azimuthally to produce a vortex line on the z axis [7]. Let $\Psi_i\,(i = 1, 2)$ be the wavefunction for the ith species of condensate in the mixture.

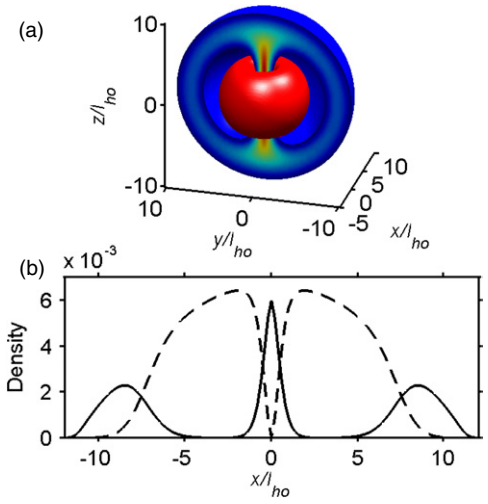

Figure 6. (a) The 3D density profile of the stable trapped Skyrmion in a two-component BEC: The central torus is the isosurface of the line component (red). The isosurface of the ring component (blue) is shown in the positive x axis. (b) The 1D density profiles: The dashed- and solid lines indicate the normalized densities for the line- and ring components respectively. The parameters in this simulation are identical to those of figure 1 in [18]: $N_1 = N_2 = 4.5 \times 10^6$ denote the numbers of atoms in species 1 and 2 respectively; $\lambda = 1$, $\omega_\perp = 2\pi \times 7.8$ Hz and $l_{\rm ho} = 3.86$ μm; $a_{11} = 5.67$ nm, $a_{22} = 5.34$ nm are the intraspecies scattering lengths and $a_{12} = 5.54$ nm is the interspecies scattering length.

Accordingly, the energy functional of the systems is described by

$$E[\Psi_1, \Psi_2] = \int \mathrm{d}\mathbf{r} \left(\frac{1}{2}|\nabla\Psi_1|^2 + \frac{1}{2}|\nabla\Psi_1|^2 + V_1|\Psi_1|^2 + V_2|\Psi_2|^2 + \frac{1}{2}g_{11}|\Psi_1|^4 + \frac{1}{2}g_{22}|\Psi_2|^4 + g_{12}|\Psi_1|^2|\Psi_2|^2 \right). \tag{13}$$

Here, for simplicity, we have assumed that all atoms have the same mass, and the two trapping potentials are overlapped perfectly, i.e., $V_1 = V_2 = (r^2 + \lambda^2 z^2)/2$. To generate the energetically stable Skyrmion configuration, we let $\Psi_1 = \psi_1(r, z)\exp[-\mathrm{i}\theta(r, z)]$ and $\Psi_2 = \psi_2(r, z)\exp(\mathrm{i}\phi)$. As a consequence, the corresponding Skyrmion configuration of winding number $W = 1$ is shown in figure 6 with the same parameters adopted in [18, figure 1]. Obviously, the results in figure 6 coincide nicely with those previous studies, and this suggests that our scheme may provide a simpler way to generate the wavefunction of a 3D Skyrmion in a two-component BEC.

It should be pointed out that due to the ansatz and its specific symmetry, the present technique does not provide sufficient information about the dynamical or energetic stability of the stationary solutions. However, this problem is particularly relevant in the case of the Skyrmion solutions. A more detailed investigation on the Skyrmion solution and its instability mechanisms can be found in [19].

4. Conclusions

In summary, we have developed a numerical scheme for obtaining the stationary vortex-ring state for an axisymmetrically trapped Bose–Einstein condensate. We derive the effective

energy functional and the associated GP equation for the condensate in the presence of a stationary vortex ring by assuming a particular phase profile for the wavefunction subject to the quantization of circulation on the rz plane. The order parameter corresponding to the equilibrium vortex-ring configuration is determined by locating the ground state of the effective GP equation which yields the maximal nucleation energy among all possible locations of the pinned-down vortex ring. This method also provides a simpler way to generate certain complicated vortical configurations such as the 3D Skyrmion in the trapped two-component BEC as shown above.

The major difference between our scheme and others is that, instead of introducing a particular velocity profile as an external field, we convert the condition of circulation quantization into effective constraining potentials and determine the wavefunction of the condensate via variational means. Our method thus avoids the difficulty of specifying the authentic velocity field in an inhomogeneous superfluid. This advantage may provide a feasible way to study the dynamics of multiple vortex rings in a trapped condensate, in which the velocity profile may develop complicated spatiotemporal behaviour while the vortex rings are moving and interacting with each other. This would involve in deriving a set of coupled equations of motion for the order parameter and the locations of different core centres, and will be the focus of our future work.

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