# Self-sustained deformable rotating liquid He cylinders: The pure normal fluid ${ }^{3} \mathrm{He}$ and superfluid ${ }^{4} \mathrm{He}$ cases 

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#### Abstract

Within density functional theory, we have studied self-sustained, deformable, rotating liquid He cylinders subject to planar deformations. In the normal fluid ${ }^{3} \mathrm{He}$ case, the kinetic energy has been incorporated in a semiclassical Thomas-Fermi approximation. In the ${ }^{4} \mathrm{He}$ case, our approach takes into account its superfluid character. For this study, we have chosen to limit our investigation to vortex-free configurations where angular momentum is exclusively stored in capillary waves on a deformed cross-section cylinder. Only planar deformations leading to noncircular cross sections have been considered, as they aim to represent the cross section of the very large deformed He drops discussed in the experiments. Axisymmetric Rayleigh instabilities, always present in fluid columns, have been set aside. The calculations allow us to carry out a comparison between the rotational behavior of a normal, rotational fluid $\left({ }^{3} \mathrm{He}\right)$ and a superfluid, irrotational fluid $\left({ }^{4} \mathrm{He}\right)$.


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## I. INTRODUCTION

Helium is the only element in nature that may remain liquid at temperatures close to absolute zero. At very low temperatures, liquid helium is the ultimate quantum fluid, able to form nanoscopic droplets and macroscopic samples as well. In particular, ${ }^{4} \mathrm{He}$ droplets are considered as ideal matrices for spectroscopic studies of embedded atoms and molecules, and for the study of superfluidity at the atomic scale, including the study of quantum vortices.

Determining the experimental size and shape of helium droplets is a challenging problem. First determinations focused on droplets made of up to several thousand atoms produced by the adiabatic expansion of a cold helium gas [1]. The experiments analyzed the scattering cross section of Kr atoms dispersed by a jet of ${ }^{4} \mathrm{He}$ or ${ }^{3} \mathrm{He}$ droplets using density functional theory (DFT) density profiles as input [2,3]. More recently, large helium droplets made of $10^{8}-10^{11}$ atoms have been created by the hydrodynamic instability of a very low-temperature ( $T$ ) liquid helium jet passing through the nozzle of a molecular beam apparatus, as reviewed in Ref. [4]. These large drops have been analyzed to determine their shape and, in the case of ${ }^{4} \mathrm{He}$, whether they host arrays of quantized vortices or not [5].

Two experimental techniques have been used to characterize large helium drops. Coherent diffractive imaging of $x$ rays from a free-electron laser [5-8] gives access to a model-independent determination of the two-dimensional (2D) projection of the drop density on a plane perpendicular to the x-ray incident direction via iterative phase retrieval algorithms. Irradiation of helium droplets with intense extreme ultraviolet pulses $[9,10]$ and subsequent measurement
of wide-angle diffraction patterns provides access to full three-dimensional information. However, so far the analysis of the densities is model dependent as their shape has to be parametrized using some guessed solid figure which is then used to produce a diffraction pattern which may be compared to the experimental one. The conclusion drawn from these experiments, which are mostly on ${ }^{4} \mathrm{He}$ drops, is that helium drops are mainly spherical and that only a small fraction of them (about 7\%) [10] are deformed and host some angular momentum, which is likely acquired during their passage through the nozzle of the experimental apparatus. The experimental results have been compared to calculations made for incompressible viscous droplets only subject to surface tension and centrifugal forces [11-15] or based on a DFT approach [16-18] specifically designed to describe liquid helium [19-22].

It has been found $[6,10]$ that spinning ${ }^{4} \mathrm{He}$ droplets follow the sequence of shapes characteristic of rotating viscous droplets $[11,14]$. This unexpected result is due to the presence of vortex arrays in the spinning droplets [17,18] that confer to them the appearance of rotating rigid-bodies.

Large ${ }^{3} \mathrm{He}$ drops have been detected as well in the coherent diffractive imaging of x-ray experiments $[7,8]$. It is worth mentioning that classical and DFT calculations for ${ }^{3} \mathrm{He}$ droplets have yielded very similar relationships between angular velocity and angular momentum [23], which is due to the fact that at the experimental temperatures $(T \sim 0.15 \mathrm{~K})$ [24] liquid ${ }^{3} \mathrm{He}$ behaves as a normal fluid with a finite viscosity.

So far, the most reliable approach to study spinning helium droplets is the DFT approach. It has, however, the limitation that the complexity of DFT calculations dramatically grows
with droplet size, making them prohibitively costly even for a few tens of thousands of atoms, which is significantly below typical experimental sizes. Addressing large droplets is especially needed to study large vortex array configurations in ${ }^{4} \mathrm{He}$ droplets as well as the recently produced spinning mixed ${ }^{3} \mathrm{He}-{ }^{4} \mathrm{He}$ droplets [25] for which classical $[26,27]$ and DFT [28] calculations are already available. To circumvent this limitation, it is often resorted to a simpler cylindrical geometry which restricts the calculations to less demanding 2D configurations while the basic physics may still be caught by the model. Indeed, self-sustained ${ }^{4} \mathrm{He}$ circular and deformed cylinder configurations have been used to describe the density of spinning ${ }^{4} \mathrm{He}$ droplets on the plane of symmetry perpendicular to the rotation axis $[6,29]$. We stress that these are self-sustained configurations, and not rotating cylindrical vessels (circular or elliptic) filled with helium for which there exists a vast literature (see, e.g., Refs. [30-32] and references therein).

In this work we describe self-sustained liquid He cylinders of infinite length under rotation. The equilibrium and stability of a rotating column of a viscid fluid subject to planar disturbances have been addressed in detail $[27,33]$ applying techniques similar to those used to describe rotating viscid droplets [11,13]. As in this study, only translationally symmetric (planar) disturbances leading to noncircular cylinder cross sections have been considered. Our final goal is to explore the behavior of large fluid drops like those used in experiments. Simulating such large drops in three dimensions (3D) is computationally intractable by any microscopic approach. The behavior of planar 2D drops is expected to be at least qualitatively similar to 3D drops [6]. Hence, axisymmetric Rayleigh instabilities, always present in fluid columns, are set aside. We remark that axisymmetric Rayleigh instabilities in superfluid ${ }^{4} \mathrm{He}$ cylinders in the nonrotating case have been the subject of a recent study based on the same 3D DFT approach employed here [34], and its extension to the case of rotating ${ }^{4} \mathrm{He}$ cylinders might be an interesting future study.

In the case of ${ }^{3} \mathrm{He}$, we have employed a classical model for viscous liquids subject to centrifugal and surface tension forces [13] and a normal liquid DFT [20,35] plus semiclassical approach, treating the ${ }^{3} \mathrm{He}$ cylinders in the DFT plus rotating Thomas-Fermi (TF) framework [23,36]. This semiclassical approach is justified by the large number of atoms per unit length in the cylinder. The DFT-TF method represents a realistic framework allowing to make the calculations affordable. It can be extended to mixed helium systems as well [21,28]. As for droplets [37], thermal effects on the energetics and morphology of the cylinder are expected to be negligible at the experimental temperatures, so we shall use a zero-temperature method [23]. Zero temperature means here a very low $T$, but above $T \sim 2.7 \mathrm{mK}$ at which ${ }^{3} \mathrm{He}$ becomes superfluid.

In the ${ }^{4} \mathrm{He}$ case, we have employed a DFT approach which takes into account its superfluid character [22], choosing to describe vortex-free configurations where angular momentum is exclusively stored in capillary waves on a deformed cross-section cylinder. Under these conditions, the calculations allow us to carry out a sensible comparison between the rotational behavior of a normal fluid $\left({ }^{3} \mathrm{He}\right)$ and of an irrota-
tional superfluid $\left({ }^{4} \mathrm{He}\right)$ for fixed values of the atom number and angular momentum per unit length. In the presence of vortices in addition to capillary waves, this comparison is obscured as one compares simply connected configurations for ${ }^{3} \mathrm{He}$ cylinders with multiply connected configurations of vortex-hosting ${ }^{4} \mathrm{He}$ cylinders. Let us recall that in the case of droplets, the presence of vortex arrays dramatically changes the appearance of the droplet [18]; at fixed angular momentum and atom number in the droplet, the higher the number of vortices, the more compact (i.e., closer to an oblate axisymmetric shape) the droplet becomes. Hence, the universal behavior found for classical drops [11] is lost. At variance, we have found that, independently of their size, the ${ }^{4} \mathrm{He}$ equilibrium configurations hosting capillary waves alone lay on a line in the scaled angular momentum and angular velocity plane [11], disclosing a de facto nearly universal behavior. Let us mention that it has recently been found [38] that, under appropriate experimental conditions, moderately deformed vortex-free ${ }^{4} \mathrm{He}$ drops prevail when the number of atoms is smaller than about $10^{8}$.

This work is organized as follows. In Sec. II we present the methods used to describe He cylinders, thoroughly described in Refs. [13,17,23] in the case of droplets. The results are discussed in Sec. III, and a summary and discussion are presented in Sec. IV. We outline in Appendix A the rationale of how we have defined dimensionless angular velocity and dimensionless angular momentum for the cylinder geometry, and present in Appendixes B $\left({ }^{3} \mathrm{He}\right)$ and $\mathrm{C}\left({ }^{4} \mathrm{He}\right)$ the results of a simple model where the cross section of the deformed cylinder is restricted to be elliptical, treating ${ }^{3} \mathrm{He}\left({ }^{4} \mathrm{He}\right)$ as a rotational (irrotational) fluid; we call this model elliptic deformations (ED) model. As we shall show, this model, although very pedagogical and often used to represent rotating bodies, becomes quickly unrealistic and it is intended here just to provide a nearly analytical model with which to compare the other elaborated approaches.

## II. MODELS

## A. Classical approach to viscous systems subjected to centrifugal and surface tension forces

The incompressible Navier-Stokes equations are solved in a reference frame rotating about a fixed axis perpendicular to the solution domain. An arbitrary Lagrange-Euler technique is employed which allows the solution domain to deform and conform to the evolving shape of the drop. The rate of displacement of the outer boundary is set by the normal velocity at the outer boundary and surface tension effects are modeled as boundary normal stresses that are proportional to the degree of boundary curvature [39]. Models are time dependent and are initialized with elliptical domains, with rotation axis passing through the origin, with semimajor and semiminor axes of $(1+\delta)$ and $(1+\delta)^{-1}$ where $\delta=0.01$. The small difference from an initial circular shape serves to seed possible nonaxisymmetric perturbations. At each time step of the simulation, the moment of inertia of the drop is calculated and used to update the rotation rate of the reference frame, assuming constant angular momentum. Models are run until the drop shapes achieve a steady state.

The equations are solved using the commercial finiteelement modeling package COMSOL MULTIPHYSICS [40]. References [26,27] give more detailed descriptions of the classical numerical model.

Classical rotating droplets subject to surface tension and centrifugal forces alone are characterized by two dimensionless variables, angular momentum $\Lambda$ and angular velocity $\Omega$, that allow description of the sequence of droplet shapes in a universal phase diagram, independently of the droplet size [11-13]. For the cylinder geometry, the expressions for $\Omega$ and $\Lambda$ are [27] (see also Appendix A)

$$
\begin{align*}
& \Omega \equiv \sqrt{\frac{m \rho_{0} R^{3}}{8 \gamma}} \omega, \\
& \Lambda \equiv \frac{\hbar}{\sqrt{8 \gamma R^{5} m \rho_{0}}} \mathcal{L} \tag{1}
\end{align*}
$$

where $\mathcal{L}$ is the angular momentum per unit length in $\hbar$ units, $\gamma$ and $\rho_{0}$ are the surface tension and atom density of liquid He at zero temperature and pressure, $m$ is the mass of the He atom, and $R$ is the sharp radius of the circular He cylinder at rest. If $\mathcal{N}$ is the number of He atoms per unit length of the cylinder, $R=\sqrt{\mathcal{N} /\left(\pi \rho_{0}\right)}$. For liquid ${ }^{3} \mathrm{He}, \gamma=0.1132 \mathrm{~K} \mathrm{AA}^{-2}$ and $\rho_{0}=0.016342 \mathrm{AA}^{-3}$. Besides, $\hbar^{2} / m=16.0836 \mathrm{~K} \mathrm{AA}^{2}$. For liquid ${ }^{4} \mathrm{He}$ one has $\gamma=0.274 \mathrm{~K} \mathrm{AA}^{-2}, \rho_{0}=0.021836 \mathrm{AA}^{-3}$, and $\hbar^{2} / m=12.1194 \mathrm{~K} \mathrm{AA}^{2}$. Similar to He droplets made of $N$ atoms, which are denoted as $\mathrm{He}_{N}$, we shall denote as $\mathrm{He}_{\mathcal{N}}$ helium cylinders with $\mathcal{N}$ atoms per unit length.

## B. DFT plus semiclassical Thomas-Fermi approach to normal fluid ${ }^{3} \mathrm{He}$

We have adapted to the cylindrical geometry the approach used in Ref. [23] to describe rotating ${ }^{3} \mathrm{He}$ droplets. Within DFT, the total energy $E$ of a ${ }^{3} \mathrm{He}_{\mathcal{N}}$ cylinder at zero temperature is written as a functional of the ${ }^{3} \mathrm{He}$ atom density per unit volume $\rho$, here taken from Ref. [20]:

$$
\begin{equation*}
E[\rho]=\int d \mathbf{r} \frac{\hbar^{2}}{2 m^{*}} \tau+\int d \mathbf{r} \mathcal{E}_{c}[\rho] \equiv \int d \mathbf{r} \mathcal{E}[\rho] \tag{2}
\end{equation*}
$$

where $\mathcal{E}_{c}$ contains the interaction term (in the Hartree approximation) and additional terms which describe nonlocal correlation effects [20]. The first term is the kinetic energy of ${ }^{3} \mathrm{He}$ with an effective mass $m^{*}$, and $\tau$ is the kinetic energy density per unit volume, both depending on $\rho$. In the TF approximation of Ref. [20] (see also Ref. [35]),

$$
\begin{equation*}
\tau=\frac{3}{5}\left(3 \pi^{2}\right)^{2 / 3} \rho^{5 / 3}+\frac{1}{18} \frac{(\nabla \rho)^{2}}{\rho} \tag{3}
\end{equation*}
$$

The second term in Eq. (3) is a Weizsäcker-type gradient correction which is necessary in order to have helium density profiles with an exponential falloff at the surface. The energy functional, represented by the energy per unit volume $\mathcal{E}[\rho]$ in Eq. (2) within the TF approximation given by Eq. (3), accurately reproduces the equation of state of the bulk liquid and yields the correct value for the ${ }^{3} \mathrm{He}$ surface tension [20].

The equilibrium configuration of the cylinder is obtained by solving the Euler-Lagrange (EL) equation arising from
functional minimization of Eq. (2):

$$
\begin{equation*}
\frac{\delta}{\delta \rho}\left\{\frac{\hbar^{2}}{2 m^{*}} \tau+\mathcal{E}_{c}\right\}=\mu \tag{4}
\end{equation*}
$$

where $\mu$ is the ${ }^{3} \mathrm{He}$ chemical potential corresponding to the number of He atoms per unit length of the cylinder. Defining $\Psi=\sqrt{\rho}$, Eq. (4) can be written as a Schrödinger-type equation [20]

$$
\begin{equation*}
\mathcal{H}[\rho] \Psi=\mu \Psi \tag{5}
\end{equation*}
$$

where $\mathcal{H}$ is the one-body effective Hamiltonian that results from the functional variation.

When the rotating cylinder, made of fermions in the normal phase, is addressed in the TF approximation, the Fermi sphere is shifted by the motion of the cylinder as a whole; this adds to its energy density $\mathcal{E}[\rho]$ a rotational term which has the rigidbody appearance $[23,36]$

$$
\begin{equation*}
R[\rho]=\int d \mathbf{r} \mathcal{R}[\rho]=\int d \mathbf{r} \mathcal{E}[\rho]+\frac{1}{2} I \omega^{2}=\int d \mathbf{r} \mathcal{E}[\rho]+\frac{L^{2}}{2 I} \tag{6}
\end{equation*}
$$

where $\mathcal{R}[\rho]$ is the Routhian density of the cylinder, $L$ is the angular momentum, $\omega$ is the angular velocity, and $I$ is the moment of inertia.

Due to the translational invariance of the system along the symmetry axis of the cylinder ( $z$ direction), the atom density per unit volume only depends on the $x$ and $y$ variables and the integral on $z$ just yields the length $\ell$ of the cylinder. Hence, Eq. (5) is a two-dimensional partial differential equation on the $x$ and $y$ variables, and from now on the energy, Routhian, and moment of inertia, integrated on the $x$ and $y$ variables, are quantities per unit length. In particular,

$$
\begin{equation*}
I=m \int d x d y\left(x^{2}+y^{2}\right) \rho(x, y) \tag{7}
\end{equation*}
$$

is the moment of inertia per unit length of the ${ }^{3} \mathrm{He}$ cylinder around the $z$ axis, and $\hbar \mathcal{L}=I \omega$ is the angular momentum per unit length. We stress that the rigid-body moment of inertia is not an imposed ingredient within the DFT-TF framework. It arises naturally from the TF approximation [23,36].

We look for solutions of the EL equation resulting from the functional variation of $R[\rho]$ :

$$
\begin{equation*}
\left\{\mathcal{H}[\rho]-\frac{m}{2}\left(\frac{L}{I}\right)^{2}\left(x^{2}+y^{2}\right)\right\} \Psi(x, y)=\mu \Psi(x, y) \tag{8}
\end{equation*}
$$

Equation (8) has been solved adapting the ${ }^{4} \mathrm{He}$-DFT-BCNTLS computing package [41] to the ${ }^{3} \mathrm{He}$ functional. To take full advantage of the fast Fourier transform [42] used to carry out the convolution integrals in the DFT mean field $\mathcal{H}[\rho]$, we work in Cartesian coordinates and impose periodic boundary conditions (PBC) on the surface of the box where calculations are carried out. In the $x$ and $y$ directions, this box has to be large enough to accommodate the cylinder in such a way that the He density is sensibly zero at the box surface, the effective wave function $\Psi(\mathbf{r})$ being defined at the nodes of a 2D $N_{x} \times N_{y}$ grid spanning the $x$ and $y$ directions. The box is made 3D by adding one single point in the $z$ direction, $N_{z}=1$.

TABLE I. Configuration characteristics of a rotating ${ }^{3} \mathrm{He}_{\mathcal{N}}$ cylinder with $\mathcal{N}=1500$ atoms $/ \AA$ calculated in this work within DFT. C: circular configurations; D: deformed, elliptic-like configurations; TL: two-lobed configurations. $\Lambda$ and $\Omega$ are the dimensionless angular momentum and velocity, and $R$ is the Routhian per unit length. AR is the aspect ratio ( $\mathrm{AR}=1$ for circular configurations), and $I / I_{\text {cir }}$ is the DFT moment of inertia in units of that of the ${ }^{3} \mathrm{He}_{1500}$ circular cylinder of sharp radius at $\Lambda=0, I_{\text {cir }}=m \mathcal{N}^{2} /\left(2 \pi \rho_{0}\right)$.

|  | $\Lambda$ | $\Omega$ | $a_{x}(\AA)$ | $b_{y}(\AA)$ | AR | $I / I_{\text {cir }}$ | $R(\mathrm{~K} / \AA)$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| C | 0 | 0 | 171.41 | 171.41 | 1 | 1 | -3641.965 |
| C | 0.20 | 0.12768 | 171.42 | 171.42 | 1 | 1.0001 | -3639.989 |
| C | 0.40 | 0.25525 | 171.45 | 171.45 | 1 | 1.0006 | -3634.064 |
| C | 0.60 | 0.38261 | 171.49 | 171.49 | 1 | 1.0013 | -3624.194 |
| C | 0.80 | 0.50964 | 171.55 | 171.55 | 1 | 1.0023 | -3610.389 |
| C | 0.90 | 0.57300 | 171.59 | 171.59 | 1 | 1.0029 | -3602.013 |
| C | 0.93 | 0.59198 | 171.60 | 171.60 | 1 | 1.0031 | -3599.310 |
| C | 0.94 | 0.59830 | 171.61 | 171.61 | 1 | 1.0031 | -3598.389 |
| C | 0.95 | 0.60463 | 171.61 | 171.61 | 1 | 1.0032 | -3597.458 |
| C | 0.96 | 0.61095 | 171.62 | 171.62 | 1 | 1.0033 | -3596.518 |
| C | 1.00 | 0.63623 | 171.63 | 171.63 | 1 | 1.0036 | -3592.658 |
| C | 1.10 | 0.69933 | 171.68 | 171.68 | 1 | 1.0043 | -3582.326 |
| C | 1.20 | 0.76227 | 171.70 | 171.70 | 1 | 1.0051 | -3571.019 |
| C | 1.50 | 0.95006 | 171.90 | 171.90 | 1 | 1.0081 | -3531.273 |
| D | 0.90 | 0.57297 | 172.43 | 170.78 | 1.010 | 1.0029 | -3602.013 |
| D | 0.93 | 0.59171 | 174.20 | 169.05 | 1.030 | 1.0035 | -3599.305 |
| D | 0.94 | 0.59709 | 177.13 | 166.19 | 1.066 | 1.0052 | -3598.384 |
| D | 0.95 | 0.59563 | 186.72 | 157.02 | 1.189 | 1.0184 | -3597.461 |
| D | 0.96 | 0.59633 | 190.93 | 153.11 | 1.247 | 1.0279 | -3596.539 |
| D | 1.00 | 0.58093 | 210.16 | 136.12 | 1.544 | 1.0991 | -3592.901 |
| D | 1.10 | 0.55159 | 237.00 | 114.55 | 2.069 | 1.2733 | -3584.134 |
| TL | 1.20 | 0.52539 | 256.81 | 100.08 | 2.566 | 1.4583 | -3575.799 |
| TL | 1.30 | 0.50254 | 273.34 | 88.81 | 3.078 | 1.6517 | -3567.855 |
| TL | 1.50 | 0.46269 | 301.70 | 71.08 | 4.245 | 2.0699 | -3552.930 |
| TL | 1.70 | 0.42981 | 326.07 | 57.22 | 5.698 | 2.5254 | -3539.125 |
| TL | 1.80 | 0.41542 | 337.25 | 51.26 | 6.580 | 2.7666 | -3532.583 |
| TL | 2.00 | 0.39071 | 357.80 | 40.72 | 8.788 | 3.2683 | -3520.123 |
| TL | 2.50 | 0.33938 | 403.92 | 18.74 | 21.550 | 4.7035 | -3492.000 |

A space step of $0.8 \AA$ has been used. We have recalculated several configurations in the circular-to-deformed bifurcation region using a space step of $0.4 \AA$ and have found that the values of the magnitudes shown in Table I are strictly the same. The imposed PBC thus make $\Psi(\mathbf{r})$ translationally invariant in the $z$ direction as required by the cylinder geometry and in practice one still handles $N_{x} \times N_{y}$ points instead of the $N_{x} \times N_{y} \times N_{z}$ points needed for droplets. The differential operators in $\mathcal{H}[\rho]$ are approximated by 13-point formulas. The stationary solution corresponding to given values of $\mathcal{N}$ and $\mathcal{L}$ is obtained starting from an initial guess $\Psi_{0}(\mathbf{r})$ and relaxing it using an imaginary-time step relaxation method [43].

It is worth mentioning that at variance with the classical model for viscous liquids subject to centrifugal and surface tension forces, universality in terms of the scaled $\Lambda$ and $\Omega$ variables is lost when droplets or cylinders are described using more refined models that incorporate other effects, e.g., liquid compressibility and surface thickness effects. Yet, these variables have been found to be very useful as they allow us
to scale the properties of the calculated droplets, which have a radius of tens of nanometers $[17,23]$ to those of the experimental ones which have a radius of hundreds of nanometers [5,7].

For any stationary configuration obtained by solving the EL equation, a sharp density surface is determined by calculating the locus at which the helium density equals $\rho_{0} / 2$. Two lengths are defined corresponding to the shortest and largest distances from the $z$ (rotation) axis to the sharp surface. We call $a_{x}$ the largest distance, and $b_{y}$ the shortest one. The aspect ratio is defined as $\mathrm{AR}=a_{x} / b_{y}$, being one for cylinders (circular cross section) and lager than one otherwise (deformed cross section).

## C. DFT approach to superfluid ${ }^{4} \mathrm{He}$

Within DFT, the energy of the ${ }^{4} \mathrm{He}_{\mathcal{N}}$ cylinder is written as a functional of the atom density per unit volume $\rho(\mathbf{r})$ as [22]

$$
\begin{equation*}
E[\rho]=T[\rho]+E_{c}[\rho]=\frac{\hbar^{2}}{2 m} \int d \mathbf{r}|\nabla \Psi(\mathbf{r})|^{2}+\int d \mathbf{r} \mathcal{E}_{c}[\rho], \tag{9}
\end{equation*}
$$

where the first term is the kinetic energy, with $\rho(\mathbf{r})=|\Psi(\mathbf{r})|^{2}$, and the functional $\mathcal{E}_{c}$ contains the interaction term (in the Hartree approximation) and additional terms which describe nonlocal correlation effects [44].

The equilibrium configuration of the cylinder is obtained by solving the EL equation resulting from the functional minimization of Eq. (9):

$$
\begin{equation*}
\left\{-\frac{\hbar^{2}}{2 m} \nabla^{2}+\frac{\delta \mathcal{E}_{c}}{\delta \rho}\right\} \Psi(\mathbf{r}) \equiv \mathcal{H}[\rho] \Psi(\mathbf{r})=\mu \Psi(\mathbf{r}) \tag{10}
\end{equation*}
$$

where $\mu$ is the ${ }^{4} \mathrm{He}$ chemical potential.
Similarly to the case of ${ }^{4} \mathrm{He}$ droplets, to study spinning ${ }^{4} \mathrm{He}$ cylinders we work in the corotating frame at angular velocity $\omega$,

$$
\begin{equation*}
E^{\prime}[\rho]=E[\rho]-\hbar \omega\left\langle\hat{L}_{z}\right\rangle \tag{11}
\end{equation*}
$$

where $\hat{L}_{z}$ is the dimensionless angular momentum operator in the $z$ direction; one looks for solutions of the EL equation resulting from the functional variation of $E^{\prime}[\rho]$,

$$
\begin{equation*}
\left\{\mathcal{H}[\rho]-\hbar \omega \hat{L}_{z}\right\} \Psi(\mathbf{r})=\mu \Psi(\mathbf{r}) \tag{12}
\end{equation*}
$$

The differential operators in $\mathcal{H}[\rho]$ and the angular momentum operator are approximated by 13-point formulas. As in the ${ }^{3} \mathrm{He}$ case, the stationary solution corresponding to given values of $\mathcal{N}$ and $\mathcal{L}$ is obtained starting from an initial guess $\Psi_{0}(\mathbf{r})$ and relaxing it using an imaginary-time step relaxation method [43].

Angular momentum can be stored in a superfluid ${ }^{4} \mathrm{He}$ sample in the form of surface capillary waves and/or quantized vortices $[6,18]$. Since we are considering only the contribution of capillary waves, we have used the so-called "imprinting" procedure starting the imaginary-time relaxation for the effective wave function

$$
\begin{equation*}
\Psi_{0}(\mathbf{r})=\rho_{0}^{1 / 2}(\mathbf{r}) e^{i \alpha x y} \tag{13}
\end{equation*}
$$

The complex phase $e^{i \alpha x y}$ imprints a surface capillary wave with quadrupolar symmetry around the $z$ axis [45], and $\rho_{0}(\mathbf{r})$


FIG. 1. Density profile of the ${ }^{3} \mathrm{He}_{\mathcal{N}}$ cylinder with $\mathcal{N}=1500$ atoms $/ \AA$ for two circular configurations corresponding to $\Lambda=0$ (red dashed line) and 1.5 (black solid line). The $\Lambda=1.5$ cylinder is metastable.
is an arbitrary, vortex-free cylinder density. The initial value of $\alpha$ is guessed, and during the iterative solution of Eq. (12) the shape of the cylinder changes to provide, at convergence, the lowest-energy vortex-free configuration for the desired $\mathcal{L}$ value, which requires adjustment of the value of $\omega$ every iteration.

Writing $\Psi(\mathbf{r}) \equiv \phi(\mathbf{r}) \exp [i \mathcal{S}(\mathbf{r})]$, the velocity field of the superfluid is

$$
\begin{equation*}
\mathbf{v}(\mathbf{r})=\frac{\hbar}{m} \operatorname{Im}\left\{\frac{\nabla \Psi(\mathbf{r})}{\Psi(\mathbf{r})}\right\}=\frac{\hbar}{m} \nabla \mathcal{S}(\mathbf{r}) \tag{14}
\end{equation*}
$$

It can be visualized with streamlines of the superfluid flow [18]. In the ${ }^{3} \mathrm{He}$ case, the velocity field consists of circumferences centered at the rotation axis, with $v(r)=\omega r$, being $r$ the distance to the axis.

Equations (10) and (12) are two-dimensional partial differential equations depending on the $x$ and $y$ variables which have been solved using the ${ }^{4} \mathrm{He}-\mathrm{DFT}-\mathrm{BCN}-\mathrm{TLS}$ computing package [41].

## III. RESULTS

We have carried out detailed DFT calculations for a cylinder with $\mathcal{N}=1500$ atoms $/ \AA$ which has a radius $R=170.93$ $\AA\left({ }^{3} \mathrm{He}\right)$ or $R=147.87 \AA\left({ }^{4} \mathrm{He}\right)$ at rest. As illustrated in Fig. 1 for ${ }^{3} \mathrm{He}$, liquid helium is fairly incompressible and hence the cross section area of the rotating $\mathrm{He}_{\mathcal{N}}$ cylinder remains sensibly equal to $\pi R^{2}$ during deformation.

## A. ${ }^{3} \mathrm{He}$ cylinders

Table I collects the DFT results obtained for ${ }^{3} \mathrm{He}$ cylinders. To determine the circular-to-deformed bifurcation point, one has to compare the Routhian $R[\rho]$ of the circular cylinder to that of the deformed cylinder for the same $\Lambda$ and $\mathcal{N}$ values; the configuration with the smaller $R[\rho]$ is the equilibrium configuration.

One can see from Table I that the difference between the Routhians of the circular and deformed cylinders is very
small in a wide interval of $\Lambda$ values between 0.900 and 0.960 , which makes rather delicate to determine the bifurcation point within the DFT. We take the angular momentum at which the aspect ratio $\mathrm{AR}=a_{x} / b_{y}$ starts to clearly differ from one as the bifurcation point, having obtained $(\Lambda, \Omega)=$ ( $0.90,0.573$ ). In the classical model, bifurcation occurs at $(\Lambda, \Omega)=(0.960,0.616)[27]$.

To compare the classical and DFT results for the Routhian (total energy including rotation energy) per unit length, one has to remember that in classical models only surface and rotation energy are considered. Consequently, we have to identify first the energies that are implicitly involved in the DFT calculation. To this end, it is convenient to split the energy per unit length of the cylinder $E / \ell$ into different terms, in a way similar in spirit as how the energy of the atomic nucleus is written as a "mass formula," namely,

$$
\begin{equation*}
E / \ell=\epsilon_{0} \mathcal{N}+2 \pi R \gamma+E_{0}=\epsilon_{0} \pi R^{2} \rho_{0}+2 \pi R \gamma+E_{0} \tag{15}
\end{equation*}
$$

where $\epsilon_{0}=-2.49 \mathrm{~K}$ is the energy per atom in liquid ${ }^{3} \mathrm{He}$ and $E_{0}$ is a constant term. Let us mention that the presence of a constant term in the nuclear mass formula is common in the most elaborated ones [46] and it appears after leading terms of $R^{3}$ (volume), $R^{2}$ (surface), and $R$ (curvature) type. In the case of the cylinder, it naturally comes after the surface term. It is worth noticing that mass formulas have also been adjusted for ${ }^{3} \mathrm{He}$ and ${ }^{4} \mathrm{He}$ droplets which include a fairly large constant term [21,35].

The parameter $E_{0}$ can be determined from the DFT values at $\Lambda=0$. For $\mathcal{N}=1500$ atoms $/ \AA, R=170.93 \AA$ and $\epsilon_{0} \mathcal{N}$ is $-3735 \mathrm{~K} / \AA$, yielding $E_{0}=28.58 \mathrm{~K} / \AA$.

We thus see that the volume and constant energy contributions have to be subtracted from the DFT Routhian for a sensible comparison with the classical results. Since in the classical calculations energies per unit length are made dimensionless dividing them by $8 \gamma R$ [27], the quantity that can be directly compared with the classical result is the dimensionless reduced DFT Routhian per unit length defined as

$$
\begin{equation*}
\frac{1}{8 \gamma R}\left\{R[\rho]-\epsilon_{0} \mathcal{N}-E_{0}\right\} \tag{16}
\end{equation*}
$$

We have represented it as a function of $\Lambda$ in Fig. 2 together with the classical result. It can be seen that they agree very well, with some minor differences showing up at large deformations.

Figure 3 shows the aspect ratio as a function of the rescaled angular momentum $\Lambda$ for ${ }^{3} \mathrm{He}$ cylinders obtained with the DFT, classical, and ED approaches. The outlines of several classical shapes are drawn in the inset.

We display in Fig. 4 the density of the ${ }^{3} \mathrm{He}$ cylinder for several values of $\Lambda$ obtained with the DFT method; superposed to the densities we have plotted several circulation lines. In the DFT approach the cross section of the cylinder becomes two-lobed at $\Lambda \sim 1.1$. The outlines of classical shapes are superimposed to the two-dimensional DFT densities. It can be seen that they are very similar to the DFT ones except for $\Lambda=1$, for which the DFT density is more deformed because this configuration is further away from the DFT bifurcation than the classical one is from the classical bifurcation point.


FIG. 2. Reduced DFT Routhian per unit length $\left(R[\rho]-\epsilon_{0} \mathcal{N}-\right.$ $\left.E_{0}\right) /(8 \gamma R)$ as a function of rescaled angular momentum. Black triangles: DFT circular configurations. Red circles: DFT deformed configurations. Solid blue line: classical circular configurations. Dashed blue line: classical deformed configurations.

This effect diminishes at larger deformations where the differences are minor.

Figure 5 shows the $\Omega(\Lambda)$ equilibrium line for ${ }^{3} \mathrm{He}$ obtained with the classical and DFT approaches. This line is very similar for both methods. As for ${ }^{3} \mathrm{He}$ droplets [23], the minor differences in the deformed branch are attributed to a better description of the droplet surface and to quantum kinetic energy contributions in the DFT approach which, together with compressibility effects, are lacking in classical models. Also shown in Fig. 5 is the result obtained with the ED model as explained in Appendix C. Just away from the bifurcation point the ED approach yields results very different from the two others, indicating that cross-section shapes quickly become nonelliptical.


FIG. 3. Aspect ratio vs rescaled angular momentum for the ${ }^{3} \mathrm{He}$ cylinder in the DFT, classical, and ED approaches. AR $=1$ corresponds to circular configurations. The lines are cubic splines of the calculated points. Also shown are the outlines of classical shapes with angular momenta $\Lambda=0.5,1,1.5$, and 2 .


FIG. 4. Two-dimensional densities for the ${ }^{3} \mathrm{He}_{1500}$ cylinder in the DFT approach. From top to bottom, they correspond to $\Lambda=$ $0.5,1,1.5$, and 2 . The color bar represents the ${ }^{3} \mathrm{He}$ density in $\mathrm{A}^{-3}$. Several streamlines are superimposed. Also shown are the outlines of classical shapes (magenta lines).

## B. ${ }^{4} \mathrm{He}$ cylinders

Table II collects the DFT results obtained for ${ }^{4} \mathrm{He}$ cylinders. Since a superfluid system cannot rotate around a symmetry axis, the cross section of rotating $(\Lambda \neq 0)$ vortexfree ${ }^{4} \mathrm{He}$ cylinders must necessarily be noncircular. The irrotational moment of inertia, defined as $I_{\text {irr }}=\left\langle L_{z}\right\rangle / \omega$, drops to zero as $\Lambda \rightarrow 0$. We have plotted $I_{\text {irr }}$ in Fig. 6 in units of the rigid-body moment of inertia $I_{\mathrm{RB}}$ [Eq. (7)]. It can be seen that $I_{\text {irr }}$ approaches $I_{\text {RB }}$ at large angular momenta, being rather different even for large deformations. For the


FIG. 5. Rescaled angular velocity $\Omega$ vs rescaled angular momentum $\Lambda$ for the ${ }^{3} \mathrm{He}_{1500}$ cylinder in the ED, classical, and DFT approaches. Black triangles, circular DFT configurations; red circles, deformed DFT configurations; blue asterisks, classical calculations [27]. The DFT configurations to the right of the vertical arrow are two-lobed. The lines are cubic splines of the calculated points.
sake of comparison, we also display the result of the ED model, that works surprisingly well even for $\Lambda$ values for which the configuration is no longer ellipticlike but two-lobed. The difference between classical and superfluid moments of

TABLE II. Configuration characteristics of a rotating ${ }^{4} \mathrm{He}_{\mathcal{N}}$ cylinder with $\mathcal{N}=1500$ atoms $/ \AA$ calculated in this work within DFT. $\Lambda$ and $\Omega$ are the dimensionless angular momentum and velocity, and $R$ is the Routhian per unit length. AR is the aspect ratio, and $I_{\text {irr }} / I_{\mathrm{RB}}$ is the DFT moment of inertia in units of that of a rigidbody ${ }^{4} \mathrm{He}$ cylinder for the same $\Lambda$ value. D : deformed ellipticlike configurations; TL: two-lobed configurations.

|  | $\Lambda$ | $\Omega$ | $a_{x}(\AA)$ | $b_{y}(\AA)$ | AR | $I_{\mathrm{irr}} / I_{\mathrm{RB}}$ | $R(\mathrm{~K} / \AA)$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| D | 0.001 | 0.43503 | 150.96 | 145.31 | 1.039 | 0.0015 | -10466.31 |
| D | 0.01 | 0.43537 | 157.12 | 139.25 | 1.128 | 0.0145 | -10465.04 |
| D | 0.02 | 0.43561 | 160.89 | 135.58 | 1.187 | 0.0289 | -10463.63 |
| D | 0.04 | 0.43606 | 166.24 | 130.43 | 1.275 | 0.0568 | -10460.80 |
| D | 0.05 | 0.43627 | 168.42 | 128.35 | 1.312 | 0.0705 | -10459.39 |
| D | 0.10 | 0.43772 | 177.09 | 120.26 | 1.473 | 0.1355 | -10452.30 |
| D | 0.20 | 0.44012 | 189.77 | 108.94 | 1.742 | 0.2510 | -10438.06 |
| D | 0.30 | 0.44188 | 200.00 | 100.37 | 1.993 | 0.3498 | -10423.77 |
| D | 0.40 | 0.44295 | 209.06 | 93.28 | 2.241 | 0.4344 | -10409.43 |
| TL | 0.50 | 0.44335 | 217.45 | 87.16 | 2.495 | 0.5069 | -10395.07 |
| TL | 0.60 | 0.44304 | 225.44 | 81.72 | 2.759 | 0.5691 | -10380.70 |
| TL | 0.80 | 0.44136 | 240.38 | 72.21 | 3.329 | 0.6680 | -10352.24 |
| TL | 1.00 | 0.43536 | 253.38 | 64.13 | 3.951 | 0.7502 | -10323.78 |
| TL | 1.20 | 0.42614 | 269.77 | 56.73 | 4.755 | 0.7980 | -10295.91 |
| TL | 1.50 | 0.40932 | 291.30 | 46.74 | 6.233 | 0.8558 | -10255.26 |
| TL | 2.00 | 0.37564 | 326.57 | 31.68 | 10.310 | 0.9096 | -10191.55 |



FIG. 6. DFT irrotational moment of inertia $I_{\text {irr }}$ in units of the rigid-body moment of inertia $I_{\mathrm{RB}}$ for ${ }^{4} \mathrm{He}$ cylinders as a function of $\Lambda$. The lines are cubic splines of the calculated points.
inertia, also appearing in ${ }^{4} \mathrm{He}$ droplets [16], is a signature of their different response to rotations.

Figure 7 shows the aspect ratio as a function of the rescaled angular momentum for ${ }^{4} \mathrm{He}$ cylinders obtained with the DFT and ED approaches. We display in Fig. 8 the density of the ${ }^{4} \mathrm{He}$ cylinder for several values of $\Lambda$ obtained with the DFT method; superposed to the densities we have plotted several circulation lines. The cross section of the cylinder becomes two-lobed at $\Lambda \sim 0.5$. The outlines of classical shapes are superimposed to the two-dimensional DFT densities. The difference between classical and DFT densities is apparent up to large $\Lambda$ values, reflecting the distinct rotational response of a normal fluid from that of a superfluid.

Figure 9 shows the $\Omega(\Lambda)$ equilibrium line for ${ }^{4} \mathrm{He}$ obtained with the ED and DFT methods. As for ${ }^{3} \mathrm{He}$ cylinders, the ED approximation quickly becomes inadequate. The finite value of $\Omega$ at very small values of $\Lambda$, also found for ${ }^{4} \mathrm{He}$ droplets [17], is the equivalent of the "rotational Meissner effect" occurring when liquid helium in a rotating cylinder is cooled through the lambda point: at sufficiently slow


FIG. 7. Aspect ratio vs rescaled angular momentum for the ${ }^{4} \mathrm{He}$ cylinder in the ED and DFT approaches. The lines are cubic splines of the calculated points.


FIG. 8. Two-dimensional densities for the ${ }^{4} \mathrm{He}_{1500}$ cylinder in the DFT approach. From top to bottom, they correspond to $\Lambda=$ $0.5,1,1.5$, and 2 . The color bar represents the ${ }^{4} \mathrm{He}$ density in $\mathrm{AA}^{-3}$. Several streamlines are superimposed. Also shown are the outlines of classical shapes (magenta lines).
rotational speeds the superfluid forms in a state of zero total angular momentum, causing the container to rotate faster [47].

## IV. DISCUSSION AND OUTLOOK

As for helium droplets [23], we have expectedly found that the rotating behavior of normal fluid ${ }^{3} \mathrm{He}$ cylinders is very similar to rotating incompressible, viscous cylinders only subject to surface tension and centrifugal forces. Even for fine details such as the aspect ratio as a function of rescaled angular momentum or the $\Omega(\Lambda)$ equilibrium line, we have found a good agreement between classical and DFT results.

Figures 4 and 8 clearly illustrate how different is instead the response to rotation of the normal fluid ${ }^{3} \mathrm{He}$ cylinder from that of superfluid ${ }^{4} \mathrm{He}$, especially at moderate angular momentum values, i.e., at aspect ratios not very different from one. Only when $\Lambda$ is large do the density profiles become similar. It is worth recalling that the number of droplets having large


FIG. 9. Rescaled angular velocity $\Omega$ vs rescaled angular momentum $\Lambda$ for the ${ }^{4} \mathrm{He}_{1500}$ cylinder in the ED and DFT approaches. The DFT configurations to the right of the vertical arrow are two-lobed. The lines are cubic splines of the calculated points.
deformations is found to be small in the experiments [10]. It is also worth seeing that even for these very deformed cylinders, the moment of inertia of superfluid ${ }^{4} \mathrm{He}$ cylinders is $10 \%-20 \%$ smaller that the rigid-body value (Fig. 6).

A close look at the appearance of the streamlines in Figs. 4 and 8 shows that while ${ }^{3} \mathrm{He}$ cylinders do rotate and streamlines are circumferences around the rotation axis, ${ }^{4} \mathrm{He}$ cylinders do not; the streamlines do not correspond to a rigid rotation, but to an irrotational flow. Lets us remember that the fluid motion is a combination of translation, rotation, and deformation of the fluid elements, and only when vorticity (defined as $\boldsymbol{\nabla} \times \mathbf{v}$ ) [48] is nonzero, may one speak of a true rotation. Vorticity is distributed inside the cylinder in the normal phase ${ }^{3} \mathrm{He}$ and it equals $2 \omega$ as for a rotating rigid body in steady rotation. Since the superfluid flow is irrotational, $\boldsymbol{\nabla} \times \mathbf{v}=0$ for ${ }^{4} \mathrm{He}$. In this case, fluid elements translate and deform, but do not rotate. An illuminating discussion of this behavior, based on a paper by Tritton [49]. can be found in Ref. [32]. The different behavior of ${ }^{3} \mathrm{He}$ and vortex-free ${ }^{4} \mathrm{He}$ cylinders in rotation is also apparent in the $\Omega(\Lambda)$ equilibrium line and in the moment of inertia as a function of the angular momentum, Figs. 5, 6, and 9 .

When the superfluid ${ }^{4} \mathrm{He}$ sample hosts linear vortices, the situation dramatically changes, as the vortex array tends to confer to the droplet or cylinder the appearance of a rotating rigid body [17,50]. To exemplify this key issue, we have redone the calculation of the rotating ${ }^{4} \mathrm{He}$ cylinder at $\Lambda=0.5$ when it hosts a large vortex array.

One single vortex along the axis of the circular cylinder has an angular momentum per unit length $\mathcal{L}=\mathcal{N}$ [51]. From the definition of $\Lambda$, Eq. (1), it corresponds to a rather small value if $\mathcal{N}=1500$ atoms $/ \AA$, namely, $\Lambda=0.09$. We have imprinted a nine-vortex array to the cylinder by using the wave function [18]

$$
\begin{equation*}
\Psi_{0}(\mathbf{r})=\rho_{0}^{1 / 2}(\mathbf{r}) \prod_{j=1}^{n_{v}} \frac{\left(x-x_{j}\right)+i\left(y-y_{j}\right)}{\sqrt{\left(x-x_{j}\right)^{2}+\left(y-y_{j}\right)^{2}}} \tag{17}
\end{equation*}
$$



FIG. 10. Two-dimensional density for the ${ }^{4} \mathrm{He}_{1500}$ cylinder hosting nine vortex lines at $\Lambda=0.5$ in the DFT approach. Several streamlines are superimposed. Also shown is the outline of classical shape (magenta line).
with $n_{v}=9$, where $\left(x_{j}, y_{j}\right)$ is the initial position of the $j$ vortex core. We have started from a deformed cylinder and have chosen an initial vortex array with a centered vortex and eight vortices around it at the same distance $d$, which is the lowest-energy configuration in the classical case [31]. During the iterative solution of Eq. (12) both the vortex-core structure and positions, and the shape of the cylinder, may change to provide at convergence the lowest Routhian configuration.

The effect caused by the presence of the vortex array on the morphology of the free-standing cylinder can be appreciated in Fig. 10: the very deformed vortex-free cylinder, with $\mathrm{AR}=2.50$ (see Table II), has become circular ( $\mathrm{AR}=1.001$ ), coinciding with the classical result. For smaller $n_{v}$ values the cylinder may still be deformed, but not as much as the vortex-free one. For instance, when $n_{v}=6$ (which is the equilibrium configuration at $\Lambda=0.5$ ), $\mathrm{AR}=1.25$. As in the case of drops, vortices and capillary waves coexist [6,18]. Let us mention that for the $\Lambda=0.5$ value used here, the $n_{v}=9$ configuration is also more stable than the vortex-free one.

It is also worth noticing that for a $n_{v}$ vortex array in a rotating cylinder of radius $R$, the total angular momentum can be written as [52]

$$
\begin{equation*}
\mathcal{L}=\mathcal{N} \sum_{j=1}^{n_{v}}\left[1-\left(\frac{d_{j}}{R}\right)^{2}\right] \tag{18}
\end{equation*}
$$

where $d_{j}$ is the distance of the $j$ vortex to the symmetry axis, which in our case reduces to $\mathcal{L}=\mathcal{N}+8 \mathcal{N}\left[1-(d / R)^{2}\right]$. This expression yields $d=96.8 \AA$ for $R=147.9 \AA$ and $\Lambda=0.5$, in perfect agreement with the DFT result.

The angular velocity leading to vortex nucleation can be straightforwardly determined, $w_{c}=\Delta E /(\hbar N)$, where $\Delta E$ is the energy difference between the one vortex and the vortex-free configurations [22]. This yields, in rescaled units, $\left(\Lambda_{c}, \Omega_{c}\right)=(0.09,0.17)$ and, hence, beyond $\Lambda_{c}=0.09$, vortex-free configurations are metastable or unstable against
vortex nucleation. For a thorough discussion of the energetic and stability of vortices in rotating ${ }^{4} \mathrm{He}$ cylinders within the DFT approach, the interested reader is referred to Ref. [29].

All configurations obtained in this work, in particular those displayed in Figs. 4 and 8, are stationary in the co-rotating frame: the framework that rotates with angular velocity $\omega$ with respect to the laboratory frame. Consequently, they would be seen from the laboratory as if they were rotating like a rigid body with the angular frequency $\omega$ imposed to obtain them [53]. The ${ }^{3} \mathrm{He}$ cylinder would undergo a true rotation, but this rotation would only be apparent for the ${ }^{4} \mathrm{He}$ cylinder. Examples of apparent rotations in the case of ${ }^{4} \mathrm{He}$ droplets, obtained within time-dependent DFT, can be found in Refs. [18,45].

Ongoing experiments on mixed helium droplets [25], which exhibit a core-shell structure with a crust made of ${ }^{3} \mathrm{He}$ atoms in the normal state and a superfluid core mostly made of ${ }^{4} \mathrm{He}$ atoms, and calculations on mixed droplets made of immiscible viscous fluids [27] call for extending the DFT calculations carried out for mixed helium droplets [23] to larger sizes, also relaxing the constraint that ${ }^{3} \mathrm{He}$ and ${ }^{4} \mathrm{He}$ moieties are concentric. When the ${ }^{4} \mathrm{He}$ core displaces with respect to the center of mass of the droplet, the moment of inertia increases from that of centered drops, influencing how angular momentum is stored in the mixed droplet. In particular, it might affect quantum vortex nucleation in the ${ }^{4} \mathrm{He}$ core, which could be hindered. The cross section of deformable cylinders is a reasonable representation of the density of a large rotating helium droplet on the plane of symmetry perpendicular to the rotation axis [6]. The use of cylindrical geometry would allow the extension of DFT calculations to helium drops of larger cross section that would otherwise be computationally prohibitive.

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## APPENDIX A: ROTATING ${ }^{3}$ He CYLINDERS HELD TOGETHER BY SURFACE TENSION: THE GENERAL CASE

In this Appendix we outline how dimensionless angular momentum $\Lambda$ and dimensionless angular velocity $\Omega$ can be introduced in the case of an incompressible cylinder of length $\ell$ and radius $R$, modeled by viscous cylinders subject to surface tension and centrifugal forces alone. To connect with the 2D DFT results, the length $\ell$ will be taken as infinite, and eventually all extensive quantities will be referred to per unit
length. We closely follow the procedure by Brown and Scriven in the case of droplets [11].

In cylindrical coordinates $(r, \phi, z)$, the radial vector to the surface is described by $\mathbf{r}=R f(\phi) \hat{\mathbf{r}}$, where $\hat{\mathbf{r}}$ is the unit vector in the radial direction and $\phi$ is the azimuthal angle. This representation handles circular, ellipticlike, and multilobed cylinders, with the limitation that $\mathbf{r}$ must not intersect the surface of the cylinder more than once.

If the cylinder rotates around its axis ( $z$ axis) at angular velocity $\omega$, the energy per unit length is given by

$$
\begin{equation*}
E=\gamma L_{c}+\frac{1}{2} I \omega^{2} \tag{A1}
\end{equation*}
$$

where $\gamma$ is the surface tension, $L_{c}$ is the perimeter of the cross section of the cylinder

$$
\begin{equation*}
L_{c}=2 R \int_{0}^{\pi} d \phi \sqrt{f^{2}(\phi)+\left(\frac{\partial f}{\partial \phi}\right)^{2}} \tag{A2}
\end{equation*}
$$

and $I$ is the moment of inertia per unit length

$$
\begin{equation*}
I=\frac{1}{2} m \rho_{0} R^{4} \int_{0}^{\pi} d \phi f^{4}(\phi) \equiv m \rho_{0} R^{4} \mathcal{I} \tag{A3}
\end{equation*}
$$

where $\mathcal{I}$ is the dimensionless moment of inertia per unit length. Writing the energy per unit length in units of $2 \gamma R$, we have

$$
\begin{equation*}
\frac{E}{2 \gamma R}=\int_{0}^{\pi} d \phi\left\{\sqrt{f^{2}(\phi)+\left(\frac{\partial f}{\partial \phi}\right)^{2}}+\frac{m \rho_{0} \omega^{2} R^{3}}{8 \gamma} f^{4}(\phi)\right\} \tag{A4}
\end{equation*}
$$

The ratio

$$
\begin{equation*}
\Sigma \equiv \Omega^{2}=\frac{m \rho_{0} \omega^{2} R^{3}}{8 \gamma} \tag{A5}
\end{equation*}
$$

is called rotational Bond number $[11,33,54]$ and is the dimensionless measure of the square of angular velocity $\Omega$. A dimensionless angular momentum $\Lambda$ is introduced such that $\Lambda=\mathcal{I} \Omega$. This yields Eqs. (1) in the main text. Equation (A4) shows that within this model the solution is universal and can be obtained once for all rotating cylinders.

We want to comment that our definition of $\Omega$ coincides with that of Ref. [33]; unfortunately, the definition of $\Lambda$ is not given in that reference.

## APPENDIX B: ROTATING ${ }^{3} \mathrm{He}$ CYLINDERS HELD TOGETHER BY SURFACE TENSION: ELLIPTIC DEFORMATIONS

It is illustrative to address the classical rotating cylinder when deformations are restricted to be elliptic, as it is nearly analytical and it is expected to be a fair approximation to describe the circular to deformed bifurcation. Proceeding as in previous Appendix A, the surface energy per unit length of the cylinder is written as $E_{s}=\gamma L_{c}$, where

$$
\begin{equation*}
L_{c}=4 a \int_{0}^{\pi / 2} d \phi \sqrt{1-e^{2} \sin ^{2} \phi} \equiv 4 a \mathbf{E}(e) \tag{B1}
\end{equation*}
$$

is the perimeter of the ellipse

$$
\begin{equation*}
\frac{x^{2}}{a^{2}}+\frac{y^{2}}{b^{2}}=1 \tag{B2}
\end{equation*}
$$

with eccentricity $e=\sqrt{a^{2}-b^{2}} / a$ (we take $a \geqslant b$ ). If the fluid is incompressible, $\pi a b=\pi R^{2}$. In Eq. (B1), $\mathbf{E}(e)$ is the complete elliptic integral of the second kind [55]

$$
\begin{equation*}
\mathbf{E}(e)=\int_{0}^{\pi / 2} d \phi \sqrt{1-e^{2} \sin ^{2} \phi} \tag{B3}
\end{equation*}
$$

Defining $\xi=a / R=\left(1-e^{2}\right)^{-1 / 4}$, where $R$ is the radius of the cylinder at rest, the moment of inertia per unit length can be expressed as

$$
\begin{equation*}
I=\frac{\pi}{4} m \rho_{0} R^{4} \frac{\xi^{4}+1}{\xi^{2}} \tag{B4}
\end{equation*}
$$

The energy per unit length in units of $8 \gamma R$ is

$$
\begin{equation*}
\frac{E}{8 \gamma R}=\frac{1}{2} \xi \mathbf{E}(e)+\frac{2}{\pi} \Lambda^{2} \frac{\xi^{2}}{\xi^{4}+1} \tag{B5}
\end{equation*}
$$

which for the circular cylinder reduces to

$$
\begin{equation*}
\frac{E}{8 \gamma R}=\frac{\pi}{4}+\frac{1}{\pi} \Lambda^{2} \tag{B6}
\end{equation*}
$$

Determining the equilibrium configuration for a given $\Lambda$ amounts to solving for $e$ (or $\xi$ ) the algebraic equation $d \mathcal{E} / d \xi=0$ :

$$
\begin{equation*}
\mathbf{E}(e)+\frac{2}{\xi^{4}-1}[\mathbf{E}(e)-\mathbf{K}(e)]+\frac{8}{\pi} \Lambda^{2} \frac{\xi\left(1-\xi^{4}\right)}{\left(\xi^{4}+1\right)^{2}}=0 \tag{B7}
\end{equation*}
$$

where $\mathbf{K}(e)$ is the complete elliptic integral of the first kind [55]

$$
\begin{equation*}
\mathbf{K}(e)=\int_{0}^{\pi / 2} d \phi \frac{1}{\sqrt{1-e^{2} \sin ^{2} \phi}} \tag{B8}
\end{equation*}
$$

The determination of the equilibrium configuration is facilitated by the existence of accurate easy-to-use approximations for $\mathbf{K}(e)$ and $\mathbf{E}(e)$ [56]. The dimensionless angular velocity is obtained from the $\xi$ value of the equilibrium configuration at the given $\Lambda$ as

$$
\begin{equation*}
\Omega=\frac{4}{\pi} \frac{\xi^{2}}{\xi^{4}+1} \Lambda \tag{B9}
\end{equation*}
$$

which reduces to $\Omega=2 \Lambda / \pi$ for the circular cylinder.
We have found that the circular-to-elliptical shape transition occurs at $\Lambda=0.966$, i.e., at $(\Lambda, \Omega)=(0.966,0.612)$. Notice that $\Sigma$ at the bifurcation point is $\Sigma=\frac{3}{8}$ [33], which yields $\Omega=\sqrt{\frac{3}{8}}=0.612$. At bifurcation, $\Omega=2 \Lambda / \pi$ and one has $\Lambda=0.966$ instead of the value close to 2 shown in Fig. 4(a) of Ref. [33] (see also Ref. [27]). For this reason, we have inferred that the definition of $\Lambda$ in that reference likely is a factor of 2 larger than ours. As shown in Fig. 5, the elliptic deformation model is unrealistic for $\Lambda \gtrsim 1.1$ and misses the appearance of two-lobed configurations. We conclude that deformations after bifurcation quickly become complex and representing the cross section of the deformed cylinder by an ellipse is a rough approximation.

## APPENDIX C: ROTATING ${ }^{4} \mathrm{He}$ CYLINDERS HELD TOGETHER BY SURFACE TENSION: ELLIPTIC DEFORMATIONS

It is also illustrative to consider the case of a vortex-free superfluid ${ }^{4} \mathrm{He}$ elliptic cylinder in which angular momentum is stored only in capillary waves. The flow is irrotational and its velocity derives from a velocity potential $\chi(x, y)=\alpha x y$, which yields $[45,51,57]$

$$
\begin{equation*}
\mathbf{v}=\nabla \chi(x, y)=\omega \frac{a^{2}-b^{2}}{a^{2}+b^{2}}(y, x, 0) \tag{C1}
\end{equation*}
$$

The $z$ component of

$$
\begin{equation*}
m \rho_{0} \int d x d y \mathbf{r} \times \mathbf{v} \tag{C2}
\end{equation*}
$$

is the angular momentum per unit length

$$
\begin{equation*}
\mathcal{L}=\frac{\pi}{4} m \rho_{0} \frac{\left(a^{2}-b^{2}\right)^{2}}{a^{2}+b^{2}} a b \omega \equiv I_{\mathrm{irr}} \omega \tag{C3}
\end{equation*}
$$

where $I_{\mathrm{irr}}$ is the irrotational moment of inertia per unit length. Writing it in terms of $R$ and $\xi$ we have

$$
\begin{equation*}
I_{\mathrm{irr}}=\frac{\pi}{4} m \rho_{0} R^{4} \frac{\left(\xi^{4}-1\right)^{2}}{\xi^{2}\left(\xi^{4}+1\right)} \tag{C4}
\end{equation*}
$$

[1] J. P. Toennies and A. F. Vilesov, Angew. Chem. Int. Ed. 43, 2622 (2004).
[2] J. Harms, J. P. Toennies, and F. Dalfovo, Phys. Rev. B 58, 3341 (1998).
[3] J. Harms, J. P. Toennies, M. Barranco, and M. Pi, Phys. Rev. B 63, 184513 (2001).
[4] R. M. Tanyag, C. F. Jones, C. Bernando, S. M. O’Connell, D. Verma, and A. F. Vilesov, in Theoretical and Computational Chemistry Series No. 11, edited by O. Dulieu and A. Osterwalder (Royal Society of Chemistry, Cambridge, UK, 2018), p. 389.
[5] L. F. Gomez, K. R. Ferguson, J. P. Cryan, C. Bacellar, R. M. P. Tanyag, C. Jones, S. Schorb, D. Anielski, A. Belkacem, C. Bernando, R. Boll, J. Bozek, S. Carron, G. Chen, T. Delmas, L. Englert, S. W. Epp, B. Erk, L. Foucar, R. Hartmann et al., Science 345, 906 (2014).
[6] S. M. O. O’Connell, R. M. P. Tanyag, D. Verma, Ch. Bernando, W. Pang, C. Bacellar, C. A. Saladrigas, J. Mahl, B. W. Toulson, Y. Kumagai, P. Walter, F. Ancilotto, M. Barranco, M. Pi, Ch. Bostedt, O. Gessner, and A. F. Vilesov, Phys. Rev. Lett. 124, 215301 (2020).
[7] D. Verma, S. M. O. O’Connell, A. J. Feinberg, S. Erukala, R. M. Tanyag, C. Bernando, W. Pang, C. A. Saladrigas, B. W. Toulson, M. Borgwardt, N. Shivaram, M.-F. Lin, A. Al Haddad, W. Jäger, C. Bostedt, P. Walter, O. Gessner, and A. F. Vilesov, Phys. Rev. B 102, 014504 (2020).
[8] A. J. Feinberg, D. Verma, S. M. O. O'Connell-Lopez, S. Erukala, R. M. P. Tanyag, W. Pang, C. A. Saladrigas, B. W. Toulson, M. Borgwardt, N. Shivaram, M.-F. Lin, A. Al Haddad, W. Jäger, C. Bostedt, P. Walter, O. Gessner, and A. F. Vilesov, Sci. Adv. 7, eabk2247 (2021).

Notice that the ratio between irrotational [Eq. (C4)] and rotational, rigid-body [Eq. (B4)] moments of inertia is

$$
\begin{equation*}
\frac{I_{\mathrm{irr}}}{I_{\mathrm{RB}}}=\left(\frac{\xi^{4}-1}{\xi^{4}+1}\right)^{2} \tag{C5}
\end{equation*}
$$

which is zero for a circular cylinder $(\xi=1)$. The energy per unit length in units of $8 \gamma R$ is

$$
\begin{equation*}
\frac{E}{8 \gamma R}=\frac{1}{2} \xi \mathbf{E}(e)+\frac{2}{\pi} \Lambda^{2} \frac{\xi^{2}\left(\xi^{4}+1\right)}{\left(\xi^{4}-1\right)^{2}} \tag{C6}
\end{equation*}
$$

As for the rotational ${ }^{3} \mathrm{He}$ fluid, determining the equilibrium configuration for a given $\Lambda$ amounts to solving for $e$ (or $\xi$ ) the algebraic equation $d \mathcal{E} / d \xi=0$ :

$$
\begin{align*}
& \mathbf{E}(e)+\frac{2}{\xi^{4}-1}[\mathbf{E}(e)-\mathbf{K}(e)] \\
& \quad-\frac{8}{\pi} \Lambda^{2} \frac{\xi}{\left(\xi^{4}-1\right)^{3}}\left[\xi^{8}+6 \xi^{4}+1\right]=0 \tag{C7}
\end{align*}
$$

The dimensionless angular velocity $\Omega$ is obtained from the $\xi$ value of the equilibrium configuration at the given $\Lambda$ as

$$
\begin{equation*}
\Omega=\frac{4}{\pi} \frac{\xi^{2}\left(\xi^{4}+1\right)}{\left(\xi^{4}-1\right)^{2}} \Lambda \tag{C8}
\end{equation*}
$$

[9] D. Rupp, N. Monserud, B. Langbehn, M. Sauppe, J. Zimmermann, Y. Ovcharenko, T. Möller, F. Frassetto, L. Poletto, A. Trabattoni, F. Calegari, M. Nisoli, K. Sander, C. Peltz, M. J. Vrakking, T. Fennel, and A. Rouzée, Nat. Commun. 8, 493 (2017).
[10] B. Langbehn, K. Sander, Y. Ovcharenko, C. Peltz, A. Clark, M. Coreno, R. Cucini, M. Drabbels, P. Finetti, M. Di Fraia, L. Giannessi, C. Grazioli, D. Iablonskyi, A. C. LaForge, T. Nishiyama, V. Oliver Álvarez de Lara, P. Piseri, O. Plekan, K. Ueda, J. Zimmermann, K. C. Prince, F. Stienkemeier et al., Phys. Rev. Lett. 121, 255301 (2018).
[11] R. A. Brown and L. E. Scriven, Proc. R. Soc. London A 371, 331 (1980).
[12] C.-J. Heine, IMA J. Num. Anal. 26, 723 (2006).
[13] S. L. Butler, M. R. Stauffer, G. Sinha, A. Lilly, and R. J. Spiteri, J. Fluid Mech. 667, 358 (2011).
[14] K. A. Baldwin, S. L. Butler, and R. J. A. Hill, Sci. Rep. 5, 7660 (2015).
[15] C. Bernando, R. M. P. Tanyag, C. Jones, C. Bacellar, M. Bucher, K. R. Ferguson, D. Rupp, M. P. Ziemkiewicz, L. F. Gomez, A. S. Chatterley, T. Gorkhover, M. Müller, J. Bozek, S. Carron, J. Kwok, S. L. Butler, T. Möller, Ch. Bostedt, O. Gessner, and A. F. Vilesov, Phys. Rev. B 95, 064510 (2017).
[16] F. Ancilotto, M. Pi, and M. Barranco, Phys. Rev. B 91, 100503(R) (2015).
[17] F. Ancilotto, M. Barranco, and M. Pi, Phys. Rev. B 97, 184515 (2018).
[18] M. Pi, J. M. Escartín, F. Ancilotto, and M. Barranco, Phys. Rev. B 104, 094509 (2021).
[19] F. Dalfovo, A. Lastri, L. Pricaupenko, S. Stringari, and J. Treiner, Phys. Rev. B 52, 1193 (1995).
[20] M. Barranco, M. Pi, S. M. Gatica, E. S. Hernández, and J. Navarro, Phys. Rev. B 56, 8997 (1997).
[21] M. Barranco, R. Guardiola, S. Hernández, R. Mayol, J. Navarro, and M. Pi, J. Low Temp. Phys. 142, 1 (2006).
[22] F. Ancilotto, M. Barranco, F. Coppens, J. Eloranta, N. Halberstadt, A. Hernando, D. Mateo, and M. Pi, Int. Rev. Phys. Chem. 36, 621 (2017).
[23] M. Pi, F. Ancilotto, and M. Barranco, J. Chem. Phys. 152, 184111 (2020); Erratum: 158, 129901 (2023).
[24] B. G. Sartakov, J. P. Toennies, and A. F. Vilesov, J. Chem. Phys. 136, 134316 (2012).
[25] A. F. Vilesov (private communication).
[26] S. L. Butler, Phys. Fluids 32, 012115 (2020).
[27] S. L. Butler, Phys. Fluids 34, 112103 (2022).
[28] M. Pi, F. Ancilotto, J. M. Escartín, R. Mayol, and M. Barranco, Phys. Rev. B 102, 060502(R) (2020).
[29] F. Ancilotto, M. Pi, and M. Barranco, Phys. Rev. B 90, 174512 (2014).
[30] A. L. Fetter, J. Low Temp. Phys. 16, 533 (1974).
[31] L. J. Campbell and R. M. Ziff, Phys. Rev. B 20, 1886 (1979).
[32] R. J. Donnelly, Quantized Vortices in Helium II (Cambridge University Press, Cambridge, UK, 1991).
[33] R. E. Benner Jr., O. A. Basaran, and L. E. Scriven, Proc. R. Soc. London A 433, 81 (1991).
[34] F. Ancilotto, M. Barranco, and M. Pi, J. Chem. Phys. 158, 144306 (2023).
[35] S. Stringari and J. Treiner, J. Chem. Phys. 87, 5021 (1987).
[36] B. Grammaticos, Phys. Rev. C 17, 1244 (1978).
[37] D. Mateo, M. Pi, J. Navarro, and J. P. Toennies, J. Chem. Phys. 138, 044321 (2013).
[38] A. Ulmer, A. Heilrath, B. Senfftleben, S. M. O. O'ConnellLopez, B. Kruse, L. Seiffert, K. Kolatzki, B. Langbehn, A. Hoffmann, T. M. Baumann, R. Boll, A. S. Chatterley, A. De Fanis, B. Erk, S. Erukala, A. J. Feinberg, T. Fennel, P. Grychtol, R. Hartmann, M. Ilchen et al., Phys. Rev. Lett. 131, 076002 (2023).
[39] M. A. Walkley, P. H. Gaskell, P. K. Jimack, M. A. Kelmanson, and J. L. Summers, J. Sci. Comput. 24, 147 (2005).
[40] COMSOL MULTIPHYSICS® v. 6.0, www.comsol.com, COMSOL AB, Stockholm, Sweden.
[41] M. Pi, F. Ancilotto, F. Coppens, N. Halberstadt, A. Hernando, A. Leal, D. Mateo, R. Mayol, and M. Barranco, ${ }^{4} \mathrm{He}-\mathrm{DFT}$ BCNTLS: A computer package for simulating structural properties and dynamics of doped liquid Helium-4 systems, https://github. com/bentls2016/.
[42] M. Frigo and S. G. Johnson, Proc. IEEE 93, 216 (2005).
[43] M. Barranco, F. Coppens, N. Halberstadt, A. Hernando, A. Leal, D. Mateo, R. Mayol, and M. Pi, Zero temperature DFT and TDDFT for ${ }^{4} \mathrm{He}$ : A short guide for practitioners, https://github. com/bentls2016/DFT-Guide/blob/master/dft-guide.pdf.
[44] F. Ancilotto, M. Barranco, F. Caupin, R. Mayol, and M. Pi, Phys. Rev. B 72, 214522 (2005).
[45] F. Coppens, F. Ancilotto, M. Barranco, N. Halberstadt, and M. Pi, Phys. Chem. Chem. Phys. 19, 24805 (2017).
[46] P. Möller, J. R. Nix, and W. J. Swiatecki, Nucl. Phys. A 469, 1 (1987).
[47] G. B. Hess and W. M. Fairbank, Phys. Rev. Lett. 19, 216 (1967).
[48] E. Guyon, J.-P. Hulin, L. Petit, and C. D. Mitescu, Physical Hydrodynamics, 2nd. ed. (Oxford University Press, Oxford, UK, 2015).
[49] D. J. Tritton, Am. J. Phys. 50, 421 (1982).
[50] D. V. Osborne, Proc. Phys. Soc. A 63, 909 (1950).
[51] L. Pitaevskii and S. Stringari, Bose-Einstein Condensation and Superfluidity, International Series of Monographs on Physics, Vol. 164 (Oxford University Press, Oxford, UK, 2016).
[52] G. B. Hess, Phys. Rev. 161, 189 (1967).
[53] G. M. Seidel and H. J. Maris, Phys. B (Amsterdam) 194-196, 577 (1994).
[54] S. Chandrasekhar, Proc. R. Soc. London A 286, 1 (1965).
[55] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series, and Products, 7th ed. (Academic Press, Oxford, 2007).
[56] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1965).
[57] A. Bohr and B. R. Mottelson, Nuclear Structure, Vol II, (W. A. Benjamin, Reading, MA, 1975).

