Quantized vortices in $^4$He droplets: a quantum Monte Carlo study

E. Sola, J. Casulleras, and J. Boronat
Departament de Física i Enginyeria Nuclear, Campus Nord B4-B5, Universitat Politècnica de Catalunya, E-08034 Barcelona, Spain

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We present a diffusion Monte Carlo study of a vortex line excitation attached to the center of a $^4$He droplet at zero temperature. The vortex energy is estimated for droplets of increasing number of atoms, from $N = 70$ up to 300 showing a monotonic increase with $N$. The evolution of the core radius and its associated energy, the core energy, is also studied as a function of $N$. The core radius is $\sim 1 \text{ Å}$ in the center and increases when approaching the droplet surface; the core energy per unit volume stabilizes at a value $2.8 \text{ K} \sigma^{-3}$ ($\sigma = 2.556 \text{ Å}$) for $N \geq 200$.

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Quantized vortices are one of the most outstanding signatures of superfluidity. They have been widely observed in liquid $^4$He at temperatures below the critical temperature $T_c = 2.17 \text{ K}$ [1]. More recently, vortices have also been detected in dilute Bose [2] and Fermi [3] gases when they are magnetically trapped, their observation being considered the most clear indication of the achievement of their superfluid phases. $^4$He droplets produced in free jet expansion experiments [4] are expected to be also superfluid due to their very low temperature ($T = 0.38 \text{ K}$). However, in this finite system the search for a direct signature of their superfluid character is more difficult. On the one hand, indirect evidence of superfluidity has been driven from the determination of the rotation spectrum of molecules adsorbed into them [5]. This very interesting phenomenon has been considered the microscopic version of the famous Andronikashvili experiment. On the other hand, the detection of vortices in droplets would be an even more conclusive proof of their superfluidity. Nevertheless, no signal of straight or circular vortices has been yet observed in experiments with $^4$He droplets, in spite of some theoretical arguments in favor of their possible metastability.

The stability of vortex excitations in $^4$He droplets was first studied by Bauer et al. [6]. They concluded that vortices are not stable in droplets due to the high excitation energy required, compared to the usual temperature at which they are produced. Later on, Lehmann and Schmied [7], studying cold droplets, smaller than the ones analyzed in Ref. [6] were led to a different conclusion. They stated that in small droplets, where only surface excitations (ripplons) are relevant, vortices should be stable against decay. Finally, density functional (DF) calculations [8, 9] have predicted that below a critical atomic number a linear vortex pinned to a dopant atom or molecule can become stable, with a lifetime long enough to allow for its experimental detection.

The excitation energy of a vortex line in a $^4$He droplet as a function of its number of atoms $N$ is one of its most fundamental properties. An accurate calculation of its value is crucial to elucidate its possible stability and formation probability in jet expansions. To our knowledge, there is only one previous microscopic calculation of the excitation energy associated to a vortex in a droplet. This calculation, performed with the path integral Monte Carlo (PIMC) method [10], was carried out for a $N = 500$ $^4$He droplet and the energy obtained was more than a factor two smaller than DF predictions [8, 9]. In the present work, we present zero-temperature diffusion Monte Carlo (DMC) results of vortex energy and vortex structure in $^4$He droplets for different number of atoms.

A vortex is an excited state of the $N$-particle Hamiltonian which corresponds to an eigenstate of the angular momentum operator. Actually, it is an eigenstate of the $z$ component of the angular momentum, $L_z$, with eigenvalue $\hbar N l$ where $l = 1, 2, \ldots$ is the quantum of circulation. In a general form, the imaginary-time dependent wave function of a vortex in a quantum liquid can be written as

$$\Psi_v(R, t) = e^{i\Omega(R, t)}\Phi(R, t).$$

By imposing that $\Psi_v$ is an eigenstate of the angular momentum $L_z$, Feynman [11] obtained his famous proposal $\Omega(R, t) = l\phi_v(R)$, with $\phi_v(R) = \sum_{j=1,N} \theta_j$, $\theta_j$ being the $j$-th polar coordinate (in cylindrical coordinates).

With the decomposition (1), the Schrödinger equation for $\Psi_v(R, t)$ splits in two coupled equations, one for the modulus

$$-\frac{\partial \Phi}{\partial t} = D(\nabla \Omega)^2 \Phi - D\nabla^2 \Phi + (V(R) - E)\Phi,$$

and one for the phase

$$\frac{\partial \Omega}{\partial t} = D \left[ \nabla^2 \Omega + 2(\nabla\Omega) \frac{\nabla \Phi}{\Phi} \right],$$

with $D = \hbar^2/2m$. If a fixed form for the phase $\Omega$ is assumed, the equation for the modulus, Eq. (2), becomes the usual Schrödinger equation with one additional term (the first one on the right hand side). In this approximation, known as fixed phase (FP), the vortex acts like a static external potential. Using Feynman’s expression

$$\begin{align*}
\Psi_v(R, t) = e^{i\Omega(\mathbf{R}, t)}\Phi(R, t),
\end{align*}$$

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for the phase, $\Omega = l \sum_{i=1}^{N} \theta_i$, this potential results
\[ V_{v}(\mathbf{R}) = \sum_{i=1}^{N} \frac{\hbar^2 \ell^2}{2m \rho_i^2} , \tag{4} \]
with $\rho_i$ the polar coordinate of particle $i$ in cylindric coordinates. Therefore, in the FP approximation the problem of having a vortex inside the droplet is reduced to a different Hamiltonian ($\hat{H} = \hat{H} + V_v$) in the Schrödinger equation to be stochastically solved. This approach was used in the PIMC calculation of the vortex energy in a $^4$He droplet \cite{Rayfield:1988} and also recently in a Monte Carlo study of the excitation energy of vortices in trapped diluted Bose gases \cite{Dalfovo:1999}.

In the present work, we will assume that the vortex line is fixed in the $z$ direction of the center-of-mass (CM) reference system of the droplet. The vortex state is then an eigenstate of the $L_{EOM}$ operator, accounting for the translational invariance of the Hamiltonian. In this case, the resulting potential ($V_v$) that must be added to the Hamiltonian in the droplet geometry is
\[ \tilde{V}_{v}(\mathbf{R}) = \frac{\hbar^2 \ell^2}{2m} \sum_{j=1}^{N} \left[ \frac{1}{\rho_j^2} - \frac{1}{N} \sum_{k=1}^{N} \cos(\theta_k - \theta_j) \right] . \tag{5} \]
Coordinates in Eq. \ref{eq:5} and hereafter are referred to the center of mass. The potential $\tilde{V}_{v}$ is very similar to the one for the bulk \cite{Rayfield:1988}, but now written using CM coordinates, and a small correction of order $1/N$ is introduced.

The FP approach to the excitation energy of a vortex line with the Feynman’s phase could be thought as a too crude approximation for an accurate microscopic treatment of the problem. An $a$ priori better method would be to consider the superposition of clockwise and anticlockwise vortices, which are degenerate in energy, and using the resulting wave function (orthogonal to the ground state) as a guiding wave function in DMC. This leads to a Fermi-like problem due to the non-positivity of the excited wave function which can be approximately solved in the fixed-node (FN) approximation. This method was used in Ref. \cite{Sadd:1999} for studying a vortex in a two-dimensional geometry. However, the results there obtained showed that FN and FP predictions are almost compatible. Moreover, both Ref. \cite{Sadd:1999} and Ref. \cite{Rayfield:1988} studied the possible improvements upon Feynman’s phase by introducing backflow correlations on it and concluded that their effect on the excitation energy is very small ($< 1\%$ in the energy per particle). Therefore, it is sound to consider that the FP method is also a good enough approximation to describe the vortex attached to a droplet.

We have carried out DMC simulations of $^4$He droplets with number of atoms $N = 70, 128, 200,$ and $300$. To extract the excitation energy associated to the vortex line we have calculated the energy of the droplets for both the ground state and the droplet with a fixed vortex in the center of mass. The ground-state trial wave function used for importance sampling in the DMC method is a Jastrow form,
\[ \Phi_0(\mathbf{R}) = \prod_{i<j} \exp \left\{ -\frac{1}{2} \left[ \frac{b}{r_{ij}} \right]^5 + \frac{\alpha^2 r_{ij}^2}{N} \right\} . \tag{6} \]
The first term in the square bracket of Eq. \ref{eq:6} is a McMillan correlation factor accounting for dynamical correlations induced by the interatomic potential $V(r_{ij})$, and the second one is a gaussian correlation to take into account the finite size of the droplet.

When the vortex is present, the Hamiltonian changes due to the potential induced by the FP approximation \ref{eq:5}. Therefore, we introduce an additional correlation factor $f(\rho)$ to reduce the variance of the energy estimation,
\[ \Phi_v(\mathbf{R}, t) = \Phi_0(\mathbf{R}) \prod_{i=1}^{N} f(\rho_i) , \tag{7} \]
with $\rho_i$ the radial position of particle $i$. Among the different options for $f(\rho)$, discussed for the bulk in Ref. \cite{Sadd:1999}, we have chosen
\[ f(\rho) = 1 - e^{-\rho/a} \]
with $a$ a variational parameter related to the radius of the vortex core. We have taken $a = 1$ Å, value which coincides with the old estimation of the core radius by Rayfield and Reif \cite{Rayfield:1988} and the more recent one by Sadd \textit{et al.} \cite{Sadd:1999}. This function satisfies $f(\rho) \to 0$ when $\rho \to 0$, reflecting the repulsive character of the potential $\tilde{V}_{v}$, and approaches 1 far from the core. We have checked that the explicit form of the function $f(\rho)$ satisfying both boundary conditions is not really important and that, as expected, the energy of the system does not depend on it.

The other two variational parameters $b$ and $\alpha$ appearing in the trial wave function \ref{eq:6} have been optimized by means of variational Monte Carlo (VMC) calculations. The optimal values are $b = 1.19 \sigma$ and $\alpha = 0.6 \sigma^{-2}$ ($\sigma = 2.556$ Å) and their dependence with the number of atoms $N$ is negligible in the range studied.

The main purpose of this work, i.e., the determination of the excitation energy associated to a vortex line attached to the CM of the $^4$He droplet, has been studied by other groups using mainly density functional theory \cite{Dallago:1999, Dalfovo:1999}. Dallago \textit{et al.} \cite{Dallago:1999} proposed a liquid-drop formula for the energy dependence on the number of particles,
\[ E_v(N) = \lambda N^{1/3} + \beta N^{1/3} \log N + \gamma N^{-1/3} , \tag{9} \]
$\lambda$, $\beta$ and $\gamma$ being parameters which were obtained by fitting Eq. \ref{eq:9} to their DF results. The final set of parameters was $\lambda = 2.868$ K, $\beta = 1.445$ K and $\gamma = 0.313$ K.
The specific dependence on $N$ in Eq. (9) is derived using the hollow-core model. In this model, the local vortex energy is integrated over all the volume occupied by particles

$$E_v(N) = \int_V dV \frac{1}{\rho^2},$$

resulting in

$$E_v(N) = \frac{2\pi \hbar^2 D_0}{m} \left[ R \ln \left( \frac{2R}{a} \right) - R + \frac{a^2}{2R} \right].$$ (11)

Notice that one can rewrite Eq. (11) in terms of $N$ just using $R = r_0 N^{1/3}$, where $r_0 = (3/(4\pi D_0))^{1/3}$, arriving in such a way to the same dependence on $N$ as Eq. (9). However, the hollow-core method is a too simple approximation to identify the parameters $\lambda$, $\beta$ and $\gamma$ using, for example, a constant density $D_0$.

Calculations performed using DF and MC evaluate the vortex energy as the difference between the total energies of the droplet with and without (ground-state) a vortex ($E_v(N) = E_1(N) - E_0(N)$). In Table I, we present our DMC results of the energies $E_1(N)$, $E_0(N)$, and $E_v(N)$ for $^4$He droplets with $N = 70, 128, 200$, and 300. The vortex energy $E_v$ comes from the difference of two energies which increase with the number of atoms $N$ and therefore its statistical error also increases with $N$.

The results contained in Table I show that the excitation energy $E_v$ increases monotonously with $N$. This can be more clearly observed in Fig. 1 where the present DMC results are compared with the liquid drop formula (9) as reported by Dalfovo et al. [8]. One can observe that the DF estimation reproduces better our results for the larger droplets than for the smaller ones. This is what one a priori expects since DF approximations work better for large droplets where application of mean field theory is more justified; in spite of this, the difference is only $\sim 4\%$ for the smallest droplet studied ($N = 70$).

The repulsive potential induced by the vortex creates a hole when $\rho \to 0$ with a characteristic modulation of the density. This behavior is shown in Fig. 2 where we have plotted the density profiles $D(\rho)$ for different values of $z$ along the vortex axis. The slice at $z = 0$ corresponds to the one in the center of the droplet and is the density profile with the highest peak. When $z$ increases, the radius of the slice is progressively smaller and also the oscillations are depressed as $z$ approaches the droplet radius. In the center of the vortex, the density goes to zero in agreement with the DMC results derived in Ref. [13] for homogeneous 2D liquid $^4$He. A relevant parameter in the microscopic description of a vortex is the size of its core, what is called the core radius $\xi$. There is not a single definition of $\xi$ but different definitions lead to quite similar results. We have used the criterion of considering for $\xi$ the position of the maximum in the azimuthal circulating current $J_\theta(\rho)$. If the vortex is described by means of the Feynman approximation, as in the present work, it follows that $J_\theta(\rho) = D(\rho)/\rho$. Therefore, we can get a direct
decomposed in the form

\[ E_{\psi}(\rho) = A \ln(\rho/\xi) + E_c \]

(12)

with \( A \) a constant, \( E_c \) the core energy, and \( \rho \) the radial coordinate in cylindrical coordinates. This model, which reproduces very well DMC results of the vortex energy in a 2D geometry [13], splits the vortex energy in a constant term \( E_c \) associated to the hole around the vortex axis and a logarithmic term containing the hydrodynamic tail. In the case of droplets, the behavior of the excitation energy is more complex due to their inhomogeneity along the \( z \) vortex axis and their finite size. In the function \( E_{\psi}(\rho) \) one finds, superimposed to the monotonously increasing law (12), a decaying trend to zero when the surface of the droplet is reached. This behavior is shown in Fig. 3 where we have plotted the function \( E_{\psi}(\rho) \) for a \( N = 70 \) \(^4\)He droplet. The function \( E_{\psi}(\rho) \) shows clearly a peak corresponding to the core of the vortex, especially for the inner slice, and a decay to zero in the surface. The size of the droplets studied is too small to see the signature of the hydrodynamic tail but we can estimate the energy of the core \( E_c \) by summing the local energy up to the estimated vortex core radius \( \xi \). Extending this sum along all the vortex axis we obtain an energy which increases with \( N \): \( E_c = 9.74(4) \) K and \( 19.2(3) \) K for \( N = 70 \) and 300, respectively. Normalizing \( E_c \) with respect to the volume of the core, the core energy per volume unit approaches a constant value of \( 2.8 \) K\(\sigma^{-3} \) for droplets with \( N \geq 200 \).

Summarizing, we have carried out the first microscopic calculation of the properties of a vortex line attached to a \(^4\)He droplet at zero temperature. The energies obtained are in good agreement with DF estimations and therefore give additional confidence on their predictions. Moreover, the magnitude of the core radius and core energy has also been studied for the first time in these inhomogeneous system. The core radius is \( \sim 1 \) \( \AA \) in the center and increases when approaching the droplet surface; the core energy per unit volume stabilizes at a value \( 2.8 \) K\(\sigma^{-3} \) for \( N \geq 200 \). We hope our results can help and stimulate further experimental work towards the long-standing purpose of detecting vortex excitations in \(^4\)He droplets.

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FIG. 3: Local energy \( E_{\psi}(\rho) \) for a \( N = 70 \) \(^4\)He droplet with a vortex axis. From top to bottom the curves correspond to increasing values of \( z \) from \( z = 0 \) in the center of the droplet up to \( z \) values close to the surface.

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