Vortex Excitation in Superfluid ^{4}He: A Diffusion Monte Carlo Study

S. Giorgini,[1,2] J. Boronat,[2] and J. Casulleras[2]
[1]*Dipartimento di Fisica, Università di Trento, I-38050 Povo, Italy*
and Istituto Nazionale di Fisica della Materia, I-38050 Povo, Italy
[2]*Departament de Física i Enginyeria Nuclear, Campus Nord B4-B5, Universitat Politècnica de Catalunya, E-08028 Barcelona, Spain*
(Received 14 June 1996)

We present a diffusion Monte Carlo study of a single vortex in two-dimensional superfluid liquid ^{4}He within the fixed-node approximation. We use both the Feynman phase and an improved phase which includes backflow correlations to model the nodal surface of the vortex wave function. Results for the particle density, core radius, and excitation energies are presented. [S0031-9007(96)01207-0]

PACS numbers: 67.40.Vs, 67.40.Db

Diffusion and Green's function Monte Carlo simulations have become a standard tool in the study of ground-state properties of Bose quantum liquids at zero temperature. However, the development of *ab initio* computational methods to investigate properties of excited states, such as the phonon-roton branch and vortex excitations in superfluid ^{4}He, is still a challenging problem at the forefront of present research in the field of computational techniques applied to condensed matter physics. In this Letter we present results on the microscopic structure of a single vortex excitation in two-dimensional liquid ^{4}He at zero temperature, obtained by employing a fixed-node diffusion Monte Carlo (DMC) method [1].

The idea that circulation in superfluid ^{4}He is quantized is due to Onsager [2], whereas the possibility that vortices might have a core of atomic dimensions was first put forward by Feynman [3] who also proposed a microscopic wave function for the vortex state. Gross, Pitaevskii, and Fetter [4] investigated the structure of vortex states in a weakly interacting inhomogeneous Bose gas using a mean field approach. The first attempt to study quantized vortices in a strongly interacting system, such as liquid ^{4}He, is due to Chester, Metz, and Reatto [5] who calculated the energy of a vortex line with the use of a variational approach involving integral equations. Only quite recently new calculations of the structure of vortex states in superfluid ^{4}He have appeared [6–9]. The very recent Letter by Ortiz and Ceperley [6] is the first attempt to tackle the problem of the vortex core structure by employing *ab initio* computational techniques. Our method in the present Letter is similar to that used by these authors, but the approach is different and our results for the core energy and the particle density near the vortex axis are significantly different from the ones obtained in Ref. [6].

A vortex excitation is an eigenstate of the N-particle Hamiltonian H and of the z component of the angular momentum L_z with eigenvalue $\hbar N\ell$, corresponding to an integer number ℓ of quanta of circulation [10]. The simplest microscopic wave function to describe a vortex state was introduced by Feynman [3]:

$$\psi_F(\mathbf{R}) = e^{i\ell\varphi_F} \prod_{i=1}^{N} f(r_i)\Phi_0(\mathbf{R}), \tag{1}$$

where $\varphi_F = \sum_{i=1,N} \theta_i$ is the Feynman phase with θ_i the azimuthal angle of the ith particle, $\Phi_0(\mathbf{R})$ describes the ground state of the system, and $f(r_i)$ is a function of the radial distance of each particle from the vortex axis, which models the density near the core. In what follows we consider only vortices with one quantum of circulation, i.e., $\ell = \pm 1$. In the recent Letter by Ortiz and Ceperley [6], a systematic method to improve the phase of the wave function is devised. Starting from the Feynman phase φ_F as zeroth order ansatz, the first correction includes backflow correlations giving an improved phase of the form

$$\varphi_{\mathrm{BF}} = \varphi_F + \lambda \sum_{i\neq j} \gamma(r_i, r_j, r_{ij}) \frac{r_j}{r_i} \sin(\theta_i - \theta_j). \tag{2}$$

The wave function constructed with the phase φ_{BF} is the vortex analog of the Feynman-Cohen backflow wave function for the phonon-roton excitation branch [11].

To go beyond a variational estimation of the properties of the vortex state, given by the above model wave functions, we have used a DMC method. This method solves the many-body Schrödinger equation in imaginary time for the function $f(\mathbf{R}, t) = \psi_T(\mathbf{R})\Phi(\mathbf{R}, t)$

$$-\frac{\partial f(\mathbf{R}, t)}{\partial t} = -D\nabla^2_{\mathbf{R}} f(\mathbf{R}, t) + D\nabla_{\mathbf{R}}[\mathbf{F}(\mathbf{R}) f(\mathbf{R}, t)] + [E_L(\mathbf{R}) - E] f(\mathbf{R}, t), \tag{3}$$

where $\Phi(\mathbf{R}, t)$ is the wave function of the system and $\psi_T(\mathbf{R})$ is a trial function used for importance sampling. In the above equation, $E_L(\mathbf{R}) = \psi_T^{-1}(\mathbf{R}) H \psi_T(\mathbf{R})$ is the local energy and $\mathbf{F}(\mathbf{R}) = 2\psi_T^{-1}(\mathbf{R})\nabla_{\mathbf{R}}\psi_T(\mathbf{R})$ is the so-called quantum drift force; $D = \hbar^2/2m$, with m the mass of the particles, plays the role of a diffusion constant, $\mathbf{R}$ stands for the $3N$-coordinate vector of the N particles of the system, and E is an arbitrary energy shift. Equation (3) is a

 0031-9007/96/77(13)/2754(4)$10.00

diffusion equation for the probability distribution $f(\mathbf{R}, t)$ which evolves in time due to diffusion, drift, and branching processes. If $\Phi(\mathbf{R})$ represents the wave function of the lowest energy eigenstate of the system not orthogonal to the trial function ψ_T, the asymptotic solution of Eq. (3) is given by $f(\mathbf{R}, t \to \infty) = \psi_T(\mathbf{R})\Phi(\mathbf{R})$ and the corresponding energy eigenvalue can be calculated exactly.

In order to deal with a real walker probability distribution function $f(\mathbf{R}, t)$, we choose as a trial function the superposition of two vortex states, one with positive and one with negative circulation, which are degenerate in energy. The importance sampling function has therefore the form

$$\psi_T(\mathbf{R}) = \cos[\varphi(\mathbf{R})] \prod_{i=1}^{N} f(r_i) \psi_T^0(\mathbf{R}), \tag{4}$$

where ψ_T^0 is the importance sampling function for the ground state and for the phase φ we have used both the Feynman phase φ_F and the backflow phase φ_{BF}. The sign problem associated with the use of the above trial wave function in the DMC algorithm has been dealt with in the framework of the fixed-node (FN) approximation [1]. This approach, which has been extensively used in the calculation of ground-state properties of fermionic systems, yields an upper bound to the energy eigenvalue [1]. The quantum drift force acting on each particle, as obtained from the trial wave function (4), can be written as the sum $\mathbf{F}^i(\mathbf{R}) = \mathbf{F}_1^i(\mathbf{R}) + \mathbf{F}_2^i(\mathbf{R})$. The first term in the sum is independent of the phase φ of the wave function, whereas the second term contains the φ dependence and has the form

$$\mathbf{F}_2^i(\mathbf{R}) = -2 \tan(\varphi) \nabla_i \varphi_i, \tag{5}$$

where φ_i is the contribution of the ith particle to the collective phase, $\varphi = \sum_{i=1,N} \varphi_i$. In the same way, the local energy $E_L(\mathbf{R})$ can be decomposed in the sum of a phase independent term E_{L1} and a phase dependent term E_{L2} which is given by

$$E_{L2}(\mathbf{R}) = D \sum_{i=1}^{N} \left((\nabla_i \varphi_i)^2 + \tan(\varphi) \nabla_i^2 \varphi_i - \frac{1}{2} \mathbf{F}_1^i(\mathbf{R}) \cdot \mathbf{F}_2^i(\mathbf{R}) \right). \tag{6}$$

Vortex states are characteristic of systems with rotational invariance, but, at the same time, simulations must deal with a finite number of particles. A simple choice is to restrict the N particles to be inside a cylindrical box with the vortex at the center and rigid boundary conditions on the walls. This is the geometry chosen for example in Ref. [6]. By confining the particles some problems arise, such as the choice of the confining potential and surface effects which can be relevant if the box size is not large enough. In the present work, we have removed the confinement in order to keep surface effects as small as possible. An important point one needs to solve when attempting to simulate a vortex excitation in an infinite system is the calculation of the collective phase $\varphi(\mathbf{R})$. For a very large system one expects that the features of the vortex state near the core are weakly influenced by the behavior of particles which are far from the vortex axis. It is thus reasonable to assume that, if the collective phase is decomposed in the sum

$$\varphi(\mathbf{R}) = \sum_{r_i \le \bar{r}} \varphi_i + \sum_{r_i > \bar{r}} \varphi_i, \tag{7}$$

where the first term sums the contributions to the phase of all the particles with distance from the vortex axis within the cutoff length $\bar{r}$ and the second term gives the contribution coming from all the other particles, the phase fluctuations in the second term are irrelevant for the core structure of the vortex and it can be safely approximated by its mean value $\sum_{r_i > \bar{r}} \varphi_i = 0$. If this prescription is employed in the calculation of the collective phase entering the expressions (5) and (6) for the drift force and the local energy, one expects that for a large enough cutoff length $\bar{r}$ the properties of the vortex state near the axis are properly simulated. However, the straightforward interpretation of the decomposition (7) would be of no practical use because the collective phase would change discontinuously by a large amount each time a particle exits or enters the region delimited by the cutoff $\bar{r}$. Instead, the procedure we have adopted is to use the decomposition (7) as a way of tagging the particles that will contribute to the collective phase for a long simulation run. The dependence of the results on the cutoff length has been studied and as will be discussed later no appreciable changes are seen for values of $\bar{r}$ larger than approximately 3σ ($\sigma = 2.556$ Å). It is worth noticing that in the limit $\bar{r} \to 0$ the collective phase vanishes and all the terms containing explicitly φ in expressions (5) and (6) for the drift force and the local energy disappear. In this case, the DMC calculation can be shown to be equivalent to the fixed-phase (FP) method employed by Ortiz and Ceperley in Ref. [6], where the phase of the wave function is fixed and the DMC algorithm is used to solve the equation for the modulus of the wave function. By taking a finite value for the cutoff $\bar{r}$, one allows for phase fluctuations in the system around the phase introduced with the trial function, and in the limit $\bar{r} \to 0$ one recovers the full FN approximation. Our results actually show that a finite cutoff is enough to account completely for the phase fluctuations.

Once established that the contribution of the more distant particles to the collective phase is irrelevant, there is no compelling reason for not extending the system using periodic boundary conditions. Surface effects exist also in this case, in the sense that particles near the walls of the box "see" the artificial density perturbations associated with the image vortices in the adjacent boxes. However, these effects are negligible for a reasonable size of the simulation cell and are definitely smaller than the density oscillations induced by rigid walls.

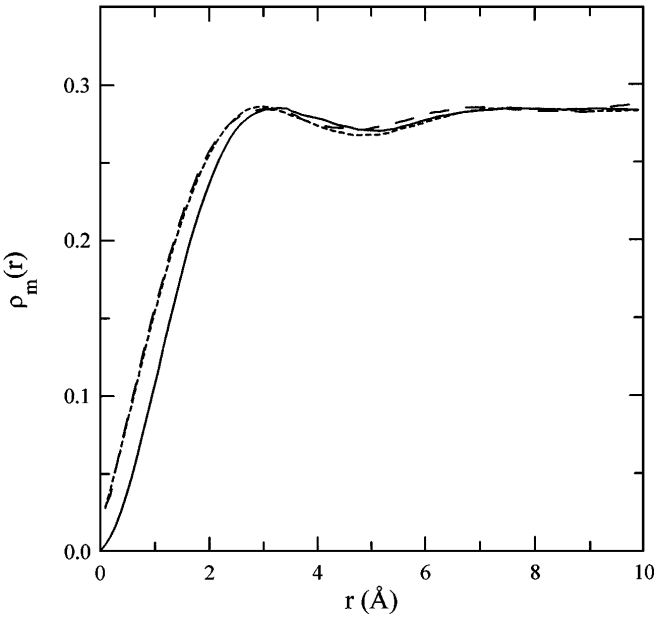

FIG. 1. Mixed density profiles. Solid line: with ψ_T^{F1}, short-dashed line: with ψ_T^{F2}, and long-dashed line: with ψ_T^{BF}.

We are now in a position to discuss our results. We consider 64 particles in a two-dimensional box of length $L = 15.0\sigma$, which corresponds approximately to the equilibrium density of the two-dimensional homogeneous liquid [12]. The atoms interact through the two-body HFD-B(HE) potential [13], which is a revised version of the HFDHE2 Aziz potential. The ground-state trial wave function we have chosen is the McMillan two-body function $\psi_T^0(\mathbf{R}) = \prod_{i<j} \exp(-b^5/2r_{ij}^5)$ with $b = 1.205\sigma$ as in the ground-state calculation of Ref. [12]. For the radial function $f(r)$, which models the structure of the vortex core, we consider two different options: $f_1(r) = 1 - e^{(-r/a)}$, and $f_2(r) = 1$. The first function gives a density in the trial function which decreases to zero at the vortex axis over a distance of order a, for which we take the value $a = 1$ Å, whereas the second one does not contain any parameter associated with the vortex core. For the backflow function γ entering Eq. (2) we have used the same functional form $\gamma(r_i, r_j, r_{ij}) = \exp[-\alpha(r_i^2 + r_j^2) - \beta r_{ij}^2]$ and the same values for the parameters α, β, and λ as in Ref. [6]. We have performed the calculation using three different trial wave functions: ψ_T^{F1} and ψ_T^{F2} which correspond to the Feynman phase φ_F with the radial terms f_1 and f_2, respectively, and ψ_T^{BF} corresponding to the backflow phase φ_{BF} with f_2. In Fig. 1 we show results for the particle density $\rho(r)$ using ψ_T^{F1}, ψ_T^{F2}, and ψ_T^{BF}. These results have been obtained by means of mixed estimators which are significantly biased by the choice of the trial wave function. As apparent from Fig. 1, the behavior near the core is strongly affected by the introduction or not of the radial term $f_1(r)$. In order to remove the influence of the trial wave function in mixed estimators of coordinate operators one can use pure estimators. In the present work we have employed the method presented in Ref. [14]. The results for the pure density profiles do not depend anymore on the use or not of the radial term $f_1(r)$ and the three cases converge to a single result. The common pure profile is presented in Fig. 2, where it clearly appears that a zero particle density is reached on the vortex axis. This result is in contrast with the prediction of a significant nonzero particle density on the axis obtained with the backflow phase in Ref. [6]. In our opinion the result of Ref. [6] can be influenced by the extrapolation technique used by the authors to improve the mixed estimator result. In fact, the usual linear extrapolation technique, which is accurate to the same order as the one employed in Ref. [6], would change their result for the particle density on the vortex axis in an amount comparable to their prediction.

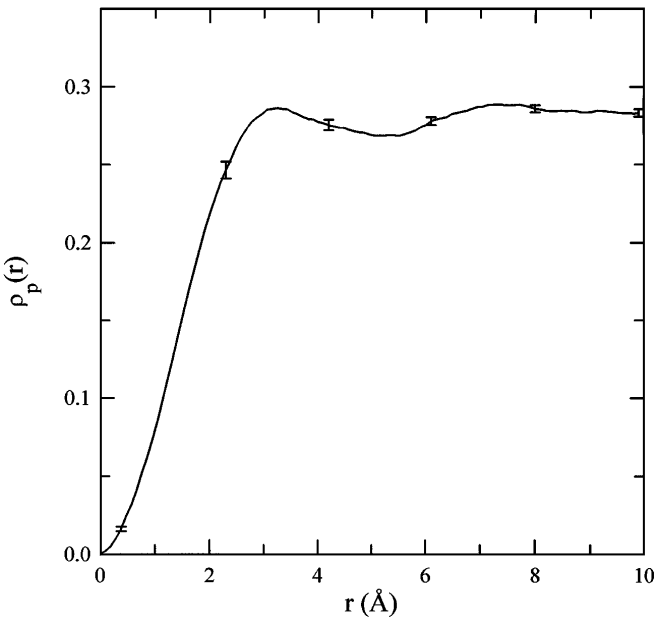

FIG. 2. Pure density profile.

In Table I are reported the energies per particle for the different trial wave functions, together with the energy per particle E_0/N in the ground state. The two results for the Feynman phase are almost equal, whereas in the case of the backflow phase the system is slightly more bounded in accordance with the improvement of the nodal surface. The cutoff length $\bar{r}$ for the calculation of the collective phase has been taken as $\bar{r} = 6\sigma$. In the case of the Feynman phase reducing the cutoff length does not give any change in the results down to the FP limit $\bar{r} = 0$.

TABLE I. Results for the energies per particle. E_{F1}/N, E_{F2}/N, and E_{BF}/N correspond to the trial functions ψ_T^{F1}, ψ_T^{F2}, and ψ_T^{BF}, respectively. E_0/N is the ground-state energy.

E_{F1}/N (K)	E_{F2}/N (K)	E_{BF}/N (K)	E_0/N (K)
−0.8162(16)	−0.8171(18)	−0.8199(18)	−0.8957(25)

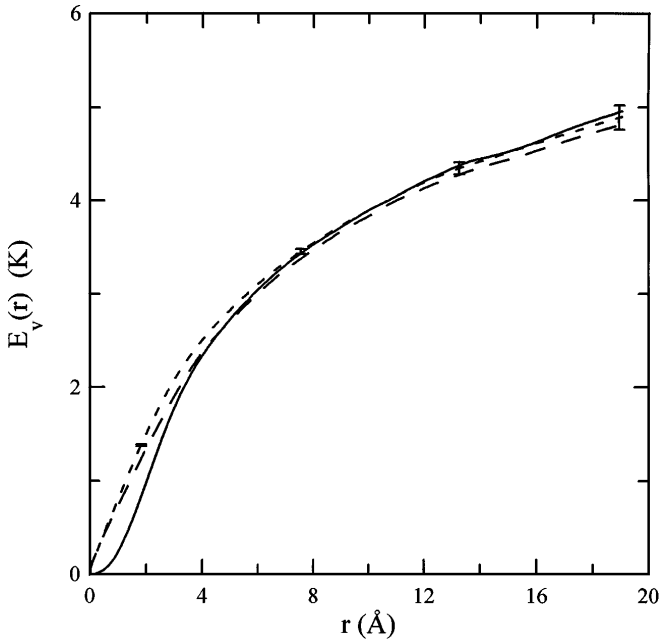

FIG. 3. Radial dependence of the excitation energy. Solid line: with ψ_T^{F1}, short-dashed line: with ψ_T^{F2}, and long-dashed line: with ψ_T^{BF}.

For the backflow phase, though, the FP energy is slightly less negative $E_{\mathrm{BF}}^{\mathrm{FP}}/N = -0.8136 \pm 0.0020$ K.

The excitation energy $E_v(r)$ of a vortex inside a disk of radius r is obtained as the difference between the total energy of the disk with and without the vortex $E_v(r) = E(r) - E_0(r)$. For large distances from the vortex axis $E_v(r)$ is usually decomposed in a hydrodynamic tail, which depends logarithmically on r, and a core energy E_c: $E_v(r) = (\pi\hbar^2\rho_0/m)\ln(r/\xi) + E_c$, where ρ_0 is the homogeneous density far from the axis and ξ is the vortex core radius. In Fig. 3 we show the vortex excitation energy $E_v(r)$ for the different choices of the trial wave function. For distances $r \gtrsim 6$ Å $E_v(r)$ shows the expected hydrodynamic behavior with a small negative shift of the backflow energy with respect to the Feynman one in agreement with the total energy results shown in Table I. For small r, the estimation of $E_v(r)$ is not exact and exhibits the influence of the trial wave function used. It is worth noticing the absence of spurious oscillations at large r, present in the results of Ref. [9], which are induced by the confining rigid walls.

The core radius ξ can be estimated, following Ref. [6], as the position of the maximum in the azimuthal circulating current $J_\theta(r)$. The radial dependence of $J_\theta(r)$ has been estimated from the pure density profile using the expression for the current in the FP approximation at the Feynman level, $J_\theta(r) = \rho_p(r)/r$. The value obtained is $\xi = 2.10 \pm 0.20$ Å which is in agreement with the result reported in Ref. [6]. By calculating the hydrodynamic contribution to the total energy for our square simulation box, we get the core energy $E_c^{F1} = 1.23 \pm 0.25$ K, $E_c^{F2} = 1.18 \pm 0.26$ K and $E_c^{\mathrm{BF}} = 1.00 \pm 0.26$ K for the Feynman and backflow phases, respectively. These values coincide with the results obtained by a fit with $E_v(r)$ for $r > 6$ Å. Our results for E_c are significantly smaller than the ones obtained in Ref. [6] and the values of E_c^F are close to the variational results of Ref. [8] based on the Feynman phase.

In conclusion, we have studied the structure of a vortex excitation in two-dimensional superfluid ^{4}He using a DMC method within the fixed-node approximation. The collective phase of the vortex has been dealt with by use of a method that allows for the use of periodic boundary conditions, removing spurious surface effects introduced by the use of confining geometries. The fixed-phase approximation is recovered as a limiting case in our approach. The result for the density profile predicts a zero particle density on the vortex axis for the two model phases used. On the other hand, the inclusion of backflow correlations in the phase gives a slightly smaller upper bound for the excitation energy. Finally, we would mention that the fixed node DMC method used in the present work permits the study of other excited states in liquid ^{4}He. Work is in progress to extend our calculations to the phonon-roton branch and the vortex-antivortex excitation in two dimensions.

This work has been supported in part by DGICYT (Spain) Grants No. PB92-0761 and No. TIC95-0429. S. G. acknowledges a postdoctoral grant from the Ministerio de Educación y Ciencia (Spain). The supercomputing facilities provided by CEPBA and CESCA are also acknowledged.

[1] P. J. Reynolds, D. M. Ceperley, B. J. Alder, and W. A. Lester, J. Chem. Phys. **77**, 5593 (1982).
[2] L. Onsager, Nuovo Cimento Suppl. **6**, 249 (1949).
[3] R. P. Feynman, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland, Amsterdam, 1955), Vol. I, Chap. II.
[4] E. P. Gross, Nuovo Cimento **20**, 454 (1961); L. P. Pitaevskii, Sov. Phys. JETP **13**, 451 (1961); A. L. Fetter, Phys. Rev. **138**, A429 (1965).
[5] G. V. Chester, R. Metz, and L. Reatto, Phys. Rev. **175**, 275 (1968).
[6] G. Ortiz and D. M. Ceperley, Phys. Rev. Lett. **75**, 4642 (1995).
[7] F. Dalfovo, Phys. Rev. B **46**, 5482 (1992).
[8] M. Saarela and F. V. Kusmartsev, Phys. Lett. A **202**, 317 (1995).
[9] S. A. Vitiello, L. Reatto, G. V. Chester, and M. H. Kalos (to be published).
[10] R. J. Donnelly, *Quantized Vortices in Helium* (University Press, Cambridge, 1991), Vol. II.
[11] R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).
[12] S. Giorgini, J. Boronat, and J. Casulleras, Phys. Rev. B (to be published).
[13] R. A. Aziz, F. R. W. McCourt, and C. C. K. Wong, Mol. Phys. **61**, 1487 (1987).
[14] J. Casulleras and J. Boronat, Phys. Rev. B **52**, 3654 (1995).