

Core Structure of a Vortex in Superfluid ^4He

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The microscopic structure of a quantized vortex core in 2D ^4He is investigated using the fixed-phase approach. We present a general method to suggest new forms for the phase of a many-particle wave function. Starting from the Feynman phase, our scheme generates *backflow* corrections with qualitatively different properties than the starting Feynman vortex. We evaluate particle density, circulating current, core radius, and energy for an isolated vortex at zero temperature using Green's function Monte Carlo.

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Even though vortices constitute a generic phenomenon in quantum systems, their microscopic structure has still not been deduced [1]. The determination of the core parameters (core radius ξ and energy E_c) and even the density at the vortex core are not yet derived from the microscopic Hamiltonian. In order to shed light on these nontrivial matters one has to consider many-body methods for strongly coupled systems. In this Letter we develop a *general* stochastic approach and apply it to the problem of a single quantum vortex in a 2D Bose superfluid confined to a disk.

The idea that vortices in a rotating bucket of ^4He might take the form of filaments with a core of atomic dimensions is due to Feynman [2]. Gross, Pitaevskii, and Fetter [3] considered a field theory description of an inhomogeneous weakly interacting Bose gas (ϕ^4 field theory). Though this approach has been successful in describing the potential flow at large distances, it gives a poor representation of the short distance behavior, mainly because of the strong correlations of ^4He atoms. A more realistic description of the core has been put forward by Chester, Metz, and Reatto [4], who considered model functions of the Feynman form and methods of classical statistical mechanics to determine the density profile and energy of the vortex configuration. Previous approaches yield a total density ρ which vanishes at the center of the core. A step forward to relax that assumption was taken by Fetter [5] who distinguished between condensate and noncondensate contributions to the z component of the total angular momentum \hat{L}_z . Based on the weakly interacting results, he conjectured that the particle density in rotating ^4He should be roughly constant, including the axis of the vortex. Strictly speaking none of the above two scenarios is exact though, as will be shown; the Feynman representation is close to the full quantum mechanical solution of an isolated vortex in ^4He .

The *fixed-phase* (FP) method [6] is a general stochastic approach to study quantum systems whose many-particle wave functions are necessarily complex. This class of problems includes fermions in external magnetic fields and topological excitations (vortices) in 2D and 3D quantum fluids, among others. For a given physical

system, whose dynamics is governed by a nonrelativistic Hamiltonian \hat{H} , one can formulate the Schrödinger eigenvalue problem as separate equations for the modulus $|\Phi|$ and phase φ of the many-body wave function $\Phi(\mathcal{R}) = |\Phi(\mathcal{R})| \exp[i\varphi(\mathcal{R})]$

$$\text{Re}\{\exp[-i\varphi]\hat{H}\exp[i\varphi]\}|\Phi(\mathcal{R})\rangle = E|\Phi(\mathcal{R})\rangle, \quad (1)$$

$$\text{Im}\{\exp[-i\varphi]\hat{H}\exp[i\varphi]\}|\Phi(\mathcal{R})\rangle = 0, \quad (2)$$

where $\mathcal{R} = (\mathbf{r}_1, \dots, \mathbf{r}_i, \dots, \mathbf{r}_N)$ denotes a point in dN dimensional configuration space. Physical states Φ can, in principle, represent particles of arbitrary statistics. The essence of the FP method consists in making a choice for φ and solving the problem for $|\Phi|$, Eq. (1), using stochastic techniques (e.g., Green's function Monte Carlo). It turns out that the equation for the modulus can be *exactly* solved with Monte Carlo methods so the remaining problem which we address in this paper is how to pick the phase.

To study a state of a given symmetry we can work with the restriction of the Hamiltonian operator to the subspace of that particular symmetry. It can be proved that the FP method provides a variational upper bound for the energy and, for a prescribed trial phase φ_T , the *lowest* energy consistent with this phase (and symmetry). In general, there are some mathematical constraints that the φ_T 's ought to satisfy; for instance, they should conserve the symmetries of the Hamiltonian (unless some are spontaneously broken), particle statistics, and be differentiable. Apart from that, physical intuition, and mean-field-type approaches, there is no procedure to generate phases systematically. In the following, we will sketch a general method to improve, in a systematic way, a given phase based on stochastic averages. The method is valid for time-reversal invariant systems, or for subspace restrictions of complex Hamiltonians which result in real symmetric operators.

For the sake of clarity, suppose we have a quantum many-body system whose Hamiltonian is $\hat{H} = -\lambda\Delta + V(\mathcal{R})$, where $\lambda = \hbar^2/2m$ and $V(\mathcal{R})$ is a general potential. $\{\Phi_\alpha\}$ are normalized eigenstates of \hat{H} with eigenvalues E_α . We are interested in finding the state Φ_V , which

is an eigenstate of $\hat{H}(E_V)$ and symmetry \hat{S} . Let us define

$$f_\tau(\mathcal{R}_0) = \frac{\Psi_G(\mathcal{R}_0)}{\exp[\tau E_G]} \int d\mathcal{R} \frac{\Psi_T^*(\mathcal{R})}{\Psi_G(\mathcal{R})} G(\mathcal{R}, \mathcal{R}_0; \tau), \quad (3)$$

where Ψ_G is a positive guiding function and

$$G(\mathcal{R}, \mathcal{R}_0; \tau) = \langle \mathcal{R} | \exp[-\tau(\hat{H} - E_G)] | \mathcal{R}_0 \rangle \frac{\Psi_G(\mathcal{R})}{\Psi_G(\mathcal{R}_0)} \quad (4)$$

is the *importance-sampled* Green's function, and Ψ_T is a trial state of a given symmetry whose phase we want to improve. Then, we can project out the ground state of a given symmetry which has a component in Ψ_T :

$$\Psi_V^*(\mathcal{R}_0) = \lim_{\tau \rightarrow \infty} \frac{f_\tau(\mathcal{R}_0)}{\exp[-\tau E_V] \langle \Psi_T | \Phi_V \rangle}. \quad (5)$$

Let us assume now that Ψ_G is the true (bosonic) ground state Φ_0 (real and normalized) and E_G is the bosonic ground state energy. Then, it can be shown that Green's function $G(\mathcal{R}, \mathcal{R}_0; \tau)$ is a probability distribution. If we separate Ψ_T and Φ_V as $\Psi_T^*(\mathcal{R}) = \Phi_0(\mathcal{R}) \exp[-\Omega(\mathcal{R})]$ and $\Phi_V^*(\mathcal{R}) = \Phi_0(\mathcal{R}) \exp[-\Omega_V(\mathcal{R})]$, where Ω and Ω_V are complex functions, Eq. (5) can be written as $\exp[-\Omega_V(\mathcal{R})] = \lim_{\tau \rightarrow \infty} \mu(\tau) \langle \exp[-\Omega(\mathcal{R})] \rangle_{\tau, \mathcal{R}_0}$, where $\mu(\tau)$ is a complex c -number, and the angular bracket $\langle \dots \rangle_{\tau, \mathcal{R}_0}$ means average over random walks beginning at \mathcal{R}_0 with a density $G(\mathcal{R}, \mathcal{R}_0; \tau)$. Since we are averaging over a probability, this expectation value can be written in a cumulant expansion [7]

$$\langle \exp[-\Omega(\mathcal{R})] \rangle = \exp[-\langle \Omega \rangle + \frac{1}{2} \langle \Omega^2 \rangle - \langle \Omega \rangle^2 + \dots]. \quad (6)$$

So far, no approximations have been made. Being interested in finding *only* corrections to the phase of Ψ_T (and not to the modulus), one can assume that Ω is purely imaginary. Then, to $\mathcal{O}(\Omega^3)$ in the cumulant expansion the corrected phase is $\Omega_V(\mathcal{R}_0) = \lim_{\tau \rightarrow \infty} \langle \Omega \rangle_{\tau, \mathcal{R}_0}$. Now consider the evolution equation for $\langle \Omega \rangle_{\tau, \mathcal{R}_0}$ in τ :

$$\partial_\tau \langle \Omega \rangle_{\tau, \mathcal{R}_0} = \lambda \int d\mathcal{R} \nabla \cdot [\nabla G - 2G \nabla \ln \Phi_0] \Omega(\mathcal{R}). \quad (7)$$

Using Green's theorem and the initial condition $\langle \Omega \rangle_{\tau=0, \mathcal{R}_0} = \Omega(\mathcal{R}_0)$, it can be integrated over imaginary time yielding $\langle \Omega \rangle_{\tau, \mathcal{R}_0} = \Omega(\mathcal{R}_0) + \lambda \int_0^\tau d\tau' \langle \Delta \Omega + 2\nabla \ln \Phi_0 \cdot \nabla \Omega \rangle_{\tau', \mathcal{R}_0}$. The solution to $[\mathcal{O}(\tau^2)]$ is

$$\langle \Omega \rangle_{\tau, \mathcal{R}_0} = \Omega(\mathcal{R}_0) + \lambda \tau [\Delta \Omega + 2\nabla \ln \Phi_0 \cdot \nabla \Omega]. \quad (8)$$

This is the main result of this paper; it tells us how to correct any trial phase analytically. Our derivation has relied upon the assumption $\Psi_G = \Phi_0$. In general, we do not know the exact ground state Φ_0 ; however, it turns out that relaxing that assumption, i.e., considering an arbitrary Ψ_G , leads to the same Eq. (8) with Φ_0 replaced by Ψ_G $[\mathcal{O}(\tau^2)]$. It is also straightforward to prove that the correction given by Eq. (8) vanishes when an exact energy eigenstate is used.

We now apply these ideas to the problem of a single vortex in liquid ^4He . A vortex is characterized by having a nonzero angular momentum, \hat{L}_Z . The Feynman vortex wave function [2] is $\Psi_T = \Phi_0 \prod_i \exp[i\theta_i]$, where θ_i is the azimuthal angle of particle i . Using the *Feynman phase* $\varphi_F = \sum_i \theta_i$ as the zeroth order ansatz we compute the first correction according to Eq. (8):

$$\varphi_B = \sum_i \left[\theta_i - 2\lambda\tau \sum_{j \neq i} \partial_{r_{ij}} u \frac{(\mathbf{r}_i - \mathbf{r}_j)}{r_{ij}} \cdot \frac{\hat{\theta}_i}{\rho_i} \right], \quad (9)$$

where we have assumed $\Phi_0 = \prod_{i < j} \exp[-u(r_{ij})]$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. In order to take into account the stochastic averaging which is neglected in Eqs. (8) and (9), we keep the form of φ_B but optimize the function u that appears in it. We call the derivative of the logarithm of the optimized function f .

As another example, and to draw the analogy with backflow correlations in liquid helium, it is instructive to analyze the phase correction when an impurity atom at position \mathbf{r}_I moves through the system with momentum $\hbar\mathbf{k}$. Then, the free-particle phase is $\Omega(\mathcal{R}_0) = \mathbf{k} \cdot \mathbf{r}_I$. Our correlated correction to that phase turns out to be $2\lambda\tau \mathbf{k} \cdot \sum_{i \neq I} \nabla_i u(r_{iI})$. This is the phase of the Feynman-Cohen *backflow* wave function [8]. By analogy, we call $\varphi_B - \varphi_F$ a backflow correction to the Feynman phase for a vortex excitation. In both cases one takes the single particle phase, and adds a pairwise sum whose strength depends on the gradient of a potential-like term. The analogous procedure for the modulus of the wave function leads from a one-body wave function, to a pair-product (Jastrow) wave function (first iteration), and to a three-body, polarization wave function (second iteration). An important feature of the corrected vortex wave function is that the density at the core is no longer identically zero and by doing a FP Monte Carlo calculation we can estimate its density. Our procedure is an indirect proof that the exact density at the core is nonzero; any pair correlation in the ground state wave function will induce a nonzero core density.

Now we describe our Monte Carlo calculations to test this procedure. We consider a system of N bosons of mass m in a disk of radius R , interacting through a Lennard-Jones potential $V_{LJ}(r)$, with an additional potential confining the atoms to the interior of the disk which mimics a static layer of helium at the edge of the disk. We use lengths in units of σ (2.556 Å), energies in units of λ/σ^2 (0.9276 K), and $\epsilon = 10.22$ K. The trial states we consider are of the form

$$\Psi_T = \prod_i \left[\frac{\tilde{z}_i}{r_i + a} \right]^\ell \Psi_0, \quad (10)$$

where ℓ is the strength of the vortex, $\tilde{z}_i = z_i + \kappa \sum_{j \neq i} f(r_{ij}, r_i, r_j) (z_i - z_j)$ with $z_i = x_i + iy_i$ defining the atomic position in complex coordinates, a and κ are variational parameters, and f is the backflow function. Ψ_0 is the McMillan-Jastrow approximation to

the ground state modified by the existence of the disk boundary

$$\Psi_0 = \prod_{i < j} \exp\left[-\left(\frac{b}{r_{ij}}\right)^5\right] \prod_i \exp[-\chi(r_i)], \quad (11)$$

with $\chi(r) = (1 + \exp[\beta(R^2 - r^2)])^{-1}(c/\sqrt{R^2 - r^2})^9$, where b , c , and β are variational parameters.

Clearly Ψ_T is an eigenstate of angular momentum, $\hbar N\ell$. The Feynman phase is recovered by setting κ equal to 0. It is clear from Eq. (10) that each particle is seeing a zero at a position different than the origin and so the particle density at the origin will not vanish (unless $\kappa = 0$, of course). We have used the form $f(r_{ij}, r_i, r_j) = \exp(-[\alpha r_{ij}^2 + \gamma(r_i^2 + r_j^2)])$ for the backflow function. The two variational parameters α and γ characterize different length scales. For γ nonzero, particles which are far from the core axis will not contribute to the backflow, so that we recover irrotational flow outside of the core.

Our simulations contained $N = 50$ ^4He atoms in a disk of radius $R = 9.31$. The ground state calculation corresponds to $\ell = 0$, while for the vortex $\ell = 1$. We first perform a variational Monte Carlo (VMC) calculation to optimize the free parameters in the trial wave function, by minimizing the fluctuations of the local energy. We use a multiparticle Metropolis algorithm to compute the expectation value of the total energy, the particle density, and current $\mathbf{J}_\theta(\mathbf{r}) = \langle \sum_{i=1}^N [\delta(\mathbf{r} - \mathbf{r}_i) \nabla_i \varphi_T] \rangle_{\mathcal{P}(\mathcal{R})}$, where expectation values are evaluated with respect to the variational distribution: $\mathcal{P}(\mathcal{R}) = |\Psi_T|^2 / \|\Psi_T\|^2$. The VMC energies for the three wave functions (ground state E_0 , Feynman vortex, and backflow vortex) are quoted in Table I and are computed by averaging the local energy $E_{\text{loc}}(\mathcal{R}) = |\Psi_T|^{-1} \hat{H} |\Psi_T| + V_{\varphi_T}$, where the phase contribution is $V_{\varphi_T} = \sum_{i=1}^N (\nabla_i \varphi_T)^2$. As will be explained below, the parameters in the backflow function are optimized in a different way, by minimizing the fixed-phase energy.

We now improve on the VMC energy by using the FP method. The calculation is almost identical to the standard diffusion (or Green's function) Monte Carlo [9]. We start our FP computation assuming some phase φ_T and an initial ensemble of $N_c = 400$ configurations \mathcal{R}_i distributed according to $\mathcal{P}(\mathcal{R})$. We then diffuse, drift, and branch each configuration as $\mathcal{R}'_i = \mathcal{R}_i + \tau \mathbf{F}(\mathcal{R}_i) + \eta$, where η is a random vector; each component is normally distributed with a variance of 2τ , and $\mathbf{F} = \nabla \ln |\Psi_T|^2$ is the gradient of the trial function. Iteration of this procedure

TABLE I. Total energies (in K) for the ground state (E_0) and vortex excitation (E_V^F and E_V^B) for a system of $N = 50$ ^4He atoms. Numbers in parentheses represent statistical error bars. Optimal parameters (see text): $a = 0.15$, $b = 1.01$, $c = 5.32$, $\beta = -0.05$, $\kappa = 0.7$, $\alpha = 0.9$, and $\gamma = 0.5$.

| | E_0 | E_V^F | E_V^B |
|-----|------------|-----------|-----------|
| VMC | -1.77(14) | 4.55(14) | 4.85(15) |
| FP | -15.59(15) | -9.68(14) | -9.88(16) |

is equivalent to applying the importance-sampled Green's function and at convergence reaches the stationary distribution $\mathcal{P}_\ell(\mathcal{R}) \propto |\Psi_T| |\Psi_\ell|$, where Ψ_ℓ is the many-body wave function with lowest energy whose phase is φ_T . This procedure leads to the *exact* boson ground state energy ($\ell = 0$) or determines an upper bound to the exact vortex energy ($\ell = 1$). For the vortex, we considered two possibilities: with and without backflow. The "mixed" observables are obtained as averages over $\mathcal{P}_\ell(\mathcal{R})$.

The modulus of the trial wave function does not affect the final estimated energy but only the rate of convergence to the final answer. However, the backflow parameters, κ , α , and γ , appearing in the phase do affect the estimated energy. To determine them, we have computed the partial derivative of the FP energy with respect to the phase parameters using the usual formula for extrapolating from the variational and mixed distribution to the exact distribution. For example, $\partial_\kappa \langle E_{\text{loc}} \rangle_{\mathcal{P}_\ell(\mathcal{R})} = 2 \langle \partial_\kappa V_{\varphi_T} \rangle_{\mathcal{P}_\ell(\mathcal{R})} - \langle \partial_\kappa V_{\varphi_T} \rangle_{\mathcal{P}(\mathcal{R})}$, and iterated until the derivative acquired its minimum absolute value. This procedure yields the values κ , α , and γ quoted in Table I as well as the FP energies. It is seen that the backflow does not lower the energy significantly.

Figures 1 and 2 show the VMC (ρ_{VMC}), FP (ρ_{FP}) and extrapolated (ρ_E) densities for the ground state, the Feynman vortex, and the backflow vortex. The large difference between VMC and FP densities is due to the lack of proper correlations in the modulus of Ψ_T . The extrapolated value is defined as $\rho_E = \rho_{\text{FP}}^2 / \rho_{\text{VMC}}$ and is properly normalized. We have checked our densities by performing path-integral Monte Carlo (PIMC) calculations at $T = 0.5$ K both in the Feynman vortex state and in thermal equilibrium. The density evaluated by PIMC has no bias. Notice that, although small, the value of the backflow vortex density at the core is nonzero contrary to what happens with the Feynman vortex. Another feature worth mentioning is the drastic reduction of the bump

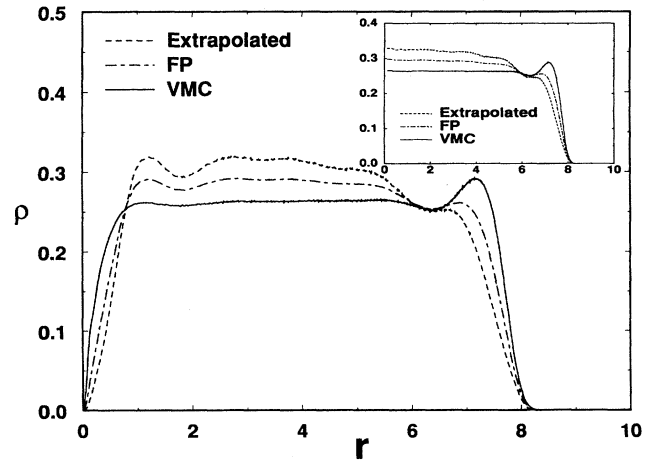


FIG. 1. The particle density ρ (in units of $1/\sigma^2$) as a function of distance (in units of σ) from the axis of the vortex using the Feynman phase. In the inset we show the density without the vortex.

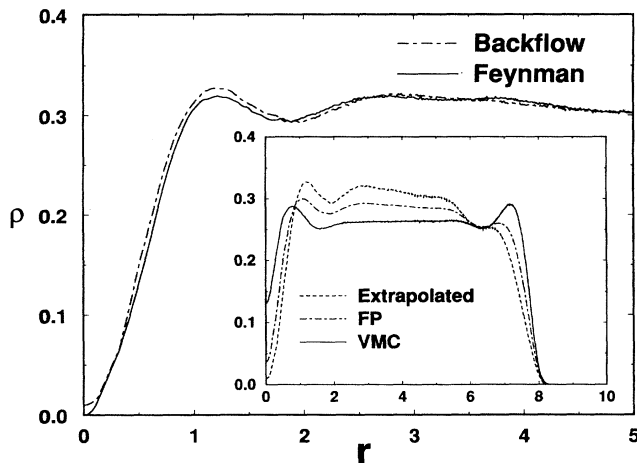


FIG. 2. Comparison between backflow and Feynman extrapolated vortex densities. Both are indistinguishable for $r > 5$. The inset displays superfluid vortex densities using backflow.

near the disk boundary as one passes from the VMC to the extrapolated quantities. Finally, Fig. 3 displays the circulating current which in the Feynman case is given by $\mathbf{J}_\theta(r) = \rho(r)/r$; the extrapolated current is defined in a similar way as ρ_E .

To our knowledge, there is no unique definition of the vortex core parameters in terms of observables. Typically these parameters are introduced phenomenologically. Here we give a definition on physical grounds. The core of a vortex is expected to rotate like a solid rod. Then, the core radius ξ delimits the boundary between solid-body rotation and potential flow. Based on this picture, we define ξ as the position where the circulating current \mathbf{J}_θ has a maximum (see Fig. 3).

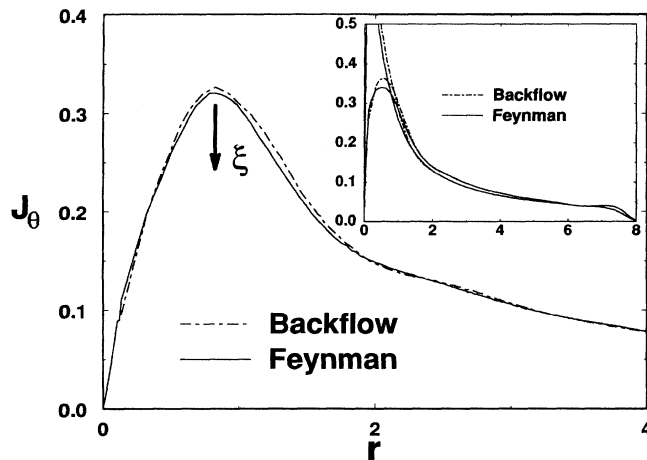


FIG. 3. The extrapolated current \mathbf{J}_θ (in units of $\hbar/m\sigma^3$) as a function of distance (in units of σ) from the axis of the vortex. The arrow indicates the value of the core radius ξ . The inset shows current profiles resulting from VMC (upper 2 curves) and FP (lower 2 curves) calculations with and without backflow.

TABLE II. Vortex core parameters: core radius ξ (in \AA) and core energy E_c (in K) in the FP and extrapolated (Ex) cases using both Feynman and backflow phases.

| | ξ^F | ξ^B | E_c^F | E_c^B |
|----|---------|---------|---------|---------|
| FP | 1.32(8) | 1.43(8) | 2.8(3) | 2.7(3) |
| Ex | 2.06(8) | 2.10(8) | 3.2(3) | 3.1(3) |

Once the core radius is defined, the core energy is evaluated as $E_c = E_V - E_0 - 2N/R^2 \ln(R/\xi)$, i.e., we subtract the asymptotic hydrodynamic energy (which is finite only for a disk of finite radius and accounts for most of the energy) from the excitation energy. We present the result of these calculations in Table II. These parameters were also estimated using the Kosterlitz-Thouless recursion relations to superfluid densities obtained with PIMC [10] obtaining $\xi = 1.9(2) \text{\AA}$ and $E_c = 2.7(2) \text{ K}$, values which are roughly the same as the ones we calculated.

In conclusion, we have studied the microscopic structure of an isolated vortex in ^4He using the fixed-phase method. We have introduced a general scheme to generate new forms for the phase. We show that the first correction to the Feynman phase is of the backflow form. Aside from a 4% correction to the density near the core axis, Feynman phase yields a very good description of a vortex in superfluid ^4He .

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