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Vortex lines in ^4He clusters

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Abstract. We present translationally invariant many-body wavefunctions which represent vortices in boson clusters. These functions are orbital angular momentum eigenstates, and a particular one within the class is an exact energy eigenstate for a cluster interacting with harmonic pairwise potentials. The results are valid for N atoms, with $N \geq 2$. Implications for superfluidity in ^4He nanodroplets are discussed.

1. Introduction

Clusters of helium atoms are interesting because of their highly quantum nature (with important delocalization and exchange symmetry effects) and in possibly exhibiting superfluidity in small quantum systems [1]. Helium droplets have also been proposed as a nanoscale cryostat for high resolution spectroscopy and studies of quantized vorticity [2–12]. Droplets produced in a supersonic expansion of cold helium gas or liquid into vacuum contain up to 10^8 atoms. The larger droplets form a superfluid matrix with extremely high thermal conductivity. Here we consider the rotational excitations of these droplets. An early investigation into the rotation of a self-bound system [13] stressed that true angular momentum eigenstates have to have translational invariance, and a class of wavefunctions with the correct translational and permutation symmetries was investigated. This approach is taken here, with emphasis on the form and structure of quantized vortices.

How large does a Bose system have to be before superfluid behaviour is manifested? One particular aspect of superfluids, the possible existence within them of quantized vortices, was thought to throw light on this question. Here we shall show that there is no indication in the many-body wavefunction of a vortex of a critical size for vortex formation. We consider a self-bound system of N helium atoms, with Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2 + V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N). \quad (1)$$

The potential energy V is assumed to be symmetric with respect to any permutation of the particle coordinates, and to be translationally and rotationally invariant. Pairwise central interactions are not assumed. Since helium atoms have spin zero, the angular momentum we consider is orbital angular momentum. We seek to find translationally invariant wavefunctions, symmetric in the N particle coordinates, which represent particular types of motion, for example vortex motion.

2. Vortex wavefunctions

A line vortex in a cylinder of helium is represented by wavefunctions of the type $\Psi = F\Phi$, where Φ is the ground state and, for a singly quantized vortex [14–19],

$$F = \prod_{j=1}^N e^{i\phi_j} s(\rho_j). \quad (2)$$

Here ϕ_j and ρ_j represent the azimuthal angle and the distance from the axis of rotation of atom j . In [17] the optimum function $s(\rho)$ was shown to satisfy a certain non-linear integro-differential equation. At small ρ , near the vortex core, s was shown to be proportional to ρ . Away from the vortex core, $s \rightarrow 1$. The z -component of the angular momentum associated with (2) is $N\hbar$.

For $N = 3$ we expect the vortex analogue (if it should exist) to have angular momentum $3\hbar$. Consider the function

$$\begin{aligned} & [x_2 + x_3 - 2x_1 + i(y_2 + y_3 - 2y_1)][x_3 + x_1 - 2x_2 + i(y_3 + y_1 - 2y_2)] \\ & \times [x_1 + x_2 - 2x_3 + i(y_1 + y_2 - 2y_3)]. \end{aligned} \quad (3)$$

This is manifestly translationally invariant, and symmetric with respect to particle interchange. We can verify that (3) is an angular momentum eigenstate, with L_z eigenvalue $3\hbar$. Now, the raising operator

$$\ell_+ = \ell_x + i\ell_y = yp_z - zp_y + i(zp_x - xp_z) = \hbar \left\{ z \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) - (x + iy) \frac{\partial}{\partial z} \right\} \quad (4)$$

annihilates any function of $x + iy$, or indeed any function of the two variables $(x + iy, r)$ where $r^2 = x^2 + y^2 + z^2$. It follows that (3) times any rotationally invariant function of x_1, \dots, z_3 is the uppermost eigenstate, and since

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_-L_+ + \hbar L_z + L_z^2 \quad (5)$$

any eigenstate of L_z with $L_z\Psi = L\hbar\Psi$ which is annihilated by $L_+ = L_x + iL_y$ is an eigenstate of L^2 with eigenvalue $\hbar^2 L(L + 1)$. Thus (3) is a three-body (three-dimensional) angular momentum eigenstate with $L = 3$. We can rewrite (3) as proportional to

$$[x_1 - X + i(y_1 - Y)][x_2 - X + i(y_2 - Y)][x_3 - X + i(y_3 - Y)] \quad (6)$$

where X and Y are the centre-of-mass coordinates for the three atoms.

For N atoms we consider wavefunctions of the type

$$\Psi = \prod_{j=1}^N [x_j - X + i(y_j - Y)]\Phi \quad (7)$$

where Φ is the rotationally invariant ground state, and

$$X = \frac{1}{N} \sum_{j=1}^N x_j \quad Y = \frac{1}{N} \sum_{j=1}^N y_j. \quad (8)$$

To make the correspondence with vortices, we note that if we define (for each particle coordinate) an azimuthal angle

$$\phi_j = \tan^{-1} \left(\frac{y_j - Y}{x_j - X} \right) \quad (9)$$

then

$$e^{i\phi_j} = \frac{x_j - X + i(y_j - Y)}{\sqrt{(x_j - X)^2 + (y_j - Y)^2}} \quad (10)$$

and the factor multiplying Φ in (7) is proportional to

$$\prod_{j=1}^N e^{i\phi_j} = e^{i\sum_{j=1}^N \phi_j}. \tag{11}$$

We find that multiplying each factor $x_j - X + i(y_j - Y)$ by any function g of $\rho_j = \sqrt{(x_j - X)^2 + (y_j - Y)^2}$ still retains us the uppermost angular momentum eigenstate with $L = N$. Thus we have found the translationally invariant analogue of (2):

$$\Psi = \left\{ \prod_{j=1}^N \frac{[x_j - X + i(y_j - Y)]}{\sqrt{(x_j - X)^2 + (y_j - Y)^2}} s \left(\sqrt{(x_j - X)^2 + (y_j - Y)^2} \right) \right\} \Phi. \tag{12}$$

This wavefunction describes a vortex in a self-bound system of N identical particles.

3. Harmonic interactions

In [13] it was shown that the wavefunction

$$\Psi = \sum_j \sum_k (x_{jk} + iy_{jk})^L \Phi \quad (L \text{ even}) \tag{13}$$

is an exact energy eigenstate for harmonic interactions,

$$V = \sum_{i < j} \sum v_{ij} \quad v_{ij} = \frac{1}{2} K r_{ij}^2 \tag{14}$$

as well as being an angular momentum eigenstate. Here we show that likewise the vortex state with $L = N$ and wavefunction

$$\Psi = \prod_{j=1}^N [x_j - X + i(y_j - Y)] \Psi \equiv \left(\prod_{j=1}^N f_j \right) \Phi \tag{15}$$

is an energy eigenstate. We use the identity ([13], (25)) which applies to $\Psi = F\Phi$ with Hamiltonians of type (1):

$$(H - E_0)\Psi = -\frac{\hbar^2}{2m} \Phi^{-1} \sum_k \nabla_k \cdot (\Phi^2 \nabla_k F) \tag{16}$$

where E_0 is the ground state energy. Here F is a product of terms in each of which x_j and y_j appear in the combination $x_j + iy_j$. The two-dimensional Laplacian vanishes for any function of $x + iy$, so the Laplacian of F is zero. Thus (16) reduces to

$$(H - E_0)\Psi = -\frac{\hbar^2}{m} \sum_k \nabla_k \Phi \cdot \nabla_k F. \tag{17}$$

Note that for $F = \prod f_j$ as in (15),

$$\nabla_1 F = \left(\frac{1}{f_1} - \frac{1}{N} \sum_{j=1}^N \frac{1}{f_j}, \frac{1}{f_1} - \frac{i}{N} \sum_{j=1}^N \frac{1}{f_j}, 0 \right) F \tag{18}$$

and that the ground state for harmonic interactions (14) is

$$\Phi = \exp \left\{ -\frac{1}{2\hbar} \sqrt{\frac{Km}{N}} \left[N \sum_{j=1}^N r_j^2 - \left(\sum_{j=1}^N r_j \right)^2 \right] \right\} \tag{19}$$

so

$$\frac{\partial \Phi}{\partial x_1} = -\frac{1}{\hbar} \sqrt{N K m} (x_1 - X) \Phi \quad \frac{\partial \Phi}{\partial y_1} = -\frac{1}{\hbar} \sqrt{N K m} (y_1 - Y) \Phi. \quad (20)$$

Thus

$$\nabla_1 \Phi \cdot \nabla_1 F = -\frac{1}{\hbar} \sqrt{N K m} \left\{ 1 - \frac{f_1}{N} \sum_{j=1}^N \frac{1}{f_j} \right\} F \Phi \quad (21)$$

and therefore

$$\sum_k \nabla_k \Phi \cdot \nabla_k F = -\frac{N}{\hbar} \sqrt{N K m} \quad (22)$$

since

$$\sum_{k=1}^N f_k = \sum_{k=1}^N [x_k - X + i(y_k - Y)] = 0. \quad (23)$$

It follows that (15) is an exact energy eigenstate for harmonic interactions, with excitation energy

$$E - E_0 = N \hbar \sqrt{\frac{N K}{m}}. \quad (24)$$

For comparison, the excitation energy of (13) is $L \hbar \sqrt{N K / m}$, so for $N \gg L$ the vortex energy is much larger (for harmonic interactions).

4. Discussion

We have shown that translationally invariant N -body vortex wavefunctions may be written down, and that a particular member of this class of wavefunction is an exact energy eigenstate in the case of harmonic pairwise interactions. The results hold for $N \geq 2$, and there is no indication of a critical cluster size being needed for vortex formation. (The mechanism of formation of helium clusters containing vortices and their detection has been discussed in section 3 of [6]; see also the references given there.)

Leggett [20] has proposed non-classical rotational inertia as an indicator of superfluidity, and a quantized vortex certainly has non-classical rotational inertia. Thus, if the existence of quantized vortices is taken as a criterion for superfluidity, the implication of this work appears to be that any number of ^4He atoms will form a superfluid droplet if the temperature is low enough (experiments are performed at about 0.37 K [4]). This statement seems to be in contradiction to the findings of [7], which reports that OCS molecules rotate freely in helium-4 droplets but not in helium-3 droplets, unless a minimum number of about 60 helium-4 atoms are added to the helium-3 droplets. These authors conclude ‘... it appears that 60 is the minimum number needed for superfluidity’. We note that an alternative explanation is possible: 60 is roughly the number of ^4He atoms required to provide shielding of the OCS molecule from collision with the fermion ^3He atoms by surrounding it with a double atomic layer. The tentative conclusion of this paper is that close to absolute zero any number of ^4He atoms forming a droplet can sustain quantized vorticity, and can thus be considered superfluid. This is in agreement with the free rotor spectra of SF_6 in very small helium clusters determined by quantum Monte Carlo calculations [21]; an earlier Monte Carlo study [22] found that ‘manifestations of superfluidity exist in a cluster of 64 atoms’, but does not put a lower bound on the number of atoms for superfluidity to exist.

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