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The long-wavelength spectrum of vortex waves in a Bose–Einstein condensate

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Abstract
Here we consider vibrations of a single quantum vortex in a Bose–Einstein condensate. Two different dispersion relations can be found in the literature; we remove the contradiction on the basis of both numerical and analytical considerations. The outcome is that the frequency of the vibrations, ω, is proportional to $k^2 \ln(1/k)$, where k is the wavenumber, assumed small compared to the inverse core size. An extension of the phase integral approximation is used in the numerical analyses.

1. Introduction

The recent spectacular achievement of Bose–Einstein condensation in trapped alkali metal gases by Cornell, Ketterle, Wieman and others [1–3] has prompted scientists to develop and tighten the theory. As vortices have been created in the medium, here we will take a new look at the vibrations of the basic, $n = 1$, vortex structure in a Bose–Einstein condensate (BEC).

A BEC is often described by a single-particle wavefunction $\psi(\vec{x}, t)$ of N bosons of mass m that obeys the nonlinear Schrödinger equation. This equation is, according to Gross and Pitaevski,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + W_0\psi|\psi|^2. \qquad (1.1)$$

An external trap potential is sometimes added when describing recent experiments. This will not be needed here. Thus we study a vortex in an unbounded condensate. W_0 characterizes the potential between bosons. A short-wave repulsive potential has been modelled by a delta function so as to obtain the cubic term. Equation (1.1) can be cast into dimensionless form via the transformation (here E is the chemical potential)

$$\psi \to \left(\frac{mE}{W_0}\right)^{1/2} \exp(-imEt/\hbar) \qquad x \to \frac{\hbar x}{\sqrt{2Em}} \qquad t \to \frac{\hbar t}{2mE}. \qquad (1.2)$$

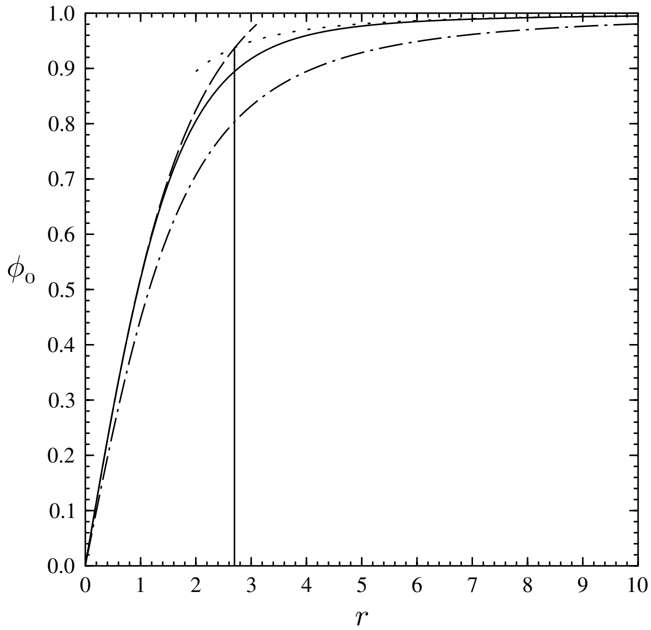

Figure 1. $\phi_0(r)$ calculated numerically and also from models: solid curve (——) for numerical results, broken curve (— — —) for $\phi_{01}(r) = 1.166r/\sqrt{4+r^2}$, dotted curve (· · · · · ·) for $\phi_{02}(r) = r/\sqrt{1+r^2}$ and dot–dash curve (— · —) for Fetter's $r/\sqrt{4+r^2}$; $\phi_{01}(r)$ and $\phi_{02}(r)$ cross at $r_0 = 2.706$.

Now (1.1) becomes

$$2\mathrm{i}\frac{\partial\psi}{\partial t} = -\nabla^2\psi - \psi(1 - |\psi|^2). \tag{1.3}$$

An equation for the equilibrium state of a single, $n = 1$, vortex is derived from (1.3):

$$\psi = \phi_0 \exp(\mathrm{i}\theta) \tag{1.4}$$

$$\frac{\mathrm{d}^2\phi_0}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}\phi_0}{\mathrm{d}r} = \phi_0(\phi_0^2 - 1 + 1/r^2). \tag{1.5}$$

We will be concerned with vibrations around the solution to (1.5) such that $\phi_0(0) = 0$, $\phi_0(r) \to 1$ as $r \to \infty$. This solution is illustrated by figure 1. We write

$$\psi = (\phi_0 + \delta\phi)\exp[\mathrm{i}(\theta + \delta\theta)] \tag{1.6}$$

and consider the perturbations

$$\delta\phi = \delta\phi(r,k)\cos(kz)\sin(\theta - \omega t) \tag{1.7a}$$

$$\delta\theta = \delta\theta(r,k)\sin(kz)\cos(\theta - \omega t). \tag{1.7b}$$

It will prove convenient to introduce $\delta\chi = \phi_0\delta\theta$. Next $\delta\phi$ and $\delta\chi$ are expanded in k, assumed small:

$$\delta\phi(r,k) = \delta\phi_0 + k\,\delta\phi_1 + k^2\,\delta\phi_2 + \cdots \tag{1.8a}$$

$$\delta\chi(r,k) = \delta\chi_0 + k\,\delta\chi_1 + k^2\,\delta\chi_2 + \cdots \tag{1.8b}$$

and a dispersion relation is obtained by one of various methods. The history is confusing, as different approximations seem to yield different solutions. Pitaevski and Fetter [4, 5] obtained

$$\omega = \tfrac{1}{2}k^2\ln(1/k) \tag{1.9}$$

which is a relation similar to that found by Kelvin for vibrations of a classical vortex in hydrodynamics [6]. This should not be too surprising, as fluid equations can be derived from (1.3) (albeit with a complicated pressure tensor and quantized circulation of the velocity). However, Rowlands [7] found $\omega \propto k^2$ and also mentioned flaws in the derivations of [4] and [5] (these flaws, however, only generated errors in higher-order terms). A bit earlier, equation (1.9) was derived by matching approximate solutions for $\delta\phi(r, k)$ and $\delta\theta(r, k)$ in two different regions ($r \ll 1/k$ and $r \sim 1/k$) [8]. As far as we can see, the derivation of [8] is free of the weaknesses of [4] and [5]. A further argument in favour of the credibility of (1.9) is that it can be reobtained as a limit of a much more complicated dispersion relation for a vortex ring, also obtained by matching two regions, but involving different mathematics. For further references for all these problems, see [9, 10] for general background, and [11] for vortex rings.

Having read the above-mentioned papers, we posed the following question: how does an expansion in k (or another small parameter) for the entire region as practised by us [12–14], in which consistency conditions in the form of integrals over all space are imposed, perform? Does it yield a dispersion relation contradicting (1.9)? To answer this question, we will take another look at Rowlands' formula. First, however, we appeal to numerics for a verdict on the veracity of equation (1.9).

2. Numerical calculations

So as to find the dispersion relation $\omega(k)$ numerically, we introduce the notation

$$u = \delta\phi + \delta\chi \qquad v = \delta\phi - \delta\chi. \tag{2.1}$$

Equations (1.3), (1.6) and (2.1) now yield a more symmetric pair for the perturbed quantities:

$$\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}u}{\mathrm{d}r} - \left(\frac{4}{r^2} + k^2 - 1 + 2\phi_0^2\right)u - \phi_0^2 v = 2\omega u \tag{2.2a}$$

$$\frac{\mathrm{d}^2v}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}v}{\mathrm{d}r} - (k^2 - 1 + 2\phi_0^2)v - \phi_0^2 u = -2\omega v \tag{2.2b}$$

where ϕ_0 solves (1.5). These equations have a unique pair of solutions that are finite at zero and vanish at infinity. Divergent solutions at either end must be eliminated. This determines $\omega(k)$ uniquely.

The first-derivative terms in equations (2.2) can be eliminated by the transformation

$$u = r^{-1/2}\tilde{u} \qquad v = r^{-1/2}\tilde{v} \tag{2.3}$$

leading to

$$\frac{\mathrm{d}^2\tilde{u}}{\mathrm{d}r^2} - \left[f_0(r) + k^2 + 1 + 2\left(\omega + \frac{1}{r^2}\right)\right]\tilde{u} - [1 - f_1(r)]\tilde{v} = 0 \tag{2.4}$$

$$\frac{\mathrm{d}^2\tilde{v}}{\mathrm{d}r^2} - \left[f_0(r) + k^2 + 1 - 2\left(\omega + \frac{1}{r^2}\right)\right]\tilde{v} - [1 - f_1(r)]\tilde{u} = 0 \tag{2.5}$$

where

$$f_0(r) = -\left\{\frac{1}{4r^2} + 2\left[f_1(r) - \frac{1}{r^2}\right]\right\} \simeq -\left[\frac{1}{4r^2} + \frac{4}{r^4} + \frac{38}{r^6} + \frac{748}{r^8}\right] \tag{2.6}$$

$$f_1(r) = 1 - \phi_0^2(r) \simeq \frac{1}{r^2} + \frac{2}{r^4} + \frac{19}{r^6} + \frac{374}{r^8} \tag{2.7}$$

and the approximate expressions follow from the asymptotic expansion of $\phi_0(r)$ for $r \to \infty$; see (A.5) in the appendix. This form of the equations is convenient for determining the asymptotic behaviour of unknown functions as $r \to \infty$. In this limit all r-dependent terms in the coefficients of equations (2.4) and (2.5) tend to zero. Neglecting them, one can easily find two pairs of solutions [8]:

$$\tilde{u} = \exp(\pm\beta_j r) \qquad \tilde{v} = s_j\tilde{u} \qquad j = \text{se, ge} \tag{2.8}$$

where β_{se} ('smaller exponent'), β_{ge} ('greater exponent') and the corresponding s_j are constants; for components of the eigenfunctions, the minus sign should be chosen. In view of (2.4)–(2.6), the validity condition for (2.8) is

$$r \gg \frac{\sqrt{2}}{k}. \tag{2.9}$$

Our approach to calculating ω for given k will be to integrate numerically equations (2.2) from $r = \epsilon \ll 1$ to r_{mch} (matching distance) and from $r = r_{\text{as}} \gg 1$ (asymptotic distance) to r_{mch}, and to choose the free parameters such that the functions u, v and their derivatives u', v' are continuous at r_{mch} (shooting method).

The boundary condition (u, u' and v, v') at $r = \epsilon$ will be calculated from power expansions around $r = 0$ (extensions of those given in [8]) of two solutions finite at $r = 0$, (u_1, v_1) and (u_2, v_2); see (A.1) in the appendix:

$$u = C_1u_1 + C_2u_2 \qquad u' = C_1u_1' + C_2u_2' \tag{2.10}$$

$$v = C_1v_1 + C_2v_2 \qquad v' = C_1v_1' + C_2v_2'. \tag{2.11}$$

The boundary condition at $r = r_{\text{as}}$ can be calculated from (2.8), but in that case r_{as} must satisfy (2.9), and becomes unacceptably large for small k. Thus, to make the calculation for small k feasible, better asymptotics must be found. By analogy to the well known phase integral approximation used for just one ordinary differential equation of the Schrödinger type [15, 16], we will assume, instead of (2.8),

$$\tilde{u} = q(r)^{-1/2}\exp\left[\mathrm{i}\int_{r_0}^{r} q(r')\,\mathrm{d}r'\right] \qquad \tilde{v} = s(r)\tilde{u} \tag{2.12}$$

where the functions $q(r)$ and $s(r)$ are 'slowly varying'. Inserting (2.12) into (2.4) and (2.5) and neglecting terms with derivatives of $q(r)$ and $s(r)$, we arrive at two equations for these two functions[1]:

$$\begin{aligned} &-q^2 - [f_0(r) + k^2 + 1 + 2(\omega + r^{-2})] - [1 - f_1(r)]s = 0 \\ &-q^2 - [f_0(r) + k^2 + 1 - 2(\omega + r^{-2})] - [1 - f_1(r)]s^{-1} = 0. \end{aligned} \tag{2.13}$$

Solving these two equations we obtain

$$q^2 = -\beta_j^2(r) \qquad j = \text{se, ge} \tag{2.14}$$

$$\beta_{\text{se}}(r) = \left\{f_0(r) + k^2 + 1 - \sqrt{4(\omega + r^{-2})^2 + [1 - f_1(r)]^2}\right\}^{1/2} \tag{2.15}$$

$$\beta_{\text{ge}}(r) = \left\{f_0(r) + k^2 + 1 + \sqrt{4(\omega + r^{-2})^2 + [1 - f_1(r)]^2}\right\}^{1/2} \tag{2.16}$$

$$s_j(r) = \frac{\beta_j^2(r) - [f_0(r) + k^2 + 1 + 2(\omega + r^{-2})]}{1 - f_1(r)}. \tag{2.17}$$

[1] A general theory of the phase integral approximations for two or more differential equations similar to (2.4), (2.5) has been developed by one of us (AAS) and will be published elsewhere; see also [17]. What is obtained here can be shown to be the lowest-order approximation in the expansion parameter.

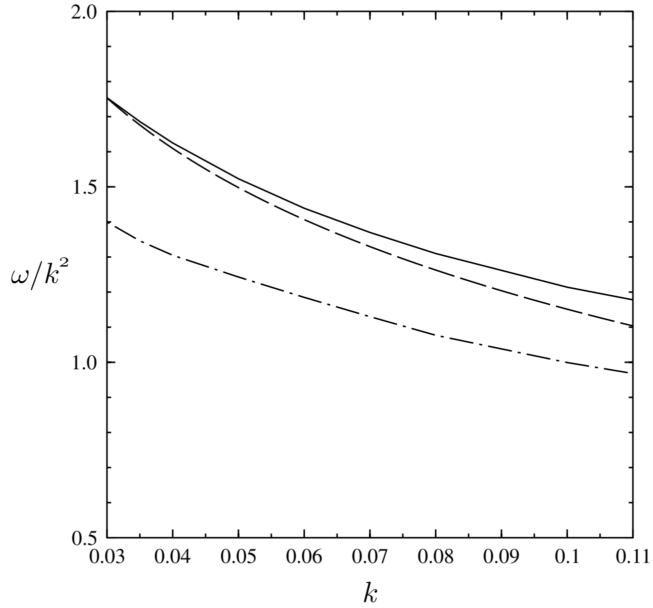

Figure 2. ω/k^2 as a function of k for long-wave perturbations: the solid curve (——) denotes numerical results, the broken curve (— — —) is the theoretical curve, $\frac{1}{2}\ln(1/k)$, and the dot–dash curve (— · —) is the Rowlands γ-coefficient (3.1) with $\delta\phi$ and $\delta\chi$ found numerically for given k.

As $q(r)$ defined by (2.14) is pure imaginary and has a double sign, this sign (for eigenfunctions) must be chosen such that $\mathrm{i}q(r) = -\beta_j(r)$, $j = \mathrm{se}, \mathrm{ge}$. Finally, for $r \geqslant r_{\mathrm{as}}$ we can write

$$u = C_{\mathrm{se}} u_{\mathrm{se}}(r) + C_{\mathrm{ge}} u_{\mathrm{ge}}(r) \qquad v = C_{\mathrm{se}} s_{\mathrm{se}}(r) u_{\mathrm{se}}(r) + C_{\mathrm{ge}} s_{\mathrm{ge}}(r) u_{\mathrm{ge}}(r) \tag{2.18}$$

where

$$u_j(r) = [r\beta_j(r)]^{-1/2} \exp\left[-\int_{r_0}^{r} \beta_j(r')\,\mathrm{d}r'\right]. \tag{2.19}$$

To fix the multiplication constant in (2.18) we will take $C_{\mathrm{se}} = 1$. The choice of lower limit of integration in (2.19) is arbitrary, but if we choose it at r_{as}, there will be no integral in the boundary condition at r_{as}; see equation (A.3) in the appendix.

Note that in the limit of $r \to \infty$, in which $f_0(r)$, $f_1(r)$ and r^{-2} tend to zero, equations (2.15)–(2.17) reproduce the results of Grant [8, p 700].

For given k, there are four free parameters in our problem: C_1, C_2, C_{ge} and ω, to be determined from four continuity conditions at r_{mch}. In our calculations we increased r_{as} until ω no longer depended on r_{as}. Typically, this limiting value of r_{as} was of the order of $1/k$ (rather than $\gg\sqrt{2}/k$).

The calculation becomes progressively more difficult as k decreases. However, with present day capabilities we have been able to take the numerical procedure down to $k = 0.03$. In the appendix we describe some further details of our calculation. The numerical program (in Fortran 77) is obtainable from the authors on request.

The results are presented as figure 2. Only by drawing ω/k^2 as a function of k were we able to answer the crucial question. Clearly $\omega \propto k^2 \ln(1/k)$ as k tends to zero.

3. Is Rowlands' formula right or wrong?

A secondary feature of figure 2 is the curve corresponding to the Rowlands coefficient γ in his $\omega = \gamma k^2$, *calculated for given* k:

$$\gamma = \frac{\langle \delta\phi_0^2\rangle + \langle \delta\chi_0^2\rangle}{4\langle \delta\phi_0\, \delta\chi_0\rangle} \qquad \langle a(r)\rangle = \int_0^\infty a(r) r\, \mathrm{d}r. \tag{3.1}$$

This coefficient does not tend to a constant as k tends to zero, but instead follows the logarithmic curve. Below, we present a qualitative explanation of why this is the case. Broadly speaking, it is due to the fact that the $k = 0$ limit is singular as far as the large-r dependence of $\delta\phi$ and $\delta\chi$ is concerned. In contradistinction to most of our k-expansion calculations, e.g. [12–14], a slow k-dependence in $\delta\chi$ must be included in the integral. When this is done, and the integrals estimated, we find

$$\omega = \tfrac{1}{2}k^2[\ln(1/k) - \text{constant}]. \tag{3.2}$$

The constant is positive and is at most of order one, and therefore insignificant when k is small. The following is a refinement of Rowlands' calculation.

Rowlands' formula, in our notation as given by (3.1),

$$\omega = k^2 \frac{\langle \delta\phi_0^2\rangle + \langle \delta\chi_0^2\rangle}{4\langle \delta\phi_0\, \delta\chi_0\rangle} \tag{3.3}$$

was obtained by expanding all quantities in k and then demanding that a global integral consistency condition be satisfied. The r-domain is treated as a whole, in contradistinction to Grant's treatment, in which behaviour in two different regions ($r \ll 1/k$ and $r \sim 1/r$) is matched and $\omega(k)$ obtained by demanding continuity across the regions.

At first glance, equation (3.3) might be read as implying that $\omega \propto k^2$. However, when the expressions in the brackets are calculated for $k = 0$, one finds $\delta\phi_0 = \mathrm{d}\phi_0/\mathrm{d}r$, $\delta\chi_0 = \phi_0/r$. The second term in the numerator diverges logarithmically (the other terms are finite). Our usual procedure, as outlined in [12–14], breaks down. The $k = 0$ limit is singular and must be treated with caution.

To obtain the correct dispersion relation from (3.3), we must allow a k-dependence in $\langle \delta\chi_0^2\rangle$, though in view of (1.8*b*) it must be much weaker than any integer power of k.

For large $r \gg 1/k$, $\delta\chi$ is proportional to $\exp(-kr)/\sqrt{r}$; see (2.2) in this limit. (Actually, there is a higher-order correction to k in the exponent that we discard here. A second, well behaved solution is proportional to $\exp(-\sqrt{2}r)/\sqrt{r}$ and will eventually lose out.)

For $k = 0$, $\delta\chi \sim 1/r$ for large r. Thus, when k is nonzero, no matter how small, we must remodel the large-r behaviour of $\delta\chi$. Simple k-expansion with $\delta\chi_0$ calculated at $k = 0$ will not give the correct result.

Before deriving an estimate for (3.3), we now present a commonsense argument for the logarithmic behaviour. As outlined above, $\delta\chi_0 = \phi_0/r$ can only be used for $r < 1/k$, roughly speaking. Thus the integral $\langle \delta\chi_0^2\rangle$ can only be taken up to $r \sim 1/k$, not $r = \infty$. As $\phi_0 \sim 1$ for this value, the integral will introduce a $\ln(1/k)$ term.

We will now try to estimate the value of (3.3) by using models for both ϕ_0 and $\delta\chi_0$.

For small r, $\delta\chi_0 \sim \phi_0/r$; for large r, say $r \gg 1/k$, the $\exp(-kr)/\sqrt{r}$ dependence can equally well be represented as $\phi_0 \exp(-kr)/\sqrt{r}$, since $\phi_0 \to 1$ as $r \to \infty$. The simplest possible model including both limits is

$$\delta\chi_0 = \frac{\phi_0\sqrt{1 + \alpha kr}}{r}\exp(-kr) \qquad \delta\chi_0(k = 0) = \frac{\phi_0}{r}. \tag{3.4}$$

We do not know the value of $\alpha > 0$. However, asymptotic behaviour only becomes important when $r \gg 1/k$. Thus α should be at most of order one. As we will see, its exact value will not influence our considerations. In view of what was said above, we do not need the improved form of $\delta\phi_0$.

For an analytic calculation, we also need a model of ϕ_0 that is an improvement on Fetter's $\phi_0 = r/\sqrt{4+r^2}$ approximation. Our model is constructed by first finding numerically the value of $a_1 = [\mathrm{d}\phi_0/\mathrm{d}r]_{r=0}$ for which $\phi_0(r)$ described by equation (1.5) tends to unity as $r \to \infty$. The next term is found by expanding ϕ_0 in r. The result is

$$\phi_{01} = \frac{2a_1 r}{\sqrt{4+r^2}} \qquad a_1 = 0.583\,189\,495\,860 \tag{3.5}$$

which is a numerical multiple of Fetter's model.

For large r we find by expanding in powers of $1/r$ that

$$\phi_{02} = \frac{r}{\sqrt{1+r^2}}. \tag{3.6}$$

These two model curves meet at $r_0 = 2.706$. Figure 1 depicts the model obtained by combining ϕ_{01} and ϕ_{02} as compared to ϕ_0 found numerically.

We will now find an approximation to (3.3) using our models. The denominator in equation (3.3) is

$$4\langle\delta\phi_0\,\delta\chi_0\rangle = 4\int_0^\infty \phi_0(\mathrm{d}\phi_0/\mathrm{d}r)\,\mathrm{d}r = 4[\tfrac{1}{2}\phi_0^2]_0^\infty = 2. \tag{3.7}$$

(Fetter's model yields the same result.)

The integral $\langle\delta\phi_0^2\rangle$ is approximately

$$\langle\delta\phi_0^2\rangle = \int_0^{r_0}\left(\frac{\mathrm{d}\phi_{01}}{\mathrm{d}r}\right)^2 r\,\mathrm{d}r + \int_{r_0}^\infty\left(\frac{\mathrm{d}\phi_{02}}{\mathrm{d}r}\right)^2 r\,\mathrm{d}r = 0.301. \tag{3.8}$$

(Fetter's model gives 0.25.)

So as to calculate the crucial term, $\langle\delta\chi_0^2\rangle$, we assume that the contribution over the interval $[0, r_0]$ is not influenced by the k-dependence, thus discarding terms $\sim k^n$, $n > 1$, as of course we may:

$$\langle\delta\chi_0^2\rangle = \int_0^{r_0}\frac{\mathrm{d}r}{r}\,\phi_{01}^2 - \int_0^{r_0}\frac{\mathrm{d}r}{r}\,\phi_{02}^2 + \int_0^\infty\frac{\mathrm{d}r}{r}\,\phi_{02}^2(1+\alpha kr)\exp(-2kr). \tag{3.9}$$

The first two integrals add up to -0.352 (zero for Fetter's model). The third term can be written as

$$I - \frac{1}{2}\alpha k\frac{\partial I}{\partial k} \qquad I = \int_0^\infty \frac{r\,\mathrm{d}r}{1+r^2}\exp(-2kr). \tag{3.10}$$

The value of $I(k)$ can be expressed in terms of ordinary and integral trigonometric functions, $\mathrm{si}(2k)$ and $\mathrm{ci}(2k)$; see [18]. Finally, when all the bits are put together, we obtain

$$\omega = \tfrac{1}{2}k^2[\ln(1/k) + \alpha/2 - 1.31] + \mathrm{O}(k^3). \tag{3.11}$$

(Fetter's model yields a similar result, but with -1.64.) Although there is no reason to expect $\alpha/2 - 1.31$ to cancel to zero, the absolute value of this constant cannot be too large. It decreases as the model is improved (e.g. from Fetter's to ours). The leading term reproduces Grant's result from Rowlands' formula, once the singular limit is understood. (Actually, Grant obtained his result as $\frac{1}{2}k^2[\ln(2/k) - 0.692] = \frac{1}{2}k^2[\ln(1/k) + 0.0011]$; we obtained $\frac{1}{2}k^2[\ln(1/k) - 0.0032]$.)

Our calculation is not significantly model dependent. For example, taking as a model

$$\delta\chi_0 = \frac{1}{r}\sqrt{\phi_0^2 + \alpha kr}\,\exp(-kr) \tag{3.12}$$

also satisfying the conditions at the two limits, one reobtains (3.11), but with α instead of $\alpha/2$.

Thus in any case we have vindicated giving the dispersion relation in the form (3.2).

4. Summary

We have been able to resolve a contradiction in the literature concerning quantum vortex vibrations in uniform BECs, superfluid ^{4}He II and indeed *any* $n = 1$ vortices described by the nonlinear Schrödinger equation with a repulsive potential. Numerical analysis confirms one of the versions found in the literature. Rowlands' formula, at first glance contradicting the more established dispersion relation, is brought in line with its rival as derived by Pitaevski, Fetter and Grant.

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Appendix. Numerical calculation; more details

The solutions of equations (2.2) that are finite at $r = 0$ can be expanded in powers of r [8], and these expansions can be written as

$$\begin{aligned} u_1 &= r^4(1 + a_2 r^2 + a_4 r^4) \qquad & v_1 &= b_0 + b_2 r^2 + b_4 r^4 \\ u_2 &= r^2(1 + d_2 r^2 + d_4 r^4) \qquad & v_2 &= r^6(g_0 + g_2 r^2 + g_4 r^4) \end{aligned} \tag{A.1}$$

where

$$\begin{aligned} a_2 &= \tfrac{1}{32}(4k^2 - 4\omega - 7) \\ a_4 &= \tfrac{1}{60}[a_1^2 b_4 + \tfrac{1}{32}(41 + 96a_1^2 - 35k^2 + 4k^4 + 38\omega + 4k^2\omega - 8\omega^2)] \\ b_0 &= 12c \qquad c = a_1^{-2} \\ b_2 &= 3c(k^2 - 1 - 2\omega) \\ b_4 &= \tfrac{1}{16}[24 + c(3 - 6k^2 + 3k^4 + 12\omega - 12k^2\omega + 12\omega^2)] \\ d_2 &= \tfrac{1}{12}(k^2 - 1 + 2\omega) \\ d_4 &= \tfrac{1}{32}[2a_1^2 + \tfrac{1}{12}(k^2 - 1 + 2\omega)^2] \\ g_0 &= \tfrac{1}{36}a_1^2 \\ g_2 &= \tfrac{1}{64}[g_0(k^2 - 1 - 2\omega) + a_1^2(d_2 - 0.25)] \\ g_4 &= \tfrac{1}{230\,400}a_1^2(127 + 464a_1^2 - 77k^2 + 10k^4 - 98\omega + 20k^2\omega + 16\omega^2) \end{aligned} \tag{A.2}$$

and a_1 is given by (3.5).

The boundary condition at r_{as} is given by equation (2.18), and its $\mathrm{d}/\mathrm{d}r$ derivative, in which

$$\begin{aligned} u_j &= (r\beta_j)^{-1/2} \qquad v_j = s_j u_j \\ u_j' &= u_j\left[-\frac{1}{2}\left(\frac{1}{r} + \frac{\beta_j'}{\beta_j}\right) - \beta_j\right] \\ v_j' &= s_j u_j' + s_j' u_j \qquad j = \mathrm{se}, \mathrm{ge} \end{aligned} \tag{A.3}$$

and all functions are taken at $r = r_{\mathrm{as}}$.

The differential equations (2.2), as well as (1.5) defining the ϕ_0-profile, were first reduced to a set of first-order equations, and then integrated by an efficient Runge–Kutta–Fehlberg algorithm of order 8(7) [19], with automatic step size control. To speed up the evaluation of ϕ_0, which enters equations (2.2), this function was first tabulated on the mesh: $r = \epsilon_0$, 0.1,

$0.2, \ldots, 14.8$. Then for $0 \leqslant r \leqslant \epsilon_0$ (=0.0006), $\phi_0(r)$ was calculated from the truncated power expansion:

$$\phi_0 = a_1 r[1 - \tfrac{1}{8}r^2 + \tfrac{1}{24}(a_1^2 + \tfrac{1}{8})r^4] \qquad a_1 = 0.583\,189\,495\,860. \tag{A.4}$$

For $\epsilon_0 < r \leqslant r_{\text{mch as}}$ (=14.861 664 9452) we integrated equation (1.5) from the nearest mesh point (which in most cases required one step of integration only), and for $r > r_{\text{mch as}}$ the asymptotic expansion for $r \to \infty$ was used:

$$\phi_0 = 1 - \frac{1}{2r^2} - \frac{9}{8r^4} - \frac{161}{16r^6} - \frac{24\,661}{128r^8}. \tag{A.5}$$

Quadruple precision (33 decimal digits) was necessary for $0.03 \leqslant k < 0.08$.

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