A three-stage analysis of standing waves in an atomic Bose-Einstein Condensate

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Abstract

We present three ways to identify the mode functions and frequencies of standing waves in a Bose-Einstein Condensate (BEC). Firstly, we treat an easier system in prolate spheroidal coordinates, which has already been solved, and we use this knowledge to implement our boundary conditions, which can be done in a rather satisfying way. Secondly, we assume a cylindrical-shaped BEC in order to get exact solutions of a more complicated (but still incomplete) system. This results in the same mode functions as used before in literature as a variational Ansatz, and therefore supports this Ansatz. Finally, we will use perturbation theory on the entire system to determine the first-order corrections on the frequencies.

When we compare our results with simulation data, we find that the frequencies (up to first order) are in the right regime, but in order to improve the accuracy, a different strategy will be needed, since the determination of the first-order mode functions (and hence the higher-order frequencies) seems to require degenerate perturbation theory.

Contents

1	Introduction	1
2	Theoretical background	2
3	Prolate spheroidal approach	4
	3.1 Separation of variables	4
	3.2 Solutions using boundary conditions	5
4	Cylindrical approach	7
	4.1 Separation of variables	7
	4.1.1 Equations for R and Φ	7
	4.1.2 Imposing the boundary conditions	7
	4.1.3 Equation for Z	8
	4.2 Solving the system	9
	4.2.1 Normalization	9
5	Perturbation theory	10
	5.1 Zeroth order	10
	5.2 First order \ldots	11
6	Comparison with experiment	12
	6.1 Conjecture for the slope of the frequencies	12
7	Conclusions, discussion and outlook	14

1 Introduction

In 1924-1925, Einstein used the work of Bose to predict a 'condensed substance', where 'as you increase the overall density, an ever increasing number of molecules drop into the ground state' [1]. This substance, now known as a Bose-Einstein condensate (abbreviated BEC), has experimentally been realised since 1995 [2]. The difficulty here is to achieve the very low temperatures needed to produce a BEC (typically in the order of 10^{-7} K). A BEC really is a different state of matter, just like for example a solid and a liquid, but because it has such an extremely low critical temperature, we do not encounter it in our daily lives.

A BEC has some interesting properties. For example, superfluidity can arise here [3]. Furthermore, BEC can be viewed as making quantum mechanics macroscopic, because the occupation of the ground state is macroscopically high. These and many other properties make BEC a phenomenon studied intensively.

In Utrecht, sodium atoms are cooled to a temperature T = 300 nK, where a BEC is formed [4]. The BEC is shaped as a tiny rugby ball or, more scientifically spoken, as a prolate spheroid¹. The theoretical description of such a BEC includes the variational model for a space-time crystal observed in this superfluid, as described in Ref. [5]. Here, a variational Ansatz is used for the density and phase of the mode functions, restricted to axial variations of the mode functions. Overall, this Ansatz led to accurate results. Only some small deviations appeared near the boundary of the condensate. The energy spectrum (frequencies) seems to have a slightly different slope as well. The goal of this thesis is to (further) improve the theoretical description of the physics in a BEC, in partic-

ular concerning these mode functions and frequencies. Not only will we permit variations in the axial direction, but also in the radial direction, because it is known that there is some (small) radial dependence, and this might explain the discrepancies. We will do this in three ways, namely (i) by using prolate spheroidal coordinates and applying our knowledge of a solvable, but drastically simplified system, (ii) by using cylindrical coordinates to treat a more complicated, but still completely solvable system, while changing the boundary of the BEC into a cylinder and (iii) by using nondegenerate perturbation theory on the entire system (with the proper boundaries). This last method will result in zeroth order functions and frequencies, and first-order corrections on these frequencies.

After a description of the theoretical background of a BEC in Sec. 2, we present the three approaches mentioned in Sec. 3 - 5. In Sec. 6, we compare our results with the experimental (simulation) data² and the results of the variational model.



Figure 1: The shape of a BEC in Utrecht: a rugby ball or prolate spheroid. In the experiment, the larger axis is approximately 1 mm.

 $^{^{1}}$ Interestingly, prolate spheroids are also used to describe several objects in astrophysics, such as moons and nebulae.

²Thanks to J. Smits for making the data available to me.

2 Theoretical background

In this section, the main objective is to explain the theoretical settings of the experiment, and deriving Eq. (5) which is the most important expression for the rest of this thesis. Most experimental parameters can be found at p.2 of Ref. [5].

In the experiment, sodium atoms are trapped using a potential

$$V(\rho, z) = \frac{1}{2}m\omega_{\rho}^{2}(\rho^{2} + \lambda^{2}z^{2}), \qquad (1)$$

with *m* the mass of the atoms, ω_{ρ} the trap frequency in the radial direction ρ and $\omega_z = \lambda \omega_{\rho}$ the trap frequency in the axial direction *z*. In the experiment with trap frequencies (ω_{ρ}, ω_z) = $2\pi * (52.7, 1.43)$ Hz the aspect ratio λ is small ($\lambda \approx 0.027$) [5].

Let furthermore μ be the chemical potential, N the number of particles and V_0 the strength of the constant³ interaction potential. Notice that ρ and z are the 'regular' or 'unscaled' cylindrical coordinates, bounded by $[0, R_{\rho}]$ and $[-R_z, R_z]$ respectively, in such a way that $\frac{\rho^2}{R_{\rho}^2} + \frac{z^2}{R_z^2} \leq 1$. Here R_i are the Thomas-Fermi radii: $R_i = \sqrt{\frac{2\mu}{m\omega_i^2}}$, for $i = \rho, z$. This defines a prolate spheroid, because in our case $R_{\rho} < R_z^4$.

Using these definitions, we can transform the well-known Schrödinger equation into

$$i\hbar \frac{\partial \psi_{macro}(\rho, z, t)}{\partial t} = \{ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\rho, z) + V_0 \ n(\rho, z, t) \} \psi_{macro}(\rho, z, t),$$
(2)

where \hbar is the Dirac constant (Planck's constant divided by 2π), $\psi_{macro}(\rho, z, t)$ the 'macroscopical wave function' and $n(\rho, z, t)$ the particle density, both defined such that $n(\rho, z, t) = |\psi_{macro}(\rho, z, t)|^2 = N|\psi(\rho, z, t)|^2$, with $\psi(\rho, z, t)$ the 'normal' wave function, which is a probability amplitude and normalized as $\int d\rho \int dz \, 2\pi\rho \, |\psi(\rho, z, t)|^2 = 1$.

By definition, $\psi_{macro}(\rho, z, t) = \sqrt{n(\rho, z, t)} e^{i\phi(\rho, z, t)}$, where $\phi(\rho, z, t)$ is the phase. Substituting this into Eq. (2) and separating into an imaginary and a real equation in the end leads to:

• the continuity equation

$$\frac{\partial n(\rho, z, t)}{\partial t} + \vec{\nabla} \cdot \mathbf{j}(\rho, z, t) = 0, \qquad (3)$$

where $\mathbf{j}(\rho, z, t) = n(\rho, z, t)\mathbf{v}(\rho, z, t)$ the current density and $\mathbf{v}(\rho, z, t) = \frac{\hbar^2}{m} \vec{\nabla} \phi(\rho, z, t)$ the velocity (equivalent to the definitions at p. 2 of Ref. [5]) and

• the Josephson equation

$$\hbar \frac{\partial \phi(\rho, z, t)}{\partial t} + (\frac{1}{2}m|\mathbf{v}(\rho, z, t)|^2 + V(\rho, z) + V_0 \ n(\rho, z, t) - \frac{\hbar^2}{2m\sqrt{n(\rho, z, t)}} \vec{\nabla}^2 \sqrt{n(\rho, z, t)}) = 0.$$
(4)

³This interaction is proportional to $\delta(\mathbf{x} - \mathbf{x}')$, because the De Broglie wavelength is huge compared to the interaction.

⁴If $R_{\rho} > R_z$, we would have an oblate spheroid.

2 THEORETICAL BACKGROUND

In the Thomas-Fermi limit or Thomas-Fermi approximation⁵, we neglect the last term in Eq. (4). Linearizing Eq. (3) and Eq. (4) around $n_0(\rho, z) = \frac{\mu-V}{V_0}$ and $\phi_0 = 0$ makes it possible to separate the problem into one equation for δn and one equation for $\delta \phi$. When the Ansatz $\delta n(\rho, z, t) = \delta n(\rho, z)e^{-i\omega t}$ and equivalent $\delta \phi(\rho, z, t) = \delta \phi(\rho, z)e^{-i\omega t}$ is made, we can rewrite our equations to be:

•
$$-\omega^2 \delta n(\rho, z) = \frac{V_0}{m} n_0(\rho, z) \vec{\nabla} \cdot \vec{\nabla} \delta n(\rho, z)$$
 and

•
$$-\omega^2 \delta \phi(\rho, z) = \frac{V_0}{m} n_0(\rho, z) \vec{\nabla} \cdot \vec{\nabla} \delta \phi(\rho, z).$$

Since these equations are completely analogous, we will in the remainder of this thesis focus on the first equation, which reads in a slightly different form:

$$-\omega^2 \delta n(\rho, z) = \frac{\mu}{m} (1 - \frac{\rho^2}{R_{\rho}^2} - \frac{z^2}{R_z^2}) \vec{\nabla}^2 \delta n(\rho, z),$$
(5)

using the definition of n_0 . From now on, δn without argument refers to this time-independent $\delta n(\rho, z)$.

When the variational method mentioned above (which neglects the radial dependence) is used to determine the functions δn and the frequencies ω , the result becomes (Ref. [5], p.3 and Ref. [4], p.7)

$$\delta n_j = K_j \cdot \left(P_{4j+2}(\frac{z}{R_z}) - P_{4j}(\frac{z}{R_z}) \right)$$
(6)

and

$$\omega_j = \omega_z \frac{\sqrt{(4j+1)(4j+2)}}{2},$$
(7)

where j = 0, 1, 2, ... is the quantum number, K_j is the normalization constant and $P_k(x)$ is the k-th Legendre polynomial⁶. These expressions and the simulation data will be used to compare our results with.

We will now analyze Eq. (5) in three different ways, resulting in approximations of the frequencies ω and the density fluctuations δn .

⁵A clear discussion of the Thomas-Fermi approximation can e.g. be found at p. 43-44 of Ref. [6]. As stated in Ref. [7] (p. 6), this approximation is valid when $\hbar\omega_{x,y,z} \ll nV_0$. This is the case, except for $V(\rho, z) \rightarrow \mu$, which corresponds to approaching the boundaries of the condensate.

⁶Legendre polynomials are defined as the solutions of $\frac{d}{dx}[(1-x^2)\frac{du(x)}{dx}]+mu(x)=0$, for which m=n(n+1), n=0,1,2,... [8]

3 Prolate spheroidal approach

A good way to start studying Eq. (5) is by using the so-called prolate spheroidal coordinates in order to get the desired frequencies and wave functions. These coordinates are useful for our condensate, because they will give an easy way to implement the boundary conditions (which is, in our case, specified on a prolate spheroid).

It is known that the Helmholtz equation, which would in our case be

$$\vec{\nabla}^2 \delta n = -\frac{m}{\mu} \omega^2 \delta n,\tag{8}$$

can be solved with these coordinates by separation of variables, which has already been done (see e.g. Ref. [9], p. 40 and Ref. [10], chapter 30.13). In this section, we will use the results of these calculations for our situation. Since we are neglecting any position dependence of n_0 (which is only a good approximation when $\frac{\rho^2}{R_{\rho}^2} + \frac{z^2}{R_z^2} \ll 1$, i.e. close to the origin), this is just a rough estimate at first, which we will improve later.

The goal is to introduce these coordinates, and to show how the boundary conditions can be introduced in a very elegant way, but we will not find any useful approximations for our more complicated system. Therefore, the detailed information such as the mode functions will not be presented here, although they are completely known. Since this approach might be very useful for further research, we wanted to implement it in this discussion.

3.1 Separation of variables

Let's introduce (ξ, η, ϕ) , such that

•
$$x = c\sqrt{(\xi^2 - 1)(1 - \eta^2)}\cos(\phi)$$

•
$$y = c\sqrt{(\xi^2 - 1)(1 - \eta^2)\sin(\phi)}$$

•
$$z = c\xi\eta$$
,

where c is half the interfocal distance: $c = \sqrt{R_z^2 - R_\rho^2} = R_z \sqrt{1 - \lambda^2}$. Furthermore, $\xi \in [1, \infty)$, $\eta \in [-1, 1]$ and $\phi \in [0, 2\pi]$.

When this coordinate system is used, one can find solutions of Eq. (8) using separation of variables (Ref. [9] and Ref. [10]) In our setup, we can use the rotational symmetry around the z-axis⁷. This simplifies the separated equations, because one quantum number becomes zero (this quantum number is denoted as m in Ref. [9] and μ in Ref. [10]). The mode functions can be expressed in terms of the so-called prolate spheroidal wave functions.

⁷The mode functions are independent of ϕ in our case. Note that η is also related to an angle. Indeed, another convention uses ν and μ with $\eta = \cos(\nu)$ and $\xi = \cosh(\mu)$. This convention shows that for $\xi \to \infty$, the prolate spheroidal coordinates will 'converge' to the regular spherical coordinates, where ξ is directly related to the radial coordinate r. This fact can also be deduced from Fig. 2.



(a) Prolate spheroid for $\xi = 1$.

(b) Prolate spheroid for $\xi = \xi_0$. (c) P

(c) Prolate spheroid for $\xi = 1.01$.



(d) Prolate spheroid for $\xi =$ (e) Prolate spheroid for $\xi = 1.2$. (f) Prolate spheroid for $\xi = 2$. 1.05.

Figure 2: Plots of prolate spheroids for different values of ξ , with c = 1 (so unscaled). Fig. 2b illustrates the situation where the ratio between the axes agrees with our experimental setup, using Eq. (10).

3.2 Solutions using boundary conditions

The advantage of prolate spheroidal coordinates is the fact that the boundary conditions can be implemented much easier, because we want our mode functions δn to be zero⁸ at a prolate spheroid.

For a fixed ξ_0 , we find

$$\forall \eta: \quad \frac{x^2 + y^2}{c^2(\xi_0^2 - 1)} + \frac{z^2}{c^2 \xi_0^2} = (1 - \eta^2) + \eta^2 = 1, \tag{9}$$

which is the defining equation of a prolate spheroid. This fact is shown in Fig. 2, where we also find that for larger ξ , the prolate spheroid becomes more 'spherical'. Notice furthermore

⁸The mode functions have to go to zero, because this is what happens near the edge, and what has been observed. It's not physical to have a discontinuity in the density at the boundaries. Notice that for the same reason, the variational model (Eq. (6)) has the difference between *two* Legendre polynomials, instead of just a single one.

that the longer axis of the prolate spheroid depends linearly on ξ (since $z = c\xi\eta$).

So, fixed values of ξ give a surface with the shape of a prolate spheroid. We thus want to specify our boundary condition for the specific ξ_0 that satisfies $R_{\rho}^2 = c^2(\xi_0^2 - 1)$ and $R_z^2 = c^2\xi_0^2$. We find

$$\xi_0 = \frac{1}{\sqrt{1 - \lambda^2}} \approx 1.00036.$$
 (10)

The prolate spheroid for this ξ_0 is shown in Fig. 2b. We can even show the line determined by $\xi = \xi_0$ in the ρz -plane⁹, resulting in Fig. 3. We conclude that the mode functions have to be zero on this ellipse in the ρz -plane (with focal points on the z-axis).



Figure 3: Plot of the line $\xi = \xi_0$ in the ρz -plane, now using the correct value $c = R_z \sqrt{1 - \lambda^2}$. Notice that the z-axis is the longer axis here.

As described by equation 30.13.15 in Ref. [10], the eigenvalues can be found by solving the equation

$$S_n^0(\xi_0, \gamma) = 0, \tag{11}$$

where this function $S_n^{k(1)}$ is the radial spheroidal function (of the first kind), while k = 0 due to the angular symmetry. The parameter γ is defined via $\gamma^2 = \frac{m}{\mu}c^2\omega^2$ and ξ_0 is given by Eq. (10). These eigenvalues can numerically be found for an arbitrary n, but they are of no use for this study.

⁹Our system is rotationally symmetric around the z-axis. Rotating Fig. 3 around the z-axis results in the scaled version of Fig. 2b.

4 Cylindrical approach

As a second approximation, we can look for solutions of Eq. (5) with the simplification that the condensate is no prolate spheroid, but a cylinder with radius R_{ρ} and length $2R_z$. This is a valid approximation when $R_{\rho} \ll R_z$, because in this situation, the term $\frac{\rho^2}{R_{\rho}^2}$ in the defining equation of a prolate spheroid can safely be neglected close to the z-axis. In our case, where $R_{\rho} = \lambda R_z$ (and $\lambda \approx 0.027$), this seems a reasonable approximation. Close to the z-axis, we can therefore reduce Eq. (5) in this cylindrical approach to

$$\frac{\mu}{m}\left(1 - \frac{z^2}{R_z^2}\right)\vec{\nabla}^2\delta n = -\omega^2\delta n.$$
(12)

We can solve this Eq. (12) using separation of variables. This approach is 'better' than our first method in the sense that the term $\frac{z^2}{R_z^2}$ will be treated as well. As we will see, the mode functions δn achieved via this method agree very well with the variational Ansatz, Eq. (6).

4.1 Separation of variables

As before, we try separation of variables¹⁰: $\delta n = R(\bar{\rho})Z(\bar{z})\Phi(\phi)$, where we make use of the substitutions $\bar{z} \equiv \frac{z}{R_z}$ and $\bar{\rho} \equiv \frac{\rho}{R_{\rho}}$, which are now dimensionless variables. Using the identities $\omega_z = \lambda \omega_\rho$ and $\frac{\mu}{mR_\rho^2} = \frac{1}{2}\omega_\rho^2$, we find¹¹:

$$\frac{-\omega^2}{1-\bar{z}^2} = \frac{1}{2}\omega_\rho^2 \cdot \{\lambda^2 \frac{1}{Z} \frac{d^2 Z}{d\bar{z}^2} + \frac{1}{\bar{\rho}} \frac{1}{R} \frac{d}{d\bar{\rho}} \left[\bar{\rho} \frac{dR}{d\bar{\rho}}\right] + \frac{1}{\bar{\rho}^2} \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2}\}.$$
 (13)

Introducing the separation constants k and m, we are able to find three separate equations: one for Z, one for R and one for Φ .

4.1.1 Equations for R and Φ

The equations for R and Φ can be solved in general, although this will not be of great importance for our study.

For Φ , we find $\frac{d^2}{d\phi^2}\Phi = -m^2\Phi$, which simply implies that $\Phi(\phi) = \Phi_0 e^{\pm im\phi}$.

The equation for R becomes $\bar{\rho}^2 \frac{d^2}{d\bar{\rho}^2} R + \bar{\rho} \frac{d}{d\bar{\rho}} R + (k^2 \bar{\rho}^2 - m^2) R = 0$. This is nothing than Bessel's differential equation for $k\bar{\rho}$, so the solution becomes $R(\bar{\rho}) = J_m(k\bar{\rho})$, where J_m is the m-th Bessel function.

4.1.2 Imposing the boundary conditions

A logical and physical¹² boundary condition is the requirement that the flux in the $\bar{\rho}$ -direction is zero at the boundary, which is to say $\frac{\partial J_m(k\bar{\rho})}{\partial\bar{\rho}}|_{\bar{\rho}=1} = 0$. This will result in discretized values

¹⁰As Griffiths states it: "separation of variables is the physicist's first line of attack on any partial differential equation." (see Ref. [11], p. 24)

¹¹Notice we can use total derivatives here.

¹²At first instance, a condition like $J_m(k\bar{\rho}) = 0$ for $\bar{\rho} = 1$ may be another guess, similar to the prolate spheroidal case, but this conditions implies that $\delta n = 0$ (i.e. no fluctuations at all) in this case, since the $\bar{\rho}$ -dependence is (almost) constant.

of k, since k is now restricted to be a zero of the first derivative of the m-th Bessel function. A lot of work has been done to find the numerical values of these zeros, see for example Ref. [12].

In our case, we are most interested in the case k = 0 and m = 0, because for those values, the ϕ -dependence is zero or equivalently $\Phi(\phi) = \Phi_0 e^0 = \Phi_0$ (which has to be the case for our angular symmetric system) and the $\bar{\rho}$ -dependence is small, so $R(\bar{\rho})$ is best approximated by a constant R_0 .

4.1.3 Equation for Z

Since the mode functions are known to be strongly \bar{z} -dependent, the equation for Z is the most interesting part. Note that this is the only equation involving ω .

The equation for Z becomes

$$(1 - \bar{z}^2)\frac{d^2}{d\bar{z}^2}Z + 2(\frac{\omega}{\omega_z})^2 Z = 2(\frac{k}{\omega_z})^2(1 - \bar{z}^2)Z.$$
(14)

Although this equation does not seem solvable for an arbitrary k, we are actually most interested in the case k = 0, since we know that the mode functions δn has the be almost $\bar{\rho}$ and ϕ -independent ([4] and [5]). Fortunately, we can solve Eq. (14) for k = 0. Notice that

$$Z(\bar{z}) = C_j \ (1 - \bar{z}^2) \frac{d}{d\bar{z}} P_j(\bar{z})$$

$$\tag{15}$$

is an eigenfunction of the operator $(1 - \bar{z}^2)\frac{\partial^2}{\partial \bar{z}^2}$, by definition of the Legendre functions. Simultaneously, we find

$$\omega = \omega_z \sqrt{\frac{j(j+1)}{2}}.$$
(16)

Similarity with variational model Eq. (15) can be rewritten in a recognizable way. We can prove the following relation:

$$(1 - \bar{z}^2)\frac{d}{d\bar{z}}P_j(\bar{z}) = \frac{j(j+1)}{2j+1}(P_{j-1}(\bar{z}) - P_{j+1}(\bar{z}),$$
(17)

which is of the exact same form as the variational Ansatz (Eq. (6))! We will now derive this equation.

We need the following properties of Legendre polynomials (Eq. 18 of Ref. [13]):

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0$$
(18)

and

$$(x^{2} - 1)\frac{d}{dx}P_{n}(x) = n[xP_{n}(x) - P_{n-1}(x)].$$
(19)

We can rewrite Eq. (18) as

$$xP_n(x) = \frac{n+1}{2n+1}P_{n+1}(x) + \frac{n}{2n+1}P_{n-1}(x).$$
(18*)

This allows us to write $(1-x^2)\frac{d}{dx}P_n(x) = n[P_{n-1}(x) - xP_n(x)] = n[P_{n-1}(x) - (\frac{n+1}{2n+1}P_{n+1}(x) + \frac{n}{2n+1}P_{n-1}(x))] = \frac{n(n+1)}{2n+1}(P_{n-1}(x) - P_{n+1}(x))$, where the first equality follows from Eq. (19)) and the second from Eq. (18*). Using \bar{z} as x and j as n, we have now proven Eq. (17).

4.2 Solving the system

As stated and explained above (Sec. 4.1.2), we are most interested in the case k = 0 and m = 0. We therefore find

$$\delta n_j(\bar{\rho}, \bar{z}, \phi) = K_j \ (1 - \bar{z}^2) \frac{d}{d\bar{z}} P_j(\bar{z}), \tag{20}$$

where K_j has to be determined by normalization¹³, which is the last step remaining in this cylindrical approach.

4.2.1 Normalization

When it comes to normalization of the mode functions (20), the question arises: which inner product are we going to use? Since the operator $(1 - \bar{z}^2)\frac{\partial^2}{\partial \bar{z}^2}$ is not symmetric, we have to symmetrize it in order to find the 'natural' inner product. This can be done by substituting $\delta n_j = \sqrt{1 - \bar{z}^2} f_j$. In this convention, the problem becomes $\hat{O}f_j = E_j f_j$, where \hat{O} $= \sqrt{1 - \bar{z}^2} \frac{\partial^2}{\partial \bar{z}^2} \sqrt{1 - \bar{z}^2}$ is a symmetric (and therefore Hermitian) operator. The inner product becomes

$$\langle f_j | f_{j'} \rangle = \int_0^{2\pi} \int_0^1 \int_{-1}^1 d\bar{z} \, d\bar{\rho} \, d\phi \, \bar{\rho} R_z R_\rho^2 \, f_j f_{j'}, \tag{21}$$

where $\delta_{j,j'}$ is the Kronecker delta¹⁴. Translating to δn gives the normalization as

$$\delta_{j,j'} = \int_0^{2\pi} \int_0^1 \int_{-1}^1 d\bar{z} \, d\bar{\rho} \, d\phi \, \frac{\bar{\rho}}{1 - \bar{z}^2} R_z R_\rho^2 \, \delta n_j \delta n_{j'}. \tag{22}$$

Plugging in the result of Eq. (20), we obtain

$$K_j = \sqrt{\frac{1}{\pi R_z R_\rho^2} \frac{2j - 1}{2j(j+1)}}.$$
(23)

To achieve this, we used Eq. (17), as well as an expression for the derivative of Legendre polynomials (Eq. 20 in Ref. [13]) and the orthogonality relation of these functions (Eq. C.8 in Ref. [8]).

Eq. (20) and Eq. (23) determine the solutions within this cylindrical approach. Some comments on the link between these functions and the variational Ansatz can be found in Sec. 6.

¹³This K_j contains C_j and the constants R_0 and Φ_0 .

¹⁴Note that the functions are real: taking the complex conjugate changes nothing.

5 Perturbation theory

At this point, we have only dealt with simplifications of Eq. (5). Does this imply that we cannot say anything about the entire system? The answer is 'no', and in this section, we will discover what can be achieved with perturbation theory.

The mode functions obtained using the cylindrical approach are already of the same form as the result of the variational Ansatz, which described the system very well, but was still $\bar{\rho}$ -independent. We conclude that the $\frac{\partial^2}{\partial \bar{z}^2}$ -term in $\vec{\nabla}^2$ is the dominant term. Therefore, we are most interested in the impact of $\bar{\rho}^2 \frac{\partial^2}{\partial \bar{z}^2}$ on the mode functions and frequencies¹⁵.

Notice the analogy between our wave functions and the 'normal' ones (as described in Sec. 2). We use this to perform the analogy of perturbation theory on our system. Let us therefore define $H = H^0 + \epsilon H^1$, where $H^0 = (1 - \bar{z}^2) \frac{\partial^2}{\partial \bar{z}^2}$ and $H^1 = -\bar{\rho}^2 \frac{\partial^2}{\partial \bar{z}^2}$. We use ϵ as perturbation constant. The time-independent Schrödinger equation (in this analogy) reads $H\delta n_j = E_j \,\delta n_j$, where in our case $E_j = -2(\frac{\omega_j}{\omega_z})^2$. As always, we write:

• $\delta n = \delta n^0 + \epsilon \, \delta n^1 + \epsilon^2 \, \delta n^2 + \dots$

•
$$E_j = E_j^0 + \epsilon E_j^1 + \epsilon^2 E_j^2 + \dots$$

which leads to specified equations in every order of ϵ .

5.1 Zeroth order

In zeroth order, we look for the $\bar{\rho}$ -independent solutions of

$$H^0 \,\delta n^0 = -2(\frac{\omega^0}{\omega_z})^2 \delta n^0,\tag{24}$$

since the $\bar{\rho}$ -dependence is known to be small and thus taken as the perturbation. We have already seen this equation, it is Eq. (14) for k = 0. We thus have the solutions, namely Eq. (15) and Eq. (16). The difference here lies in the inner product used for the prolate spheroid, but at the end, the $\bar{\rho}$ -independent solutions cannot be different! Therefore, we have to 'change' our inner product, which was defined via Eq. (21), into

$$\langle \delta n_j | \delta n_{j'} \rangle = \int_0^{2\pi} \int_{-1}^1 \int_0^{\sqrt{1-\bar{z}^2}} d\bar{\rho} \, d\bar{z} \, d\phi \, \frac{\bar{\rho}}{(1-\bar{z}^2)^2} R_z R_\rho^2 \, \delta n_j \delta n_{j'}, \tag{25}$$

since this gives the exact same (natural) inner product for $\bar{\rho}$ -independent mode functions δn_j as one would have in the cylindrical case¹⁶. The C_j 's thus have to satisfy

$$\delta_{j,j'} = R_z R_\rho^2 C_j C_{j'} \int_0^{2\pi} \int_{-1}^1 \int_0^{\sqrt{1-\bar{z}^2}} d\bar{\rho} \, d\bar{z} \, d\phi \, \bar{\rho} \, \frac{d}{d\bar{z}} P_j \, \frac{d}{d\bar{z}} P_{j'}.$$
(26)

It happens to be the same problem of finding the total normalization constant in the cylindrical case, so we find (compare with Eq. (23))

$$C_j = \sqrt{\frac{1}{\pi R_z R_\rho^2} \frac{2j - 1}{2j(j+1)}}.$$
(27)

¹⁵Note that we didn't do anything with this term until now.

¹⁶To check this: just perform the $\bar{\rho}$ integral here together with the one used in Eq. (22).

As a reminder, we give the expression for ω^0 :

$$\omega^0 = \omega_z \sqrt{\frac{j(j+1)}{2}}.$$
(28)

5.2 First order

In first order, we can use the well-known result for the first-order correction terms on the frequencies (Ref. [11], p. 251, Eq. 6.9):

$$E_j^1 = \langle \delta n_j^0 | H^1 | \delta n_j^0 \rangle, \tag{29}$$

or in words: the first-order corrections can be found by calculating the expectation value of the perturbation in the zeroth (or unperturbed) state. In our case, we find

$$E_j^1 = -(C_j)^2 R_z R_\rho^2 \int_0^{2\pi} \int_{-1}^1 \int_0^{\sqrt{1-\bar{z}^2}} d\bar{\rho} \, d\bar{z} \, d\phi \, \frac{\bar{\rho}^3}{1-\bar{z}^2} \frac{d}{d\bar{z}} P_j \frac{d^2}{d\bar{z}^2} \{(1-\bar{z}^2)\frac{d}{d\bar{z}} P_j\}, \tag{30}$$

using the inner product of Eq. (25). The elegant result is

$$E_j^1 = \frac{j(j+1)}{2}.$$
 (31)

This can be used to determine ω^1 , because $E_j^1 = -4 \frac{\omega^0 \omega^1}{\omega_z^2}$. This leads to our first-order result:

$$\omega^1 = -\frac{1}{4} \,\omega^0. \tag{32}$$

It would now be nice (and logical) to go further and calculate the first-order mode functions, the second-order frequencies, etc. However, things start to go wrong from this point. Notice that we cannot express the first-order mode functions as a linear combination of zeroth-order mode functions, since the last are $\bar{\rho}$ -independent, while the first are not! In other words: we haven't used a complete basis in zeroth order. It was a valid approach, since we know (experimentally) that the $\bar{\rho}$ -dependence is very small, and therefore we can view it as a 'perturbation'. But in order to proceed in this way (and improve the accuracy of the frequencies), we need a different strategy.

Of course we can solve this problem by allowing $\bar{\rho}$ -dependent solutions in zeroth order, but this results in an infinite degeneracy, as can easily be seen from Eq. (24). We will come back to this point later, in Sec. 7. First, let's answer the following question: How good are our results until now, compared to the experimental data?

6 Comparison with experiment

In this section, we want to formulate an answer to the question stated above. Summarizing the result of our approach using perturbation theory, we state that

$$\omega_j = \frac{3\,\omega_z}{4}\sqrt{\frac{j(j+1)}{2}},\tag{33}$$

where this is the frequency up to first order (so $\omega = \omega^0 + \omega^1$), using Eq. (28) and Eq. (32). For the mode functions, we had

$$\delta n_j = \sqrt{\frac{1}{\pi R_z R_\rho^2} \frac{2j-1}{2j(j+1)}} \ (1-\bar{z}^2) \frac{d}{d\bar{z}} P_j(\bar{z}),\tag{34}$$

using Eq. (27) and Eq. (15). In the experiment, only the mode functions with an index of the form 4j+1 will be excited, for symmetry reasons.

Concerning the mode functions, we can say that these are in good agreement with the experimental results. As stated before, our mode functions are of the same form as the ones taken as variational Ansatz in literature. For a comparison between these and the experiment, we refer to Ref. [5].

Recall that in this variational Ansatz, the frequency is determined to be

$$\omega_j^{var} = \omega_z \frac{\sqrt{(4j+1)(4j+2)}}{2}.$$
(35)

When these frequencies are compared, we find a slight difference in the slopes when the quantum number j becomes large (i.e. the j(j+1) can be approximated by j^2). Notice that, for $j \to 4j + 1$, ω_j has a slope of $\frac{3\omega_z}{\sqrt{2}} \approx 2.12 \cdot \omega_z$, whereas ω_j^{var} has a slope of $2 \cdot \omega_z$. In Fig. 4, our result is shown, including the data of the experiment, and the theoretical

In Fig. 4, our result is shown, including the data of the experiment, and the theoretical prediction of the variational model. Here, the difference in these slopes can just be observed, and we can see that our result is, unfortunately, further away from the data than the frequency obtained via the variational model. Our result seems to be not accurate enough. This can be interpreted as follows: when we look at the zeroth-order frequency, which is given by Eq. (28), then this is hardly visible in Fig. 4, since the lowest point (at j = 16) will be at $\omega_j/\omega_\rho \approx 1.23$ (i.e. this (magenta) line cuts off a tiny piece of the top left corner of Fig. 4). This indicates that our first-order correction term did the good thing: it changed our total frequency in a beneficial way (fortunately!), but in this case, we need more than only the first order. We therefore conclude that our perturbation approach cannot be used to get the desired accuracy.

6.1 Conjecture for the slope of the frequencies

Although we are unable to work out the perturbation approach for higher orders, there is something more to say here¹⁷. Notice that the first-order correction term of the frequencies

 $^{^{17}}$ We do not prove any of the statements in this subsection: it is meant to be an invitation and motivation for further research.



Figure 4: Plot of the frequencies ω_j , scaled at $\omega_{\rho} = \omega_z/\lambda$ is shown as a function of j. The orange dashed line shows our result up to first order (Eq. (33)), whereas the magenta dashed line gives an impression of the zeroth-order result. The black line refers to the frequency obtained via the variational Ansatz (Eq. (35)). As has been explained in Ref. [5] (Fig. 4), the red dots are the frequencies for the simulation data by phase-imprinting and the blue dots are the frequencies obtained by the integration of the mode function found from the simulation data. More details about this data can be found in both Ref. [4] and Ref. [5].

only caused the total slope to change, but it didn't affect the starting point at j = 0 (which is still zero). This is stated in the fact that ω^1 is just a constant (namely $-\frac{1}{4}$) multiplied by ω^0 (Eq. (32)). Having this in mind, it seems reasonable to expect the same behavior for ω^2 . Let us state the following conjecture:

$$\omega^2 = -\frac{1}{16} \,\omega^0. \tag{36}$$

This seems reasonable, because it has the same structure as ω^1 , but the constant $-\frac{1}{16}$ is quadratically smaller than $-\frac{1}{4}$ (i.e. the slope of ω will be further fine tuned). Although this is just a conjecture at this point, we can look at the consequences of this second-order correction, illustrated in Fig. 5. Notice that the total frequency up to second order becomes

$$\omega^{conj} = \frac{11}{16}\omega_0. \tag{37}$$

As we can see, this conjecture makes the total frequency to be absolutely spot on (especially for the blue dots)! This observation makes the conjecture of Eq. (36) a very interesting one, although we did not prove it at this point and it might still be incorrect.



Figure 5: Plot of the frequencies ω_j^{conj} (up to second order), scaled at $\omega_{\rho} = \omega_z/\lambda$ is shown as a function of j as a green dashed line, together with the zeroth-order (magenta) and the first-order result (orange). As before (Fig. 4), the blue and red dots correspond to the (simulation) data, determined in two different ways and the black line shows the result of the variational model.

7 Conclusions, discussion and outlook

In conclusion, we have worked out three different ways to explore the physics in an atomic Bose-Einstein condensate, with the main focus on the mode functions and the frequencies.

The prolate spheroidal approach was very rough, but nevertheless, it was a good starting point to investigate our system, especially when it comes to the boundary conditions. Further research can focus on (different methods¹⁸ of) solving Eq. (5) with extra term(s) in n_0 (e.g. position-dependence), which might give useful approximations for the mode functions and frequencies, because those were not found in our situation.

In the cylindrical approach, we solved the entire system, within our experimental limits, i.e. angular symmetry. This approach is valid close to the z-axis, and when $R\rho \ll R_z$, which is satisfied due to the small parameter λ . Moreover, we found a good explanation for the variational Ansatz used before in literature¹⁹, via Eq. (17).

Finally, when we made use of perturbation theory on the full system, we arrived at expressions for the mode functions in zeroth order and the frequencies up to first order, which were given by Eqs. (15), (27) and (33). When we compare this expression for the frequencies with the experimental values, we conclude that the slope matches quite well, but there is still some deviation. In order to make the theoretical description more accurate, a different approach seems to be required, e.g. degenerate perturbation theory. Hopefully, this will lead to a second-order correction of the frequency, which might very well be the one we stated as a conjecture.

 $^{^{18}}$ It looks like separation of variables cannot be used when these extra term(s) are added, although more research is needed here.

¹⁹Remember this Ansatz: $\delta n_j \propto P_{4j+1} - P_{4j-1}$.

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