

# EXACT DIAGONALIZATION OF THE HAMILTONIAN OF ROTATING TRAPPED BOSONS FOR N=3

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## Abstract

The aim of this delivery is to study a rotating system of a small number of interacting bosons confined to harmonic potentials in two dimensions, we will consider a trap frequency  $\omega$  and a rotating frequency  $\Omega$ . By exact numerical diagonalization of the many-body Hamiltonian we determine the ground state energy, the density profile and the pair correlation. Our numerics will consist on a system with a number of bosons  $N = 3$  and the angular momentum,  $L \leq 6$  such as the Laughlin state is included. We will characterize the Laughlin state properties from the results we will obtain. We will consider a ratio of  $\Omega/\omega$  from 0.7 up to 1.

## 1 Exact diagonalization of the Hamiltonian

In aim to simulate the physics of gauge fields using ultracold atoms, we will consider rotating condensates. We will study a system consisting in a trapped interacting Bose where its Hamiltonian in second quantization reads,

$$\mathcal{H} = \sum_{k,l} H_{sp}^{k,l} \hat{a}_k^\dagger \hat{a}_l + \frac{g_{2D}}{2} \sum_{k,l,p,q} I_{k,l,p,q} \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_p \hat{a}_q, \quad (1)$$

where  $\hat{a}_k$  annihilates a particle in the state  $k$  and  $\hat{a}_k^\dagger$  creates a particle in the same state. The Hamiltonian can be studied separating two different terms, the single particle energy and the interaction energy. The single particle Hamiltonian,  $H_{sp}$  is defined as,

$$H_{sp}^{k,l} = \int dz_1 dz_2 \psi_k^*(z_1) H_{sp} \psi_l(z_2), \quad (2)$$

and will act over the eigenfunctions as,

$$H_{sp} \psi_k = (1 + k(1 - \frac{\Omega}{\omega})) \psi_k \quad (3)$$

where the eigenfunctions have the form  $\psi_k(z) = \frac{1}{\sqrt{\pi k!}} z^k e^{\frac{|z|^2}{2}}$  and  $\epsilon_k = (1 + k(1 - \frac{\Omega}{\omega}))$  is the single particle energy of level  $k$ .

The interaction term will be determined by  $I_{k,l,p,q}$  that is an overlap integral over four oscillator eigenfunctions and reads,

$$I_{k,l,p,q} = \int dz \psi_k^*(z) \psi_l^*(z) \psi_p(z) \psi_q(z), \quad (4)$$

and the corresponding integrals can be calculated analitically and, in our case, the expression reads,

$$I_{k,l,p,q} = \frac{1}{2\pi} \frac{1}{a_\perp^2} \frac{1}{\sqrt{k!l!p!q!}} \frac{1}{2^{k+l}} (k+l)! \delta_{k+l-p-q} \quad (5)$$

where we will consider  $a_{\perp} = 1$  and it corresponds to  $a_{\perp} = \sqrt{\frac{\hbar}{m\omega}}$ .

To study the many particles basis we will work in the Fock configuration where the occupation-number representation may be written in the following form,

$$|\psi\rangle = |n_0 \ n_1 \ n_2 \dots n_K\rangle \quad (6)$$

where  $n_k$  is the particle number in the single particle state  $k$  and the total particle number must be conserved,

$$\sum_k n_k = N. \quad (7)$$

This state can be construct as,

$$|n_0 \ n_1 \ n_2 \dots n_K\rangle = \frac{1}{\sqrt{n_0!n_1!\dots n_K!}} (a_0^\dagger)^{n_0} (a_1^\dagger)^{n_1} \dots (a_K^\dagger)^{n_K} |vac\rangle. \quad (8)$$

And, the anihilation and creation operators over a Fock state acts as,

$$\begin{aligned} a_k^\dagger |n_0 \ n_1 \ n_2 \dots n_K\rangle &= \sqrt{n_k + 1} |n_0 \ n_1 \ n_2 \dots n_{k+1} \dots n_K\rangle \\ a_k |n_0 \ n_1 \ n_2 \dots n_K\rangle &= \sqrt{n_k} |n_0 \ n_1 \ n_2 \dots n_{k-1} \dots n_K\rangle \end{aligned} \quad (9)$$

and have the commutation relation  $[a_k, a_l^\dagger] = \delta_{kl}$ . The number operator is thus  $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$  with eigenvalue  $n_k$ .

To construct the basis in this representation we will have a set of Fock states that will form the Fock basis. For that, we will have a fixed number of particles  $N$ , Eq. (7), and a maximum angular momentum  $L$  given by,

$$L_{max} = N(N - 1), \quad (10)$$

in the notation we where using in the Fock states, the maximum angular momentum  $L_{max}$  was denoted by  $K$ . We will consider a system of  $N=3$ , therefore  $L_{max} = 6$  following Eq.(10). The total angular momentum of a Fock state is computed as,

$$L = \sum_i n_i \cdot i. \quad (11)$$

In our computer program we will start by constructing the Fock basis where we will compute all the possible combinations of Fock states formed by 3 particles with angular momentum  $L \leq 6$ . This two constrains read,

$$\sum_{i=0}^6 n_i = 3 \quad \sum_{i=0}^6 n_i \cdot i \leq 6. \quad (12)$$

The full Hamiltonian can be computed by having into account that the free part of the Hamiltonian contributes to the diagonal terms with an amount  $\sum_k \epsilon_k n_k$  where the single particle energy is the one described in Eq.(3). Meanwhile, the interaction part yields the contribution,

$$\langle \mathcal{H}_{int} \rangle = \frac{g_{2D}}{2} \sum_{k,l,p,q} I_{k,l,p,q} \langle \alpha' | a_k^\dagger a_l^\dagger a_p a_q | \alpha \rangle \quad (13)$$

where  $|\alpha\rangle$  are the Fock states.

To compute numerically the diagonalization of the Hamiltonian matrix we will split the complete Fock space into subspaces to reduce considerably the dimension of the matrix. These subspaces will be labeled by the total angular momentum of the many particle state. Which means that we will have a block for each angular momentum and we will treat them individually for each of the seven blocks we will obtain.

In our computer program we will obtain the diagonal matrix corresponding to the single particle Hamiltonian and then we will compute Eq. (13) that will give us another Hamiltonian matrix, this time not diagonal. We will add the two contributions to the Hamiltonian to obtain the full Hamiltonian matrix, which is also non diagonal due to the interaction contribution.

The full Hamiltonian matrix will be diagonalized using a routine to diagonalize hermitian matrices and we will obtain the eigenenergies and the corresponding eigenstates of the system in the Fock basis.

## 2 Ground state of the system

The diagonalization of the full Hamiltonian will give us the eigenenergies of the system, by selecting the lowest energy of the eigenenergies we will obtain the ground state of the system. Thus we will have the energy of the ground state for each angular momentum and the corresponding eigenvector that will give us the Fock coefficients to be able to construct the ground state in terms of the Fock basis.

If the full diagonalized Hamiltonian reads,

$$\mathcal{H} = \begin{bmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \ddots & 0 \\ 0 & \ddots & 0 & E_K \end{bmatrix} \quad (14)$$

the ground state will be the state that fulfills  $E_{gs} = \min_i(E_i)$ . Once obtained the ground state for each block of angular momentum  $L$ , the corresponding eigenvectors will give us the Fock coefficients. Thus the ground state with energy  $E_{gs}$  can be write in terms of the Fock basis as,

$$|GS\rangle = \sum_{\alpha} C_{\alpha} |\alpha\rangle, \quad (15)$$

where  $C_{\alpha}$  are the Fock coefficients and  $|\alpha\rangle$  are the state of the Fock basis.

### 2.1 Yrast line

Having the ground state of each angular momentum we are able to obtain the *Yrast line* that is the line which connects the levels of the lowest energy to each angular momentum. This is interesting to consider in nuclear many-body problems. In our study it is interesting to study how the ratio  $\Omega/\omega$  produces a variation in the Yrast line. In Fig. 1 can be seen results for a ratio of  $\Omega/\omega$  going from 0.7 up to 1.

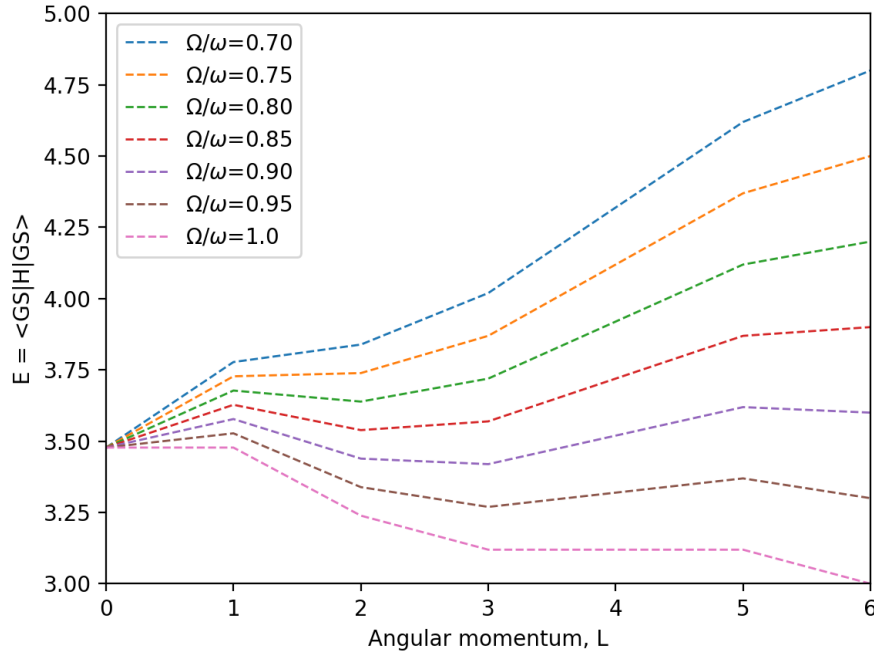


Figure 1: Yrast line for different ratios of  $\Omega/\omega$ . It is plotted the energy of the lowest state (ground state) as a function of the angular momentum.

We are considering rotating trapped condensates, the ratio  $\Omega/\omega$  describes the relation between the rotating frequency  $\Omega$  and the trap frequency  $\omega$ . Considering this single particle spectrum, Eq. (3), if we increase the rotation, such that  $\Omega = \omega$  we have all the single particle states become degenerate. In terms of the ratio this happens when we consider  $\Omega/\omega = 1$  which from Fig. (1) we can observe that this situation corresponds to the lowest Yrast line.

## 2.2 Density profile

Now, we have the full Hamiltonian diagonalized and this will allow us to have the coefficients for the ground state. This enables us to find the ground state density distribution  $\rho(r)$ . The density operator reads,

$$\hat{n}_\psi = \sum_{k,l} |k\rangle n_{kl} \langle l|, \quad (16)$$

where  $|k\rangle$  is a single particle state, and  $n_{k,l} = \langle \psi | a_l^\dagger a_k | \psi \rangle$ . Then, the density in terms of the density operator is,

$$\rho(z) = \langle z | \hat{n}_\psi | z \rangle. \quad (17)$$

For a state in the form of Eq. (15) the density can be computed as,

$$\rho(z) = \langle GS | \rho(z) | GS \rangle = \sum_{i,j} \psi_i^*(z) \psi_j(z) \sum_{\alpha, \alpha'} C_\alpha^* C_{\alpha'} \langle \alpha | a_i^\dagger a_j | \alpha \rangle \quad (18)$$

where the wavefunctions have the form of Eq. (3).

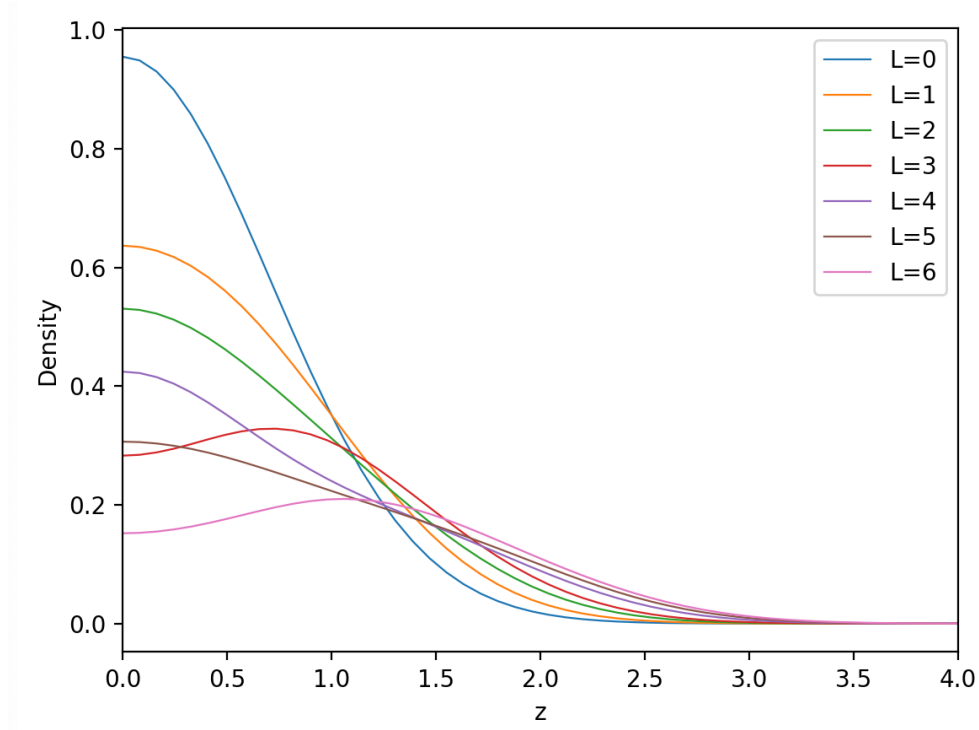


Figure 2: Density profile as function of the radius computed for different angular momentum  $L=0,1,2,3,4,5,6$ . System formed by  $N=3$  and the ratio  $\Omega/\omega$  for each angular momentum is  $\Omega/\omega = 0.8$  for  $L = 0$ ,  $\Omega/\omega = 0.8$  for  $L = 1$ ,  $\Omega/\omega = 0.9$  for  $L = 2$ ,  $\Omega/\omega = 0.9$  for  $L = 3$ ,  $\Omega/\omega = 0.9$  for  $L = 4$ ,  $\Omega/\omega = 0.98$  for  $L = 5$  and  $\Omega/\omega = 0.98$  for  $L = 6$ .  $L=6$  corresponds to the Laughlin state.

An important state to consider will be the so-called *Laughlin state*. Laughlin proposed the following wavefunction for bosons,

$$\psi_{\mathcal{L}} = N \prod_{i < j} (z_i - z_j)^2. \quad (19)$$

The intuition behind this proposed wavefunction is that it will become zero when two particles are in the same position. Therefore, this would give an idea that the interaction will be very low. The density created by this wavefunction will be almost constant and it will be highly correlated because if we find a particle in one position we can't find another particle in the same position (discussed in more detail in Section 2.3).

For a system formed by 3 bosons,  $N=3$ , the Laughlin wavefunction would read,

$$\psi_{\mathcal{L}} \propto (z_1 - z_2)^2 (z_1 - z_3)^2 (z_2 - z_3)^2 \quad (20)$$

where the angular momentum will be  $L=6$ .

In Fig. 2 the Laughlin state corresponds to  $L=6$  (pink line) and it can be seen how from all the densities shown for the different angular momentum, the one corresponding to the Laughlin state has the most constant density as it was expected.

### 2.3 Pair correlation

Pair correlations study the correlations among pairs of atoms. It is assumed that the first atom is placed at the center of the trap, and we compute the probability of finding a second atom at an arbitrary position. This probabilities can be seen in Fig. 3. To compute the pair correlation for the ground state we follow a procedure similar to what has been done for the density profile. Then, for states in the form of Eq. (15) where we have the Fock coefficients for the states of the Fock basis that construct the ground state, the pair correlation reads,

$$\eta(z, z') = \langle GS | \eta | GS \rangle = \sum_{\alpha, \alpha'} C_{\alpha}^* C_{\alpha'} \sum_{i, j, k, l} \psi_i^*(z) \psi_j^*(z') \psi_k(z) \psi_l(z') \langle \alpha' | \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l | \alpha \rangle. \quad (21)$$

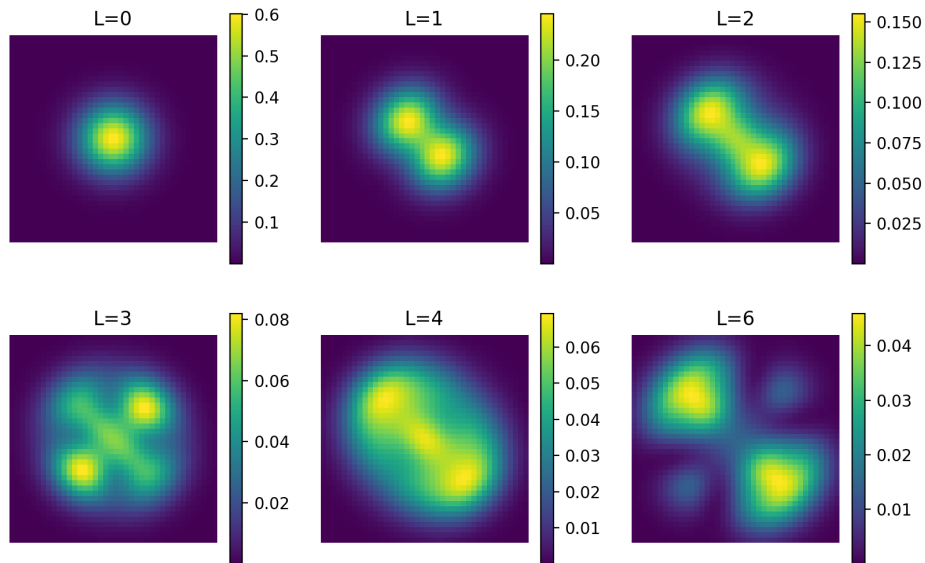


Figure 3: Pair correlation among the atoms for different values of the angular momentum. (a)  $L=0$ , (b)  $L=1$ , (c)  $L=2$ , (d)  $L=3$ , (e)  $L=4$  and (f)  $L=6$ .

In Fig. 3 can be seen the different probability distributions of finding a second atom for different angular momentum.

Some interesting situations can be discussed in more detail from the results obtained in Fig. 3. For  $L = 0$  Fig. 4 (a) the second atom is most likely to be found at the same position as the first atom, which means that we have no correlation among the atoms. This will imply that the many-body state is Bose condensate as we will expect for this value of the angular momentum. On the other hand, in Fig 4. (b) we can see the pair correlation of the Laughlin state,  $L = 6$  as deduced in Eq. (20), in this case we find full correlation since the probability of finding the atom in the same position of the first atom is zero. In this type of solutions if we measure one particle it will be correlated to the other particles, thus we could compare this behaviour with what we would expect in a mean field wavefunction, where if we measure a particle it does not affect the others.

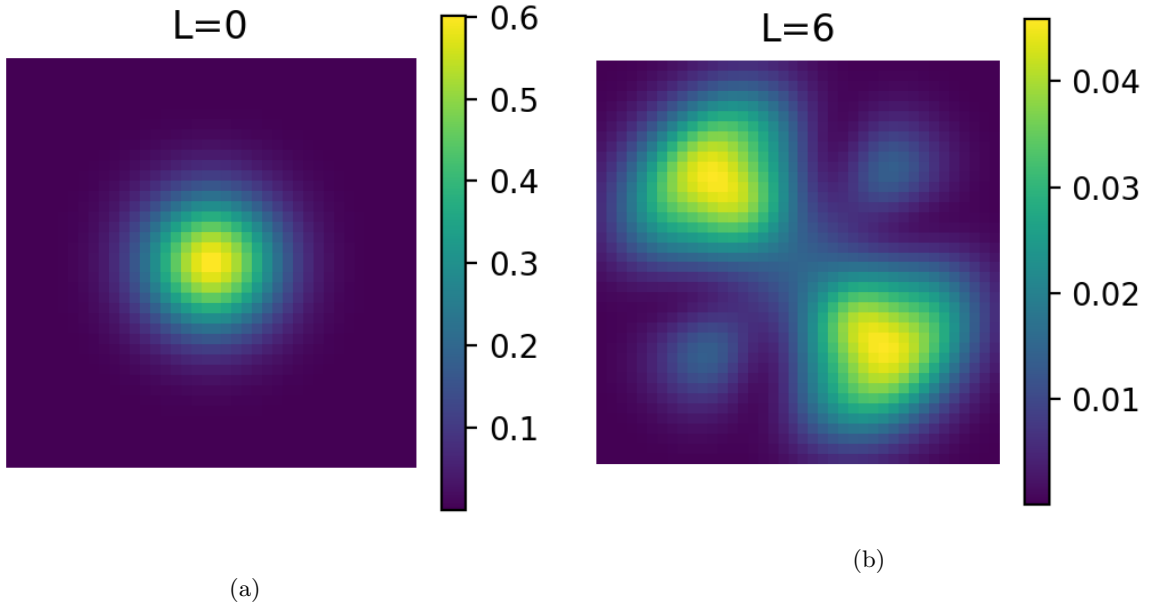


Figure 4: Closed up to the pair correlation distributions for the most interesting angular momentum in our study that will be discussed. (a)  $L=0$  (Bose condensation) (b)  $L=6$  (Laughlin state).