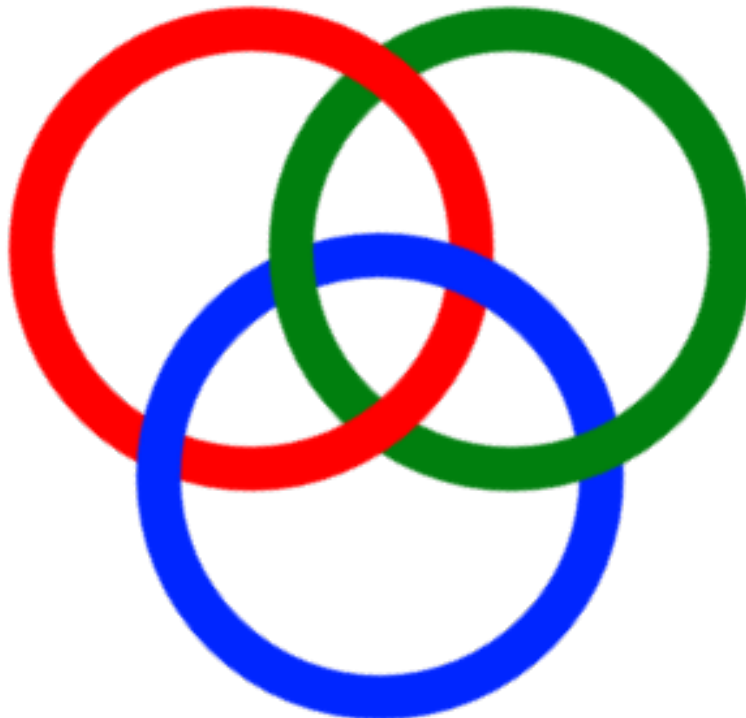# Squeezed quantum few-body systems

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Abstract

    This thesis examines the nature of identical, squeezed two- and three-boson systems, and mass-imbalanced three-boson systems with a gaussian particle interaction tuned to be at resonance in the relevant sub-systems, and present squeezed spectra. The energies in question were found by using the stochastic variational method with fully correlated, non-shifted gaussians as a basis. The mass imbalance was at 1:100 and 1:100:100 in the two- and three-body systems respectively. The plateaus of squeezing in one, two and three directions on the identical two-body system yielded energies of -0.4651, -1.4170, and -2.683, in good correspondence to previous measurements, in a unit basis where the gaussian width of the interaction is unit length, and the mass of the bosons are unit mass. The three-identical-boson ground state yielded -0.2375, and the imbalanced yielded -0.1810 and -0.0790 for its ground state and first excited state respectively. The monodirectional squeezing of the imbalanced system yielded a plateau of -8.199 and the identical bosons yielded -2.091, with the first excited state being pushed down to -0.008 relative to the two-body system.
In total, the calculations are in agreement with the relevant theory, and the method proved useful.

Contents

1 Introduction

Quantum physics has been an ever-growing subject of research since its discovery, and it would seem that it time and time again surprises us, and defies our intuition. One of the ways in which it does this, is through the Efimov effect, which predicts a model-independent, long-range three-body attraction with infinitely many bound states in three dimensions, when the ranges of the two-body interactions are zero, and the sub-systems are exactly at the threshold of binding. It is then of interest to examine how the lowest lying bound states would behave, should one insert a more realistic interaction between the particles in question, and artificially alter its dimensionality through squeezing, as the conditions of the effect is broken.

This paper examines the binding energies of two-body systems consisting of both identical and mass-imbalanced bosons, the latter consisting of one boson with a hundredth of the mass of the other, with a gaussian interaction initially tuned to be at zero binding energy in the case when they're free, and its behaviour when squeezed with a harmonic potential, along with the ground state and first excited state of two three-body systems made up of both identical and mass-imbalanced bosons, the former is examined when undergoing unidirectional squeezing.

The method applied is the stochastic variational method, in which one constructs one's wavefunction by expanding it in an appropriate set of basis functions, gaussians in this case, and selecting the parameters for these randomly from an appropriate distribution.

The specific type of gaussians chosen is the fully correlated, unshifted gaussians, in which a basis function can be written $\exp(\sum_{ij} \vec{r}_{ij}^T A \vec{r}_{ij})$, where A is an appropriate 3×3 matrix, and $\vec{r}_{ij}$ is the vector separating particle i and j.

We can thus present points from the spectrum that occurs when one squeezes two bosons of identical unit mass in one, two and three directions, along with that from the ground state of a three-body system of identical bosons, and its first excited state, when squeezed in a single direction, and the squeezed ground state of the three-body system of $m_1 = 100 = m_2$, $m_3 = 1$, and the un-squeezed states of some of the above, along with tests of the code by calculations of states from Hydrogen and Helium.

2 Theory

It is well known that the dimensionality of a system greatly affects some of its properties. A hypothetical sound wave in a single dimension would not dissipate its energy nearly as fast as a three-dimensional one.

In a more appropriate example for the subject at hand, it has been shown that the centrifugal barrier in a quantum mechanical two-body system at zero angular momentum has the opposite sign than in its three-dimensional counterpart. This means that particles, in conditions restricting them to such a dimensionality, will be attracted to one another in stead of being repulsed, letting them form bound states in two dimensions that would otherwise be unbound in three. In order for this to happen, however, one requires a small attraction beyond the effective potential.[3]

The interaction is somewhat more complicated in the case with three particles, as other factors than the centrifugal barrier and the two-body potentials begin to play into the system's hamiltonian.

2.1 Efimov states

An interaction, initially discovered by Vitaly Efimov, emerges, which is only present when there are more than two bodies in the system. If at least two of the two-body sub-systems are at resonance, resulting in an infinite scattering length, which most importantly means that they are at the threshold of being unbound, and interact at zero range, then a scale-invariant potential appears, that allows for energy levels that increment as:

$$E_n = E_0 \lambda^{-2n}$$

Such states are called Efimov states, and correspond to the interaction being mediated in the system by one or more of the particles, moving between the others. They are also called "Borromean states" if all of the sub-systems are unbound, analogous to the symbol of the Borromean rings, where, if one removes a single ring, they all fall apart, but as long as all three rings are there, they stick together. Similarly, should one remove a particle, the system will disassociate, but until then, it will maintain a bound ground state.

This, however, has a dimensional requirement. If one only allows integer dimensions, it only appears in three dimensions. In fewer dimensions, Borromean states do not exist, although bound states certainly do, but in stead of there existing an infinite amount of bound states, the amount is finite.

If one squeezes the system by adding a harmonic oscillator potential to it, all but the ground state and first excited state of from the Efimov attraction should be moved up in energy, while the rest, for large enough oscillator strengths, disappear. This can be thought of as a lightly bound three-body state decaying to a bound two-body system and a free particle, and happens because the two-body energy becomes lower than the three-body energy.

The ground state and the first excited state, however, should be pushed down relative to the two-body threshold.[4]

The Efimov potential and scale invariance

In order for the reader to understand this three-body force, one has to understand the form of the potential.

The potential that Efimov derived comes from calculating the hamiltonian of three identical bosons that interact at infinitely short ranges near resonance, i.e. nearly unbound two-particle subsystems, and then applying appropriate boundary conditions and coordinate transformations, in the end finding a Schrödinger equation with a wavefunction of two coordinates. This can be broken down into a spatial part $F_n(R)$, and an angular part $\phi_n(\alpha)$.

Here R is the so-called hyper-radius, defined such that $R^2 = r_{12}^2 + \rho_{12,3}^2$, where r_{12} is the norm of the vector between particle 1 and 2, and $\rho_{12,3}$ is proportional to the norm of the vector between the center of mass of particle 1 and 2, and particle 3.

α is the angle between these two vectors.

Much like an effective centrifugal potential appears in the three-dimensional Schrödinger equation from choosing spherical coordinates, a potential of the form

$$V_n = \frac{s_n^2 - \frac{1}{4}}{R^2},$$

appears.

Worth noting is that the n in the equation is not the primary quantum number, dictating what energy state one is looking at. The parameters s_n stems from boundary conditions on $\phi_n(\alpha)$. The appropriate equation for solving s_n has one imaginary root, leading to one attractive potential, and finally to bound states. The resulting value of λ is then given as $\lambda = e^{\pi/|s_0|}$, where s_0 is the imaginary root of the appropriate equation. [4].

The next question to ask is then why this particular potential leads to infinitely many states, and why they're all scaled relative to one another.

This becomes apparent when one looks at the scaling relations of the kinetic energy operator.

Consider the Hamiltonian for a a single particle in one dimension with a potential $V(x)$:

$$(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x))\psi_1(x) = E_1\psi_1(x) \qquad (1)$$

If we then attempt a solution with another trial function named $\psi_2(x) = \psi_1(\lambda x)$, we obtain:

$$E_2\psi_2(x) = (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x))\psi_2(x)$$

$$= \lambda^2(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial (\lambda x)^2} + \lambda^{-2}V(x))\psi_1(\lambda x)$$

If we then have a potential that scales so that $V(x) = \lambda^2 V(\lambda x)$ for a given λ, which is the case for a potential of the form $V(x) \propto x^{-2}$, then the equation would become:

$$E_2\psi_2(x) = \lambda^2(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial (\lambda x)^2} + V(\lambda x))\psi_1(\lambda x)$$

This is, all but for the factor of λ^2 in front of the parenthesis on the right hand side, the Schrödinger equation for ψ_1 with $x \to \lambda x$, which must therefore have the same eigenvalue.

$$(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial (\lambda x)^2} + V(\lambda x))\psi_1(\lambda x) = E_1\psi_1(\lambda x) = E_1\psi_2(x)$$

$$\Rightarrow E_2\psi_2(x) = \lambda^2 E_1\psi_2(x)$$

$$\Rightarrow E_2 = \lambda^2 E_1$$

One can then repeat the arguments and propose a function $\psi_n(x) = \psi_{n-1}(\lambda x)$, but the result is already apparent: An infinite series of energy levels emerge where $E_{n+1} = \lambda^2 E_n = \lambda^{2n}E_0$. Of course, if the arbitrarily named E_0 is smaller than zero, one obtains a ground state energy that is not E_0, but E_∞, going towards $-\infty$. Naturally, this is simply a naming

convention, and, if a finite, negative ground state exists, the energies will be ordered in ascending order with n so that

$$E_n = E_0\lambda^{-2}$$

The physics of the spatial scaling $x \to \lambda x$ for the wavefunction can be intuitively understood by looking at a gaussian with width b:

$f(x) = \exp(-x^2/b^2)$. If $x \to \lambda x$, $f \to \exp(-x^2/(b/\lambda)^2)$, which is equivalent to the transformation $b \to b/\lambda$, effectively narrowing the function. It can also be understood from the physics of the free particle, where $x \to kx$ in the wavefunction corresponds to a decrease in the wavelength for $k > 1$. Therefore, if ψ is a wavefunction and $E_0 < 0$, the wavefunction should, given the aforementioned scaling conditions of the potential, collapse onto its center and be infinitely bound.

However, if appropriate boundary conditions are applied to a wavefunction, a corresponding boundary condition is applied to the energy as well as to the values that λ is allowed to take, ensuring a finite ground state, and a discrete scale invariance. Naturally, we will not observe pure Efimov states, as a gaussian potential has finite range, and this itself sets a boundary condition for the wavefunction, ensures a finite ground state, and possibly also creates excited states on its own. However, if one looks at very large systems, which highly excited states tend to be, one can expect to see some Efimov-like states, as one could, for very large systems, treat the gaussian interaction like a zero-range potential.

Mass dependencies

The Efimov effect does not only appear for bosons of identical mass, but also for different particles. The equation governing the solutions for s_n is particularly mass-dependent. For two bosonic particles of mass M, and one bosonic particle of mass m, the equation of interest for three resonantly interacting pairs with angular momentum $l = 0$ is:

$$(cos(s_n\frac{\pi}{2}) - \frac{2}{s_n}\frac{sin(s_n\gamma)}{sin(2\gamma)})cos(s_n\frac{\pi}{2}) - 2(\frac{2}{s_n}\frac{sin(s_n\gamma')}{sin(2\gamma')})^2 = 0$$

$$\gamma = arcsin(\frac{M}{M+m})$$

$$\gamma' = arcsin(\sqrt{\frac{m}{2M+m}})$$

Some interesting limits and values of the emerging scaling value are [4]

$$\lim_{M/m\to 0}(\lambda) = 15.74$$

$$\lim_{M/m\to\infty}(\lambda) = 1$$

$$for\ M/m = 1,\ \lambda \approx 22.7$$

Therefore, if one wishes to calculate many Efimov states, it is favourable to consider the states where two bosons of high mass interact with a single boson of low mass.

This dependency on the ratio of the masses can be put in a classical analogy, in which the lighter particle will move faster

between the other two particles due to its smaller mass.

Understanding the scaling relations of the kinetic energy operator in respect to the mass of a system also gives rise to some shortcuts one can take. Since we take interest in the calculations of the potentials that give rise to resonant two-body systems, we can utilise a mass-scaling, so that that calculating a single potential is sufficient to trivially calculate the rest. The many calculations, that would otherwise be required, can be circumvented, if one enforces a scaling of the interaction potential. Say one has calculated a two-body interaction for a system with reduced mass μ, tuned its ground-state energy to be near, or exactly zero, and wants to also calculate an interaction for a different two-particle system of reduced mass μ'.

One then has a Schrödinger equation without the center of mass for the ground state function $\psi = \psi(r_{12})$, if $V = V(r_{12})$:

$$(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r_{12}^2} + V)\psi = E\psi$$

One can then understand the scaling of the mass as a scaling of the energy, by looking at the primed system:

$$(-\frac{\hbar^2}{2\mu'}\frac{\partial^2}{\partial r_{12}^2} + V')\psi' = E'\psi'$$
$$= \frac{\mu}{\mu'}(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r_{12}^2} + \frac{\mu'}{\mu}V')\psi'$$

The operator within the parenthesis is the hamiltonian for a mass μ system with a potential $\frac{\mu'}{\mu}V'$. If we, by construction of our interaction potential, let $V = \frac{\mu'}{\mu}V'$, then $\psi' = \psi$ is a solution, and since ψ is the ground state solution of the un-primed system, that particular function will be the ground state of the primed system. Hence:

$$\frac{\mu}{\mu'}(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r_{12}^2} + \frac{\mu'}{\mu}V')\psi'$$
$$= \frac{\mu}{\mu'}(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r_{12}^2} + V)\psi$$
$$= \frac{\mu}{\mu'}E\psi = E'\psi$$
$$V' = \frac{\mu}{\mu'}V \Rightarrow E' = \frac{\mu}{\mu'}E$$

Thus, to keep the new system near resonance, one only has to ensure that the reduced masses of the subsystems are similar. Of course, when $E = 0$, this has no bearing, and the ground state of the primed system is kept to be equal to that of the un-primed system. This, however, also implies that, if the un-primed sub-system is only near-resonant, a simple rescaling of the interaction potential at sufficiently large μ/μ' is not a valid approach.

2.2 The correlated gaussian method

The main idea of this method, is to expand the wavefunction as a linear combination of gaussian functions, so that if the supervector $\vec{r}$ consists of N single particle vectors as such:

$$\vec{r} = \begin{pmatrix} \vec{r_1} \\ \vec{r_2} \\ . \\ . \\ \vec{r_N} \end{pmatrix}$$

then the wavefunction in position space can be given as follows:

$$\psi(\vec{r}) = <\vec{r}|\psi> = \sum_j c_j <\vec{r}|g_j>$$

$$<\vec{r}|g_j> = \exp(-\vec{r}\cdot A_j\vec{r})$$
$$dim(A_j) = dN \times dN \ in \ d \ dimensions$$

The exponent is also often written $-r^T A_j r$ for brevity of notation. It is of great importance that the A matrices are positive definite, as the gaussians, otherwise, may not be quadratically integrable.

One can then infer that the ket-state $|\psi>$ must be an eigenstate of the hamiltonian,

$$\hat{H}|\psi> = E|\psi>,$$

where E is the energy. This leads to a generalised eigenvalue problem, if we collect the parameters c_j as the j'th index of a vector $\vec{c}$, and

$$H_{ij} \doteq <g_i|\hat{H}|g_j>$$
$$and$$
$$M_{ij} \doteq <g_i|g_j>$$

as the ij'th elements of the matrices H and M:

$$\hat{H}|\psi> = E|\psi> = E\sum_j c_j|g_j>$$
$$<g_i|\hat{H}|\psi> = \sum_j <g_i|\hat{H}|g_j>c_j = (H\vec{c})_i$$
$$= E\sum_j <g_i|g_j>c_j = (EM\vec{c})_i$$

The i indicates that both of these equations are just the i'th index of the resulting vector of multiplying H on $\vec{c}$ and EM on $\vec{c}$ respectively.

Naturally, not any gaussians will do. There exists a theorem, stating that the eigenvalue will either be greater than, or equal to the corresponding energy state. More accurately, if the eigenvalues of a set of gaussians are ordered such that $E_{i+1} > E_i \ \forall \ i$, and those that corresponds to physical energies are sorted such that $\epsilon_{i+1} > \epsilon_i \ \forall \ i$, then $E_i \geq \epsilon_i \ \forall \ i$, and the equality will only hold if $<\vec{r}|\psi> = \sum_j c_j <\vec{r}|g_j>$.[2]

Thus, the problem reduces to finding the matrix elements of relevant potentials, along with a computational problem of finding the correct gaussians to span the wavefunction.

2.3 Coordinates

When interested in the internal structure of the system, one can draw great benefit from choosing one's coordinates in such a manner, that the center of mass disconnects from one's equations, as this effectively reduces the problem from an N-particle problem to an (N-1)-particle problem. A set of coordinates are typically chosen such that the transformed vector $\vec{x} = U\vec{r}$, where U is a matrix, has, on its first three entries, the vector from particle 1 to particle 2, then, on its second three entries, the vector between the center of mass of particle 1 and 2, to particle 3, and, in general, if we see it as a supervector:

$$\vec{x}_i = (\frac{1}{\sum_j^i m_j} \sum_n^i m_n \vec{r}_n) - \vec{r}_{n+1}$$

with

$$\vec{x}_N = \frac{1}{\sum_j^N m_j} \sum_n^N m_n \vec{r}_n = \vec{R}_{CM}$$

This, for N=3, leads to the matrix transformation:

$$U = \begin{pmatrix} I_d & -I_d & 0 \\ \frac{m_1}{m_1+m_2}I_d & \frac{m_2}{m_1+m_2}I_d & -I_d \\ \frac{m_1}{m_1+m_2+m_3}I_d & \frac{m_2}{m_1+m_2+m_3}I_d & \frac{m_3}{m_1+m_2+m_3}I_d \end{pmatrix}$$

Where I_d is the unit matrix in d dimensions. The transformation matrix has an inverse. By explicitly concerning ourselves with the consequences on the internal system's energy, we can understand that an A-matrix in a gaussian basis function can be manipulated as follows

$$-r^T A r = -r^T U^T (U^{-1})^T A U^{-1} U r$$
$$= -x^T (U^{-1})^T A U^{-1} x,$$

and, by absorbing the inverse transformation matrix in A and disposing of the center of mass coordinate, can be treated as $d(N-1) \times d(N-1)$ dimensional.

Relative coordinates

Many, if not all, interaction potentials between particles have a dependency on the distance vector connecting them. It is therefore also worth noting their expressions in this basis.
Let us denote $\vec{r}_i - \vec{r}_j = \vec{r}_{ij}$, then we let $\vec{w}_{ij}$ and $\vec{S}_{ij}$ be supervectors, and define and calculate their connection as follows:

$$\vec{r}_{ij} = \vec{w}_{ij}^T \vec{x} = \vec{S}_{ij}^T \vec{r}$$
$$(\vec{S}_{ij})_q \doteq (\delta_{i,q} - \delta_{j,q})I_d$$
$$\vec{S}_{ij}^T \vec{r} = \vec{S}_{ij}^T U^{-1} U \vec{r}$$
$$= \vec{S}_{ij}^T U^{-1} \vec{x} = \vec{w}_{ij}^T \vec{x}$$
$$\vec{S}_{ij}^T U^{-1} = \vec{w}_{ij}^T$$

These prove useful when dealing with interactions, such as the Coulomb interaction, that only depend on these.
For three identical particles with unit mass, the supervectors are given as:

$$\begin{pmatrix} \vec{S}_{12}^T \\ \vec{S}_{23}^T \\ \vec{S}_{13}^T \end{pmatrix} = \begin{pmatrix} I_d & -I_d & 0 \\ 0 & I_d & -I_d \\ I_d & 0 & -I_d \end{pmatrix}$$
$$\begin{pmatrix} \vec{w}_{12}^T \\ \vec{w}_{23}^T \\ \vec{w}_{13}^T \end{pmatrix} = \begin{pmatrix} I_d & 0 & 0 \\ -\frac{1}{2}I_d & I_d & 0 \\ \frac{1}{2}I_d & I_d & 0 \end{pmatrix},$$

and it is both apparent and intuitive that the center of mass does not enter into such calculations, as this would imply that the distances between the individual particles are inherently dependent on the position of the system.

Harmonic potentential's coordinates

If we consider three non-interacting particles in a harmonic potential of strength a, the potential will have the form:

$$h_z = a(z_1^2 + z_2^2 + z_3^2)$$
$$= \sum_j \frac{1}{2}m_j \omega_j^2 z_j^2$$

The ground state of a harmonic oscillator will be a gaussian, and will have a width associated with it, related to the amplitude:

$$a = \frac{1}{2}m_j \omega_j^2 = \frac{2\hbar^2}{m_j b_j^4}$$

Thus, whenever one is operating in a coordinate basis where this operator is diagonal, meaning that it does not mix coordinate vectors in this basis, one can calculate the width of the system through this mechanism, and one has:

$$m_j^{1/4} b_j = m_i^{1/4} b_i$$

The potential can be rewritten to

$$h_z = a r^T W_z r,$$

where W_z is a diagonal matrix that picks out the z-components of the vector r. Further transformations to an x-basis, would result in the following:

$$h_z = a x^T (U^{-1})^T W_z U^{-1} x$$

There are conditions for the matrix between the x-vectors to be diagonal in the last three rows and columns, allowing us to separate the center of mass. If we for a moment consider a spherically symmetric trap, and thus omit the I_d from our U-matrix, we see the conditions appear, since if it is diagonal for a potential $\sum_i z_i^2$, it is also diagonal for one of the form $\sum_i x_i^2 + y_i^2 + z_i^2$:

$$U^{-1} = \begin{pmatrix} \frac{m_2}{m_1+m_2} & \frac{m_3}{m_1+m_2+m_3} & 1 \\ -\frac{m_1}{m_1+m_2} & \frac{m_3}{m_1+m_2+m_3} & 1 \\ 0 & -\frac{m_1+m_2}{m_1+m_2+m_3} & 1 \end{pmatrix}$$

$$(U^{-1})^T = \begin{pmatrix} \frac{m_2}{m_1+m_2} & -\frac{m_1}{m_1+m_2} & 0 \\ \frac{m_3}{m_1+m_2+m_3} & \frac{m_3}{m_1+m_2+m_3} & -\frac{m_1+m_2}{m_1+m_2+m_3} \\ 1 & 1 & 1 \end{pmatrix}$$

$$(U^{-1})^T U^{-1}$$
$$= \begin{pmatrix} \frac{m_2^2+m_1^2}{(m_1+m_2)^2} & \frac{m_3}{m_1+m_2+m_3}\frac{m_2-m_1}{m_1+m_2} & \frac{m_2-m_1}{m_1+m_2} \\ \frac{m_3}{m_1+m_2+m_3}\frac{m_2-m_1}{m_1+m_2} & \frac{2m_3^2+(m_1+m_2)^2}{(m_1+m_2+m_3)^2} & \frac{2m_3-m_1-m_2}{m_1+m_2+m_3} \\ \frac{m_2-m_1}{m_1+m_2} & \frac{2m_3-m_1-m_2}{m_1+m_2+m_3} & 3 \end{pmatrix}$$

Diagonality is only achieved when $m_1 = m_2 = m_3$. This is highly problematic, as the center of mass coordinates cannot be directly removed in such calculations, and will greatly increase the time for each calculation. However, if one has different potential strengths for different particles, one gains:

$$h_z = \sum_j a_j z_j^2 = r^T a W_z r$$

$$a = \begin{pmatrix} a_1 I_d & 0 & 0 \\ 0 & a_2 I_d & 0 \\ 0 & 0 & a_3 I_d \end{pmatrix}$$

Due to the symmetry of the U-matrix, we can, for a qualitative look at when the resulting matrix $(U^{-1})^T a W_r U^{-1}$ is diagonal, omit I_d:

$$(U^{-1})^T a U^{-1}$$
$$= (U^{-1})^T \begin{pmatrix} a_1\frac{m_2}{m_{12}} & a_1\frac{m_3}{m_{123}} & a_1 \\ -a_2\frac{m_1}{m_{12}} & a_2\frac{m_3}{m_{123}} & a_2 \\ 0 & -a_3\frac{m_1+m_2}{m_{123}} & a_3 \end{pmatrix} =$$
$$\begin{pmatrix} \frac{a_1 m_2^2+a_2 m_1^2}{m_{12}} & \frac{m_3}{m_{123}}\frac{a_1 m_2-a_2 m_1}{m_{12}} & \frac{a_1 m_2-a_2 m_1}{m_{12}} \\ \frac{m_3}{m_{123}}\frac{a_1 m_2-a_2 m_1}{m_{12}} & \frac{(a_1+a_2)m_3^2+a_3(m_{12})^2}{(m_{123})^2} & \frac{(a_1+a_2)m_3-a_3(m_{12})}{m_{123}} \\ \frac{a_1 m_2-a_2 m_1}{m_{12}} & \frac{(a_1+a_2)m_3-a_3(m_{12})}{m_{123}} & a_1+a_2+a_3 \end{pmatrix}$$

Some items have been constracted so that $m_{12..j} = m_1 + m_2 + ... + m_j$. The conditions for diagonality become apparent, and are where $a_i/m_i = a_j/m_j \forall \ i,j$ in the system, which is equivalent to having the kinds of systems where each particle has the same oscillating frequency, such that the potential becomes

$$h_z = \frac{1}{2}\omega^2 \sum_j m_j z_j^2$$

By no longer keeping the potential strength, a, invariant across different particles, but in stead maintaining a/m, the relation between different widths of the trap on different particles, is rewritten to

$$\sqrt{m_j}b_j = \sqrt{m_i}b_i$$

2.4 Matrix elements

Once appropriate coordinates have been decided upon, one must analytically calculate the matrix elements of the hamiltonian H, and the overlap M.

The overlap

If we denote $|g> = \exp(-x^T A x)$, and $A + A' = B$ for simplicity, then we have:

$$<g|g'> = \int_{\mathbf{R^{D(N-1)}}} e^{-x^T B x} d^{D(N-1)} x$$
$$\doteq \int e^{-x^T B x} dx \quad \text{(notation convention for D dimensions)}$$

Suppose, then, that B was diagonal. Then our problem reduces to a product of one-dimensional single coordinate integrals:

$$<g|g'> = \prod_i^{D(N-1)} \int e^{-x_i^2 B_{ii}} dx_i = \prod_i^{D(N-1)} \sqrt{\frac{\pi}{B_{ii}}}$$
$$= \sqrt{\frac{\pi^{D(N-1)}}{det(B)}}$$

Since the determinant of a matrix is independent of its basis vectors, the result must remain unchanged, should B not be diagonal. Hence, the overlap reduces to:

$$M_{ij} = <g_i|g_j> = \sqrt{\frac{\pi^{D(N-1)}}{det(A_i + A_j)}}.$$

It is also worth noticing the symmetry $A_i + A_j = A_j + A_i \Rightarrow M_{ij} = M_{ji} \ \forall \ i,j$. In fact, all matrices whose elements depend take from the gaussians only the matrix $A_i + A_j$ must, of course, hold this symmetry.

As a final note on this element, should one consider the case of spherically symmetric gaussians, in which one has one element in the A-matrices per three coordinates, it naturally follows that one should replace the determinant with itself to the power of three.

The kinetic energy operator

The first thing of interest, after having calculated the overlap, is to separate the kinetic energy of the whole system from that of the subsystems. Hence, we follow the approach of Varga and Suzuki [1]. We denote the momentum in the single particle basis as $\vec{p_i}$ for particle i, and in x-basis as $\vec{\pi_i}$, for the i'th vector in x, and operate in a set of units where $\hbar = 1$.

Then, in the case with spherical gaussians, where one has a

coordinate per vector $\vec{r}$:

$$p = \begin{pmatrix} \vec{p_1} \\ \vec{p_2} \\ \vec{p_3} \end{pmatrix} = U^T \begin{pmatrix} \vec{\pi_1} \\ \vec{\pi_2} \\ \vec{\pi_3} \end{pmatrix}$$

$$= U^T \pi$$

$$K_{CM} = \frac{\pi_N^2}{2 \sum_i m_i}$$

$$\sum_i^N \frac{1}{2m_i} \vec{p_i}^2 - K_{CM} = \frac{1}{2} \sum_i^N \sum_j^N (\frac{1}{m_i} \delta_{ij} - \frac{1}{\sum_k^N m_k}) \vec{p_i} \cdot \vec{p_j}$$

$$= \sum_i^{N-1} \sum_j^{N-1} \Lambda_{ij} \vec{\pi_i} \cdot \vec{\pi_j}$$

$$\Lambda_{ij} = \frac{1}{2} \sum_k^N U_{ik} \frac{1}{m_k} U_{jk},$$

where i and j range from 1 to N-1. In the fully correlated case, where we have a parameter for each coordinate of each particle vector, every parameter of the U-matrix has been multiplied with I_d, and thus must every component of Λ as expressed here. Hence, if we denote a diagonal matrix L of dimension D*N in D dimensions, with entries $L_{kk} = 1/m_q$, where $q = k/D$ rounded up to the nearest integer, on the diagonal, then Λ is all but the last three rows and columns of the matrix $\frac{1}{2} U L U^T$, and it contains, in our chosen coordinates, the reduced masses of the subsystems on its diagonal, and zeroes on every other entry. We can then, after removing the center of mass coordinate from our x-vector, rewrite our kinetic energy operator as

$$\hat{K} = -\frac{\partial}{\partial \vec{x}} \Lambda \frac{\partial}{\partial \vec{x}^T}.$$

It is solved in the following way.[2]

$$< g|\hat{K}|g' > = \int e^{-x^T A x} (-\frac{\partial}{\partial \vec{x}} \Lambda \frac{\partial}{\partial \vec{x}^T}) e^{-x^T A' x} dx$$

If we integrate by parts, we obtain:

$$< g_i|\hat{K}|g_i > = \int (\frac{\partial}{\partial \vec{x}} e^{-x^T A_i x}) \Lambda (\frac{\partial}{\partial \vec{x}^T} e^{-x^T A_j x}) dx$$

$$= \int (4 x^T A_i \Lambda A_j x) e^{-x^T (A_i + A_j) x} dx$$

This can with great benefit be written as

$$< g_i|x^T F x|g_j >$$

as solving this general case also solves the harmonic oscillator. Suppose, initially, that the sum of the A-matrices, B, is diagonal, and that F is a general matrix with the appropriate dimensions. Then:

$$x^T F x = \sum_{i,j} F_{ij} x_i x_j$$

is an uneven function of a given x_i for $i \neq j$. Since we integrate over all space in our inner product, and since gaussians are even functions, every off-diagonal term of F vanishes, leaving us with:

$$< g_i|x^T F x|g_j > = \int e^{-\sum_k x_k^2 B_{kk}} \sum_q F_{qq} x_q^2 dx$$

$$= \sum_q \prod_{k \neq q} \int e^{-x_k^2 B_{kk}} dx_k \int e^{-x_q^2 B_{qq}} F_{qq} x_q^2 dx_q$$

Let us look at a single integral of the type:

$$k_q = \int e^{-x_q^2 B_{qq}} F_{qq} x_q^2 dx_q = \int e^{-y^2 b} f y^2 dy \quad \text{(for brevity)}$$

$$k_q = \frac{-f}{2b} \int y(-\frac{2}{b} y e^{-y^2 b}) dy$$

$$= \frac{-f}{2b} \int y \frac{\partial}{\partial y} e^{-y^2 b} dy$$

$$= \frac{-f}{2b} (y e^{-y^2 b}|_{-\infty}^{\infty} - \int e^{-y^2 b} dy)$$

$$= \frac{f}{2b} \int e^{-y^2 b} dy$$

$$= \frac{F_{qq}}{2 B_{qq}} \int e^{-x_q^2 B_{qq}} dx_q$$

Combining this with the rest yields:

$$< g_i|x^T F x|g_j > = \sum_q \prod_k \int e^{-x_k^2 B_{kk}} dx_k \frac{F_{qq}}{2 B_{qq}}$$

$$= \prod_k \int e^{-x_k^2 B_{kk}} dx_k (\sum_q \frac{F_{qq}}{2 B_{qq}})$$

We readily recognise the product as the overlap, and since B is diagonal in the chosen basis, we can write

$$< g_i|x^T F x|g_j > = < g_i|g_j > \frac{1}{2} trace(B^{-1} F)$$

$$= M_{ij} \frac{1}{2} trace(B^{-1} F)$$

Since the trace, just like the determinant, is independent of the basis chosen, this holds true for non-diagonal B-matrices. With the kinetic energy operator, we had

$$F = 4 A_i \Lambda A_j$$

$$\Rightarrow K_{ij} \doteq < g_i|\hat{K}|g_j > = 2 trace(A_i \Lambda A_j (A_i + A_j)^{-1}) * M_{ij}$$

Note that the trace has a cyclical property so that $trace(ABCD) = trace(DABC) = ...$

Building up the A-matrices to be symmetric, so that $A^T = A \ \forall \ A$, then $(B^{-1})^T = ((A_i + A_j)^{-1})^T = B^{-1}$, meaning that A matrices, B matrices, and a B^{-1} matrices commute with each other, and we can adjust the operator to:

$$trace(A_i \Lambda A_j B^{-1}) = trace(\Lambda A_j B^{-1} A_i)$$

$$= trace(\Lambda B^{-1} A_j A_i) = trace(\Lambda B^{-1} A_i A_j)$$

$$= trace(\Lambda A_i B^{-1} A_j) = trace(A_j \Lambda A_i B^{-1})$$

And therefore, as the overlap satisfies $M_{ij} = M_{ji}$,

$$K_{ij} = 2trace(A_i \Lambda A_j B^{-1}) M_{ij} = 2trace(A_j \Lambda A_i B^{-1}) M_{ji}$$
$$= K_{ji}$$

Harmonic oscillator

Revisiting our coordinate-calculations, we substitute F as all but the last three rows and columns of the chosen matrix

$$F_{ij} = \frac{1}{2} m\omega^2 ((U^{-1})^T W U^{-1})_{ij}$$
$$(i, j = 1, ..N - 3)$$
$$\Rightarrow h_{ij} \doteq < g_i | \hat{h} | g_j > = trace(F(A_i + A_j)^{-1}) * M_{ij}$$

It's trivial that the matrix is symmetric, so that $h_{ij} = h_{ji}$.

Gaussian interactions

With a gaussian interaction of the sort

$$\hat{V} = \exp(-x^T C x)$$

the matrix element is calculated in the same way as the overlap:

$$V_{ij} = < g_i | \hat{V} | g_j > = \int e^{-x^T (A_i + A_j + C) x} dx$$
$$= \sqrt{\frac{\pi^{D(N-1)}}{det(A_i + A_j + C)}}.$$

The symmetry $V_{ij} = V_{ji}$ is apparent from this calculation.

2.5 The method in practice

The relevant A-matrices can be constructed in a plethora of ways. One way of doing it is to have them constructed by defining their diagonal elements as $A_{ij} = \delta_{ij} \frac{1}{b_i^2}$, where each b_i in a given matrix can be chosen from an exponential distribution with a relevant mean, b, and then scrambling them by multiplying with a Q-matrix from a QR decomposition of a random matrix, and then make the transformation $A \rightarrow (U^{-1})^T A U^{-1}$, and cutting off the last three rows and columns. This leads to a full correlation matrix, but is slow and tedious. Another, is to build one's matrix from the relative coordinates, so that

$$< \vec{r} | g > = \exp(- \sum_{i,j} (\vec{r}_i - \vec{r}_j)^T \alpha_{ij} (\vec{r}_i - \vec{r}_j) + \sum_k \vec{r}_k^T \alpha_k \vec{r}_k)$$

where α_{ij} and α_k are $D \times D$ matrices, then scrambling them and making a transformation to the x-basis, effectively constructing the A-matrices from the $\vec{w}_{ij}$ vectors mentioned in the section about relative coordinates. The effectiveness of the code, and thus the likelihood of having the best result after some amount of trials, is dependent on both the coordinates chosen and the parameter b from the exponential distribution. In the case of N=2, one automatically builds one's matrix from these by separating the center of mass coordinate.

The code that solves the eigenvalue problem works by having a set of A-matrices initially randomly collected, after which each underwent a number R of trials, calculating the corresponding rows in the H and M matrices each time, and keeping the one which gave the lowest eigenvalue, before moving on to the next. Once each A-matrix had undergone its trials, the process started over, and repeated the process Z times, totalling a R*Z trials for each function. Then the basis was expanded with some amount, and the procedure started over.

The parameters in the matrices must necessarily be chosen at random, as many other approaches, such as starting from the smallest value of b and moving forwards, would likely reach a local minimum in a situation where one is looking for a global one.

Matlab was used for solving the eigenvalue problem through Cholesky decomposition. In essence it dissolves the overlap matrix M into LL^T, where L is a lower triangular matrix, such that

$$H\vec{c} = EM\vec{c} = ELL^T\vec{c}$$
$$L^{-1}H(L^{-1})^T L^T \vec{c} = EL^T \vec{c}$$
$$\Rightarrow L^{-1}H(L^{-1})^T \vec{c} = E\vec{c}$$

This procedure, however, requires that M is a positive definite matrix [3]. An exception to its positive definiteness, is when one has several identical gaussians. Ideally, this should not be the case, as our basis should be linearly independent, but due to the randomness of the selection process, it can become very close. Suppose one puts into the system $< \vec{r} | g_1 > = < \vec{r} | g_2 >$, with a basis set of two gaussians.

Then one has the matrix:

$$M \propto \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

which is singular. Having a similar matrix for H would give Matlab major difficulties with calculating physical eigenvalues.

3 Hydrogen

Every number compared with here, and in the chapter of helium represents a citation from [6] and [5] combined.

As we are interested in both two-body and three-body systems, it is vital that we can test the code written to calculate this, by using a known system, and therefore hydrogen is chosen. In order to simulate this, however, one needs to calculate the matrix element for the coulomb interaction.

This is not trivial.

In order to solve the problem, the potential is expanded into gaussians, such that

$$\frac{a_0}{r} \approx \sum_j c_j exp(-b_j r^2)$$

15 gaussians were used in this case. The approximation is easily done through the method of least squares, in which one minimises the function

$$\chi^2 = \sum_i^n (\frac{F(r_i) - y(r_i)}{\Delta y})^2.$$

This begs for clarification. We approximate the function $y = \frac{a_0}{r}$, by first separating it into several bits, $y_i = a_0/r_i$. This approximation is done with the function $F(r) = \sum_k^m c_k f_k(r)$, where $f_k(r) = exp(-b_k r^2)$, with the uncertainty $\Delta y = 1$.

This is equivalent to solving the problem

$$A\vec{c} = y$$

where c is a column vector that on its k'th entry has c_k, and A is a matrix, such that $A_{i,k} = exp(-b_k r_i^2)$, and y is a column vector, whose i'th entry is a_0/r_i.

The best solution for the parameters, c_k, is, thankfully, easily found in Matlab, by calculating $c = A\backslash y$.

The parameters are collected from a logarithmic distribution, and fifteen gaussians were chosen, to be compared on 5000 points, and run through an optization loop to minimise the parameter χ^2. Small widths were preffered to large widths, as the potential diverges at $r = 0$, and a shortcoming in fitting the potential at small r, is therefore a greater problem in calculation compared to a shortcoming at large r [3]. To test the approximation of the potential, the hydrogen atom is calculated, as the matrix element for two particles is analytical if the gaussian is spherically symmetric. In the case of two-particle systems, the transformation matrix becomes

$$U = \begin{pmatrix} I_d & -I_d \\ \frac{m_1}{m_1+m_2}I_d & \frac{m_2}{m_1+m_2}I_d \end{pmatrix},$$

and the full A-matrices become of dimension $d \times d$ when the center of mass is disposed.

As a test of the rest of the code without the approximated potential, a set of spherical gaussians - that is, those with $A = aI_d$, where a is a scalar, are chosen, as the expectation value can then be rewritten in spherical coordinates in three dimensions:

$$< g_i |\frac{1}{r_{12}}| g_j >$$
$$= \int_{R^3} exp(-(a_i + a_j)(r_{12x}^2 + r_{12y}^2 + r_{12z}^2)\frac{1}{r_{12}}dr_{12x}dr_{12y}dr_{12z}$$
$$= \frac{4\pi}{-2(a_i + a_j)} \int_0^\infty \frac{\partial}{\partial r_{12}} exp(-(a_i + a_j)r_{12}^2)r_{12}dr_{12}$$
$$= \frac{2\pi}{(a_i + a_j)}$$

With this potential, the ground state is found for spherical gaussians, although the evidence thereof is not relevant to show here, as it is essentially a preliminary test of a framework for a test of an approximation for a test of the final code.

3.1 Results

Once the preliminary tests were concluded, and the potential found, the code was set to work on the ground state and the first two excited states. The excited states were found by adding more gaussians to the already minimised basis containing the previous states, holding those not added constant, and only altering the added gaussians, such that the basis of gaussians of the second excited state contains both the gaussians for the first excited state and the ground state.
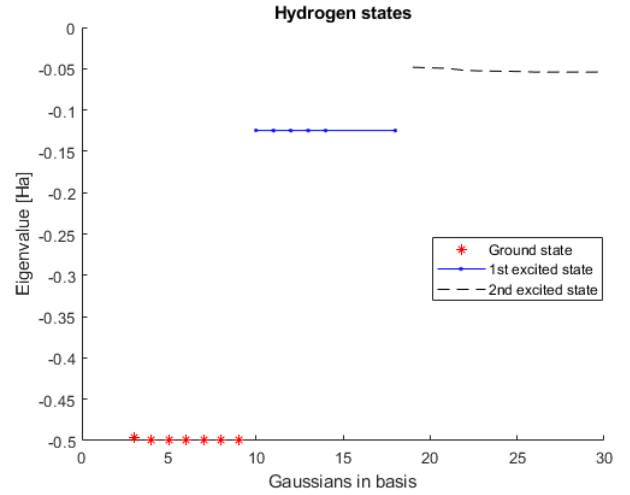

Figure 1: Convergence of the three lowest-lying hydrogen states.

In figure 1, one can see the energy levels. For a closer look, see the appendix. The convergence of the first state leads to an eigenvalue of $-0.4996\ Ha$, which is in good correspondence with the expected value of $-0.5\ Ha$, so our approximation can, at the very least replicate a ground state.

The second state at $-0.1248\ Ha$ is in fair correspondence with

the 2s state at $-0.1252\ Ha$, and the third state at $-0.054\ Ha$ corresponds well to the 3s state at $-0.056\ Ha$. The reason no p-states are considered, is that they deviate on about $10^{-7}\ Ha$, and that the gaussians do not allow for uneven parity, which those states have.

3.2   Partial conclusion

From all of this, we conclude that we have an adequate approximation of the coulomb-potential, and that two-body problems can readily be solved by the code.

4   Two-body interactions

What we take interest in here, is the emergence of a bound state from a transition to a quasi-2D system, of a two-body system of identical bosons of mass 1, that is otherwise at zero energy, with a gaussian interaction. This has been done before, and from [3], we acquire the interaction potential:

$$V(r) = -S \exp(-(r/b_{int})^2)$$
$$S = 2.684$$
$$b_{int} \doteq 1$$

where the width of this gaussian is the unit in relations to which we will compare every other length unit. The unit of energy is not denoted, it is an arbitrary energy unit that depends on what one chooses the length scale and the mass scale to be, as both the mass and length is unitless and arbitrary, so must it be. By having such a potential, the center of mass only goes into the kinetic energy operator, and separates trivially in Jacobi-coordinates, and is therefore readily disposed of.

4.1   The free case of mass-imbalance

In order to confirm that this system is indeed near resonance, the problem was solved with spherical gaussians, as the problem in the two-particle system then reduces to a spherical one. However, this has already been done in [?], and therefore another extreme case of interest was examined: The mass-imbalanced system. A system where one particle had the mass $m_1 = 100$, and the other had $m_2 = 1$, was looked upon, and therefore, as per the mass-scaling relations, the strength of the interaction was transformed to $S' = (\frac{1}{2})/(1/(1/100 + 1) * S = 1.35542$.
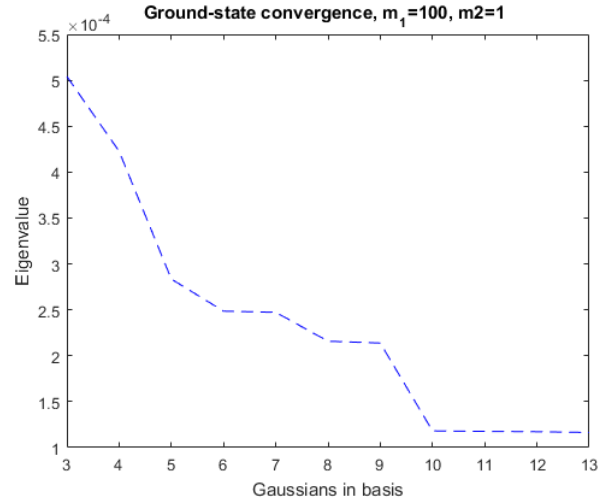
Figure 2: Convergence to the ground state for a mass-imbalanced system of two bosons with a gaussian interaction.

The result of the calculation is shown in figure 2, and is obviously very small, of a magnitude 10^{-4}, if the convergence is to be believed, and therefore the system is near resonance when free.

4.2   The squeezed identical case

In understanding the interplay between the two-body systems and the three-body system, we must calculate the squeezed spectrum of the two bosons, by applying an oscillator term to our Hamiltonian. Simply plotting the eigenvalue as a function of the width of the trap is insufficient, as actually squeezing a quantum state necessarily gives it more energy, so one might expect more sophisticated methods to be needed. Fortunately, one would be mistaken, and we can simply subtract the ground state of the harmonic oscillator from the system [4]. This ground state energy is, if one ensures that each particle has the same associated frequency, equal to the amount of particles,N, multiplied with the amount of directions in which one squeezes, multiplied with $\frac{1}{4\pi}h\omega$, where ω is the associated (angular) frequency, and h is Planck's constant. Of course, when one changes to appropriate coordinates, one can dispose of the center of mass, and in stead of subtracting N ground states, one only subtracts N-1, which, in the two-particle case, corresponds to only one ground state per direction.

The calculations were obtained by making a set of fully correlated gaussians with widths chosen to be around 2, and at $b_{osc} = 1$ and lower, selecting the affected diagonal components of the A-matrix from a distribution with mean b_{osc}, and keeping off-diagonal elements of the corresponding rows and columns to be equal to zero, thus effectively enforcing that the selection process would restrict particle motion in the corresponding direction. It is worth noting, that the smaller the oscillator width, the more difficult convergence becomes to obtain.
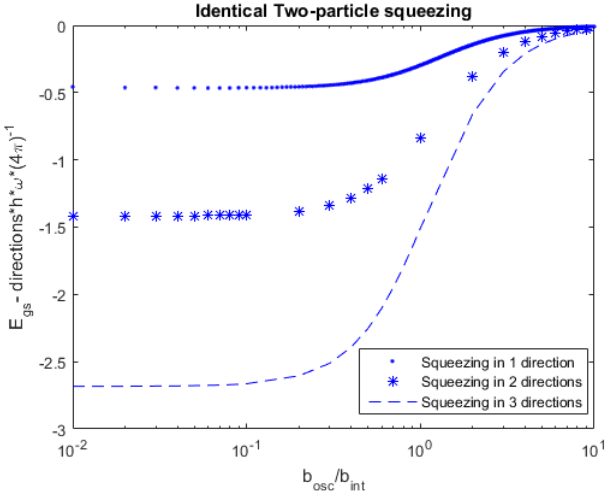
Figure 3: Ground state energies for squeezing in one, two and three directions for two identical bosons as a function of the width of the oscillator.

This is depicted in figure 3, and the first convergence to a minimum, by squeezing in a single direction, seems to be in fair correspondence with that produced by [3].

The plateaued energies are -0.4651 for the first plateau, -1.4170 for the second plateau, and -2.683 for the final plateau.

Of purely physical interest, however, are the following observations.

The first point is that they all converge to something very small for large widths, which is expected, as the particles are then effectively free.

The second point is that at a width of about $0.1\ b_{int}$, there appears to be the beginning of a plateau, and the system, apparently, no longer responds to changes of the trap's width. It would seem that a change to a different dimension is effectively obtained fully around this width.

The third is that, the more we confine a directional freedom, the more bound a system becomes.

The fourth point is that this system, when confined to a single point, seems to have an energy that is very close to its potential's strength.

The final point is that this figure is easily convertible to systems of other reduced masses if the center of mass separates.

Due to the harmonic oscillator's amplitude and frequency being written as

$$\frac{1}{2}\mu\omega^2 = \frac{2\hbar^2}{\mu b_{osc}^4}$$
$$\omega = \frac{2\hbar}{\mu b_{osc}^2}$$

the potential, for a constant oscillator-width, satisfies the scaling relations of the mass that were previously mentioned, and therefore $E'_{gs} = \frac{1}{2\mu'}E_{gs}$ for a different system. Similarly, the ground state of the oscillator, which we subtract from E_{gs} to get the figure, also have a $1/\mu$ dependency for a constant

width, and scales accordingly, meaning that if one finds another two-body system where the center of mass disconnects in the harmonic oscillator, or wants to scale the masses of the particles with some number, one simply has to divide these energies with twice that number to reproduce the squeezing spectra.

5 Helium

In order to test the code's capabilities with three particles, the helium atom's ground state and first excited state was calculated. This was done with fully correlated gaussians, by selecting the diagonal widths of the A-matrices pre-scramble from a distribution with average width of $3\ a_0$, setting the unit of mass equal to that of the electron, and choosing the nucleus mass of ^4He. By utilising the coulomb potential's expansion in gaussians, as found earlier, some deviation from the actual values were expected, but not by a lot. What matters the most, of course, is the ground state's value, as the precision of excited state relies somewhat on its minimisation, as calculating power is a limited commodity, and as the object is to test the method's and the code's capabilities. The excited state was built on the first 115 gaussians of the ground state.

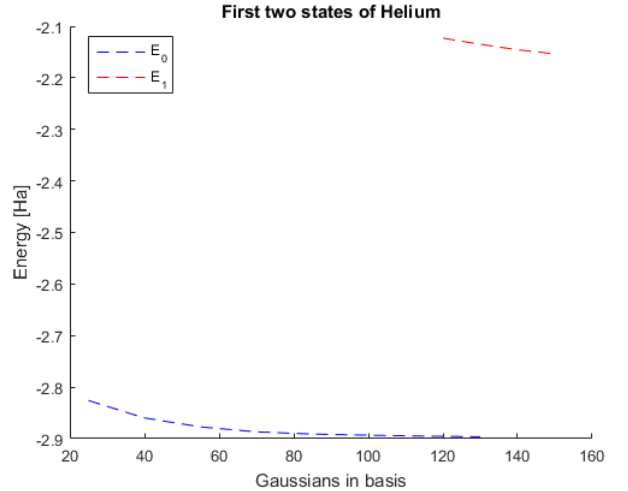The results can be seen on figure 4. For an individual look at the figures, see the appendix.

Figure 4: Convergence of the two lowest states in helium against gaussians in the basis.

The ground state converged slowly, but eventually reached $-2.8963\ Ha$, having dropped 0.001 over the last 15 gaussians, which is fairly close to the expected result of the 1s1s-state's energy of $-2.9034\ Ha$, and gives us an adequate precision.

Similarly, although only four datapoints had been taken on the excited state before time demanded we moved on, it reached $-2.1535\ Ha$, with the final drop over ten gaussians was $0.013\ Ha$, which is also fairly close to the expected value of $-2.1750\ Ha$ of the 1s2s, and these combined thus stand as a

proof that the code, and method, can calculate the eigenvalues
of relevant quantum systems of an acceptable precision.

6   Three-boson interactions

After having made a convenient set of tests for the program in the form of calculating helium states, the matter of interest is at hand - the three-body interactions. At first, the ground states of the free three-body systems were calculated in a similar fashion to the helium atom, by building the matrices from the w_{ij} vectors. The identical particles seemed to converge faster, when its diagonal was chosen with a mean of 3 b_{int}, while the mass-imbalanced system of $m_1 = 1$, $m_2 = m_3 = 100$ preferred widths of 2 b_{int} on average. The steps taken in the amount of gaussians are not always consistent, and are certainly not one by one, as this would amount to a massive computation time, as these calculations were run at 2000 rounds per gaussian over 7 sweeps before each increment of the basis. No excited bound state could be found for the identical bosons, but several were visible when calculating the mass-imbalanced system. This is suspected to be a remnant of the efimov effect, as the value of $|s_0|$ is about equal to 4.061 for $M/m = 100$, giving a scale factor of about $\lambda^2 \approx 4.69$, rather than $\lambda^2 \approx 515.29$ for the identical bosons. The amplitude of the interaction potential was also re-scaled per the mass-scaling relations obtained earlier, to ensure the resonance of the sub-systems in three dimensions.
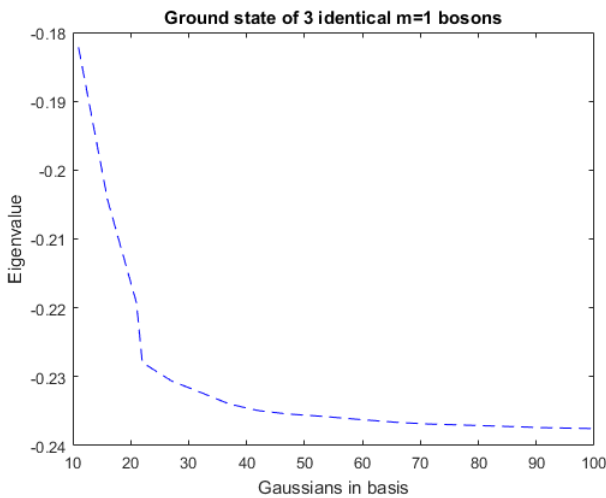
6.1   No squeezing

Figure 5: Convergence of the ground state of identical particles to an eigenvalue of -0.2375.

On figure 5, the convergence towards the ground state for the identical, un-squeezed bosons is plotted against the amount of gaussians in the basis. The ground state was found to be -0.2375, changing with 10^{-4} over the last 10 gaussians.

The convergence towards the ground state can be seen on figure 6, and amounts to a value of -0.1810, which, surprisingly, is less tightly bound than the identical bosons, changing with

$4 * 10^-5$ over the last 15 gaussians.
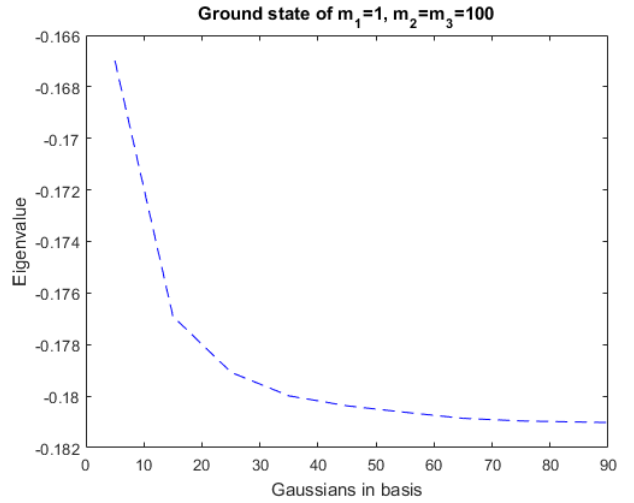These are very accurate results, and are thus stated confidently.

Figure 6: Convergence of the ground state of mass-imbalanced bosons to an eigenvalue of -0.1810.

First excited state of mass-imbalanced system

The excited states, however, are more time consuming, and usually more difficult to obtain good convergence for. An argument is that one should build atop the already minimised gaussians for the ground state, as the lowest eigenvalue sets a hard barrier for the second lowest, since it must necessarily be smaller, and sure enough, unsuccessful attempts were made towards convergence of an excited state from nothing. A stepping stone is without a doubt needed. Therefore, this approach was chosen, in which a basis was built upon 90 gaussians, and then supplied with further 15, and then went in steps of 10 gaussians to 195.
The results can be seen on figures 7.
It has converged to a final value of -0.0790 while varying with 10^{-4} over the last 10 gaussians, so the accuracy seems to be satisfactory. We note that this excited state could hypothetically be dictated solely from the properties of the potential, but still has a ratio relative to the ground state, corresponding to a scaling factor of $\lambda = 1.58$.

Again, we can with a fair certainty express a confidence in the results, based on the final deviations.
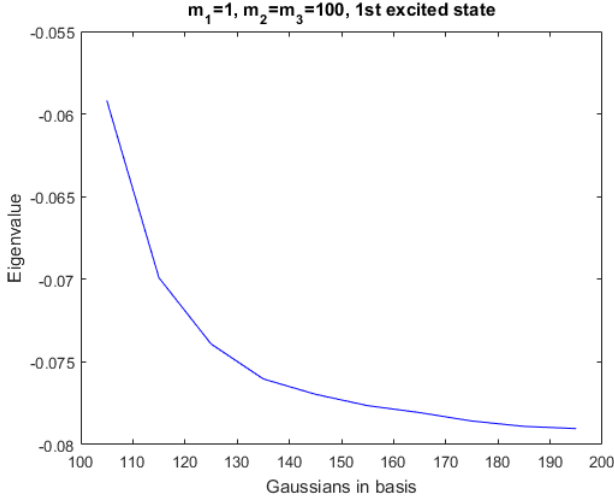
Figure 7: Convergence of the first excited state of mass-imbalanced bosons, built on top of the entire ground state, converging to an eigenvalue of -0.0790.
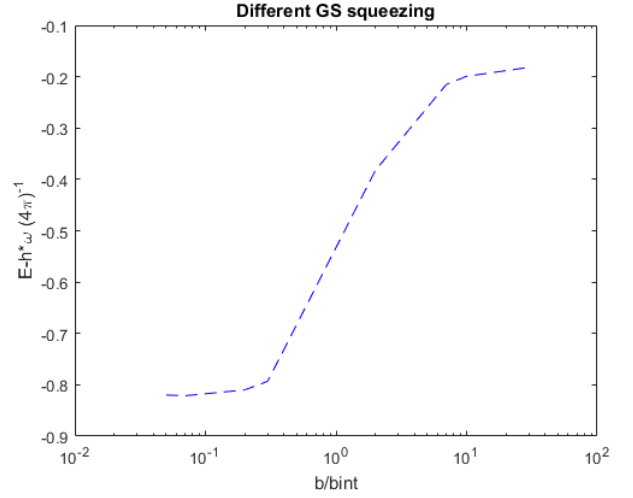

Figure 8: Squeezing of the mass-imbalanced three-body system to a pancake with a 2D value of -8.1990, and a value at $b_{osc} = 30$ b_{int} at -0.1820.

6.2   Squeezed mass-imbalanced three-body states

Having found the ground states, the first excited state of the mass-imbalanced system, and their associated widths in three dimensions, it is interesting to replicate a three-body equivalent to the two-body squeezing presented earlier. However, due to restrictions in time, only squeezing in a single direction has been an option. Inferring that the center of mass must disconnect when squeezing the mass-imbalanced system by enforcing a mass-specific harmonic trap, there has been created a corresponding spectrum for the ground state of the mass-imbalanced system, shown in figure 8 as a function of the oscillator width for the distance between particle 1 and 2. We remind the reader that not every vector feels the same width in this case, but the same frequency. Similarly to the two-body case, each datapoint below 0.5 had its A-matrices confined in the direction of the trap, and each above it had permitted motion. Initially, each was calculated with 75 gaussians in a for-loop, after which convergence was checked to make sure they were usable, and further gaussians were added where needed. The range of b_{osc}/b_{int} spans from 0.04 to 30, and has end-point values of -8.199 and -0.1820 respectively.

It appears from the figure that the system plateaus rather abruptly, but this may be an artefact of the amount of data-points.

Discussion of sub-systematic impacts

What is of high interest in this case, is that there are two kinds of two-body systems being squeezed here. Around 0.04, the two identical particles of mass 1 have an energy of -0.4651. If one swiftly considers that one could just as easily have chosen another coordinate system, in which one's Jacobi-coordinates had the distance vector between particle 2 and 3 on its first entry, we also understand that this system would necessarily have the same associated frequency, as it, as shown, separates as a front factor to the corresponding matrix in the calculation of the matrix element, and the system would then satisfy the aforementioned relation:

$$b_{23} = \sqrt{\mu_{12}/\mu_{23}} b_{12}$$
$$= \sqrt{\frac{2/100}{1/100 + 1}} 0.04 \ b_{int}$$
$$\approx 0.006 \ b_{int}$$

The 100-100-subsystem has already plateaued at this point, in fact, it did so around $b_{12} = 0.7$. However, we also understand that this goes unnoticed, as the energy it ends on satisfies the mass-scaling relations, and is quite small $E_{23} = \frac{1}{100}E_{identical}$, whereas the different-mass system plateaus at $E_{12} = 0.505 E_{identical}$.
This is also reflected in the place that the curve reaches its minimum. Had the heavy systems of equal mass been the source of a lowering of the binding energy, its plateau would come far further to the right.

6.3   Squeezed identical three-body system

Although not satisfying any scaling relations that do not affect all the masses equally, the squeezed spectrum for three identical bosons of unit mass is still a fairly interesting figure to present. As with the mass-imbalanced system, a for-loop was initiated for each datapoint, calculating 75 fully correlated, un-shifted gaussians, and adjusting and adding in gaussians where necessary. However, of further interest was the behaviour of the excited states near the crossing of the two-body threshold.

The squeezed ground state of the three- and two-body systems of identical particles are plotted against the width of the trap as experienced by the two-body sub-systems, along with a few points of the first excited state, which became visibly bound during the squeezing, at figure 9. The excited datapoints were calculated one by one by building on top of the ground states, as this, in the previous section, seemed to allow for a higher precision, in spite of taking a lot of time.

The final result is seen on figure 9, and the spectrum relative to the two-body spectrum is plotted at figure 10.
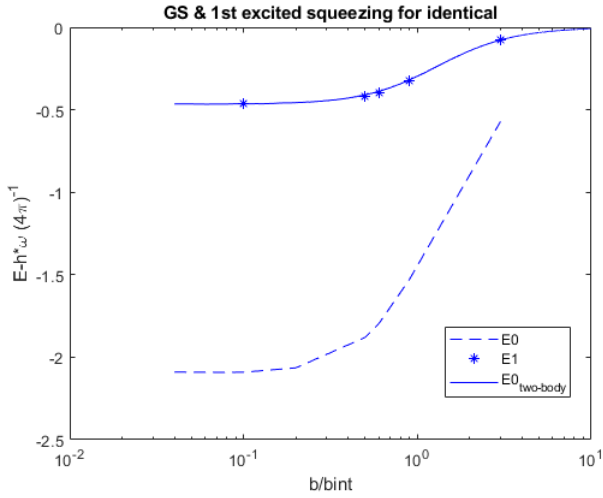

Figure 9: The ground state and first excited state of the squeezed identical mass three-body system along with the two-body spectrum against the width of the trap
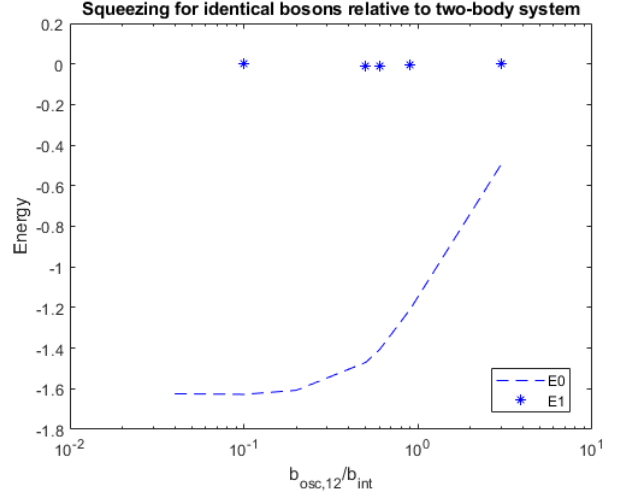

Figure 10: The ground and first excited state of the squeezed three-body system with the two-body spectrum subtracted, against the width of the trap.

As is apparent from figure 8 and, in part, 9, the three-body states unsurprisingly converge to their three-dimensional equivalents for large b_{osc}. The convergence for identical bosons reached a minimum of -1.628.

6.4   Discussion of the squeezed states

The precision of the datapoints of the first excited state is varying, and varied with as much as -0.0064 on the last 30 gaussians from 205 to 235 gaussians on the datapoint at 0.1, and as little as 10^{-4} for the last $7 * 10^{-4}$ over the last 20 from 185 to 205 gaussians on the point at 0.9 for the excited state, but nonetheless, it seems it is as precise as it is going to get within reasonable computational hours.

The theory has mentioned that the ground state and the first excited state of the efimov spectrum would both be pushed down relative to the two-body system when squeezed to such a quasi-2D configuration [4], and the same appears to be true for these states as well, although the first excited state is very close to the threshold, lying about 0.008 below the threshold at best. Interestingly enough, the mass-imbalanced system starts out at a higher energy, but ends up at a lower energy than the identical boson system.

7 In conclusion

We have presented the reader with a theory about few-body states, their behaviour when squeezed, and a method to solve this. The method, when compared to other methods, for instance calculating with only spherical gaussians, allows the basis functions a high enough degree of malleability to adequately approximate both hydrogen and helium states, although the results in those sections may as well be due to an imperfection in the approximation of the potential as it could be due to an adequacy of the code.

Nonetheless, we have shown you the first three even parity states of hydrogen, approximated to $-0.4996\ Ha$, $-0.1248\ Ha$, and $-0.054\ Ha$, which are all within reasonable parameters, we have shown you the ground state of the mass-imbalanced system, along with a squeezed spectrum in every direction for the identical boson system, the monodirectional squeezing being in reasonable correspondence with earlier presented values [3], at the plateaued energies -0.4651, -1.4170 and -2.683 for one-, two- and three-directional squeezing, we have shown you the two lowest helium states of even parity, approximated to $-2.8936\ Ha$ and $-2.1535\ Ha$, against the expected $-2.9034\ Ha$ and $-2.1750\ Ha$, leaving the ground state in good correspondence with the expectations, and finally we have shown you three-body systems of mass-imbalanced and identical bosons with their sub-systems initially at resonance. The ground state of the identical bosons fell to -0.2375 with a deviation of 10^{-4} over the last 10 gaussians in a set of 100 gaussians, and the ground state of the mass-imbalanced system fell to a groun state of -0.1810, deviating with $4*10^{-5}$ over the last 15 gaussians in a set of 90. Some might remark on the surprise that the latter is more weakly bound than the former, but it is unsurprising as two of the three interaction stengths are approximately unchanged, while the last is reduced by quite a deal as per the mass-scaling relations, in order to keep the sub-systems at resonance, so this result is also in favour of us having found an accurate ground state. The first excited bound state of the identical boson system could not be found, but that from the mass-imbalanced system was. Its convergence reached -0.0790, deviating with 10^{-4} over the last 10 gaussians, having been built on top of 95 gaussians. The squeezed three-body spectra yielded expected results in terms of convergence to their three-dimensional counterparts in the case of wide traps, although a very wide trap is necessary to prove it in the case of the mass-imbalanced system, as one sub-system experiences a width that is 0.141 times the size of the other two. For that of the identical bosons, we can technically present no data on the convergence, as the calculations were deemed to not have reached their minimal eigenvalues, and focus was placed on the excited state in stead. The identical squeezed spectrum seemed to reach minimum at -2.091, while the mass-imbalanced system reached one at -8.1990, being significantly more tightly bound than the identical system. When compared to the two-body threshold, above which lies a continuum of states for a set of bound two-body systems plus a single free particle, the three-body spectrum's ground state does not seem to change its form, while the first excite state is heavily affected, but both are still pushed down relative to the two-body threshold, even if it's just by -0.008, which is in correspondence to the expected result from [4].

Knowing that articles are being written about using shifted gaussians in stead of fully correlated gaussians, one must comment on the usefulness of the method. For now, fully correlated gaussians seem to be functional in solving various three-body problems.

8   Appendix: Hydrogen

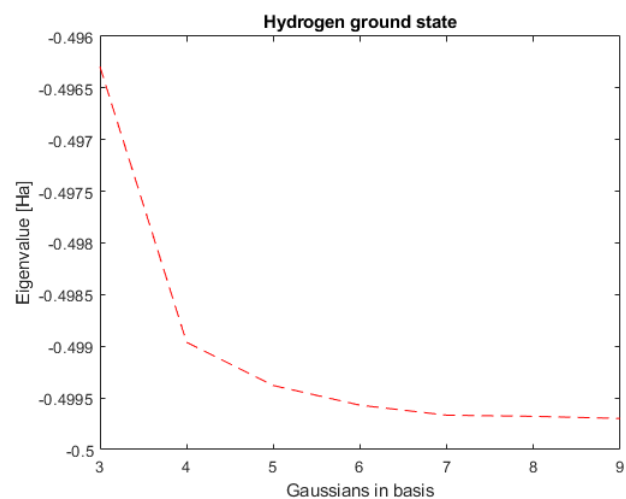We here present the convergence for the first three even parity
states of hydrogen.

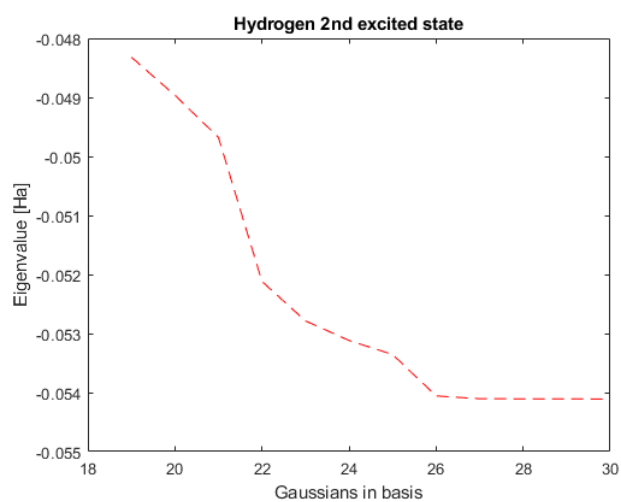Figure 11: Convergence of the lowest lying hydrogen state, the
1s

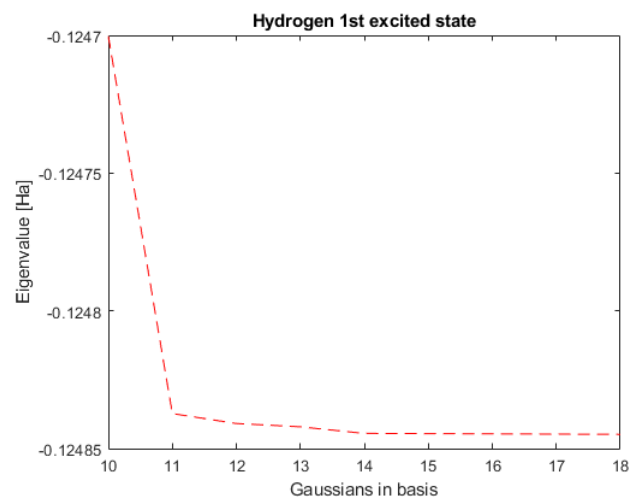Figure 13: Convergence of the second excited state, correspond-
ing to a 3s

Figure 12: Convergence of the first excited state, corresponding
to a 2s

9 Appendix: Helium

We here present the convergence for the first two even parity states of Helium.

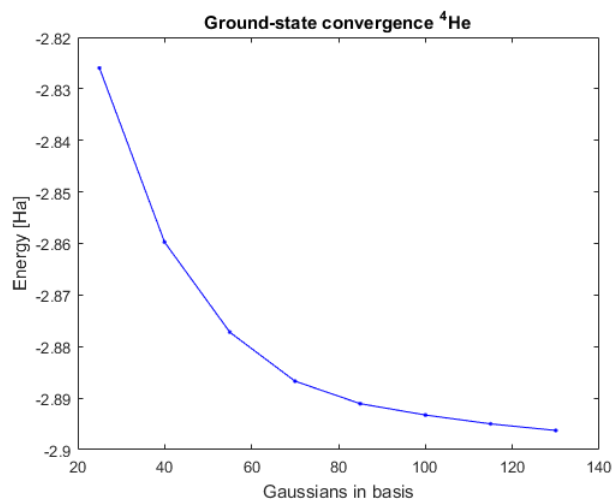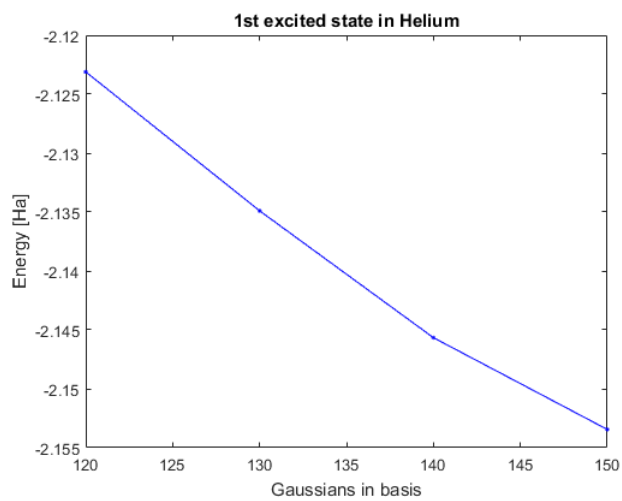Figure 14: Convergence of the ground state of Helium

Figure 15: Convergence of the first excited state of Helium

Bibliography

[1] *Yasuyuki Suzuki & Kálmán Varga, 2011, "Stochastic Variational approach to Quantum-Mechanical Few-body problems", pp. 11*

[2] *Dmitri Vladimir Fedorov, 9 November 2017, "Correlated Gaussian method in Quantum Mechanics"* `https://en.wikibooks.org/wiki/Correlated_Gaussian_method_in_Quantum_Mechanics`

[3] *Frederik Skovbo, 2017, "BOUND STATES IN CROSSOVER FROM THREE TO TWO DIMENSIONS USING FULLY CORRELATED GAUSSIAN BASIS"*

[4] *P. Naudon, S. Endo, 2016, "Efimov Physics: A review", arXiv:1610.09805* `https://arxiv.org/abs/1610.09805`

[5] *J.E. Sansonetti, W.C. Martin, and S.L. Young (2005), Handbook of Basic Atomic Spectroscopic Data (version 1.1.2). [Online], [2018, June 1]. National Institute of Standards and Technology, Gaithersburg, MD.* `http://physics.nist.gov/Handbook`

[6] *Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team. "NIST Atomic Spectra Database Ionization Energies Data". Gaithersburg, MD: NIST.* `https://physics.nist.gov/PhysRefData/ASD/ionEnergy.html`