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Variational resolution of the bound states problem of a non-relativistic five-body quantum system

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Ψ	Wave function
E	Energy
H	Hamiltonian operator
i	Imaginary number
h	Planck constant
$\hbar$	Reduced Planck constant
$\hat{H}_r$	Hamiltonian relative operator
$R_{n,l}$	Radial wave function
Δ	Laplace operator
$\overrightarrow{P}_i$	Momentum operator of particle the ith particle
$\overrightarrow{r}_i$	Coordinate vector of particles i
$d_{\wp}$	Probability of presence
$\overrightarrow{R}$	Center of mass vector
V	Potential energy
t	Time
m_i	Mass of i^{th} particle
$\mathbf{M}$	Total mass of the system
$\hat{T}$	kinetic energy operator
$\overrightarrow{\rho}$	Jacobi coordinates
k_{ij}	Coupling constant
μ, μ_ρ	Reduced mass
$E_{0var}^{(N)}$	Upper bound for the ground energy for N-body system
E_{exact}	Exact energy of the system

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Dedication

To the gleaming handles of my life, my parents.

To my little family, my wife and children.

To my honorable teacher Dr. Kh. Boudjemaa

To all my friends.

Introduction

The study of the properties of interacting non relativistic quantum few-body systems is one of the most active branches of modern theoretical physics. The dynamics of such systems is governed by the few-body Schrödinger equation. Due to the large number of degrees of freedom involved and the nature of the interactions between particles, the equations of motion of these systems are not exactly solvable in most cases. Even the one-body problem for a rotationally invariant potential or the two-body problem in translationally and rotationally invariant interaction are solvable only for very particular forms of the interaction potential [1]. The complexity of the problem grows exponentially with the number of particles. The one-body and two-body problems are said to be trivial, while the three-body problem is considered as the simplest non-trivial problem and does not admit exact solutions even in classical mechanics. In all these cases, it is necessary to resort to approximate resolution methods. Among these methods, let us mention the expansion on hyperspherical harmonics [2], Faddeev's equations [3], derivation of upper bounds by systematic expansion on correlated gaussians [4], derivation of lower bounds [5].

In the work presented in this thesis, we are interested in the approximate solution of the stationary Schrödinger equation for spinless five-body system applying the variational principle. We use an expansion over correlated gaussians to derive upper bounds for the ground state energy and the associated wave function of a five-body system for certain mass configurations and which is an extension of a similar earlier study carried out for the three-body [6] and the four-body [7] cases.

This document is organized as follows:

The first chapter constitutes a review on the basic notions of quantum mechanics where we

present the stationary Schrödinger equation which describes the time-independent states of a particle. Particular attention has been paid to problems of central forces where it is shown that the problem of two mutually interacting particles reduces to the problem of a one-dimensional particle.

Chapter two will be devoted to an exactly solvable quantum problem. This is about the harmonic oscillator. We present the study of one-dimensional and three-dimensional harmonic oscillators in a quantum framework. The resolution of the two-body harmonic oscillator will also be presented in detail.

In the third chapter, we will focus on the few-body problem interacting via two-body forces deriving from harmonic potentials. This type of systems is often called "N-body harmonic oscillator". We are particularly interested in the five-body problem. The method adopted to solve this problem is based on changes of variables thus making it possible to reduce the problem of the five-body harmonic oscillator to a set of four decoupled harmonic oscillators where the energy of the system will be the sum of the energies of these oscillators.

The main objective of our work will be the subject of the fourth chapter.We will present in detail the method of expansion on correlated gaussians applied to five-body systems, which is a method based on the variational principle. This method will allow us to obtain an approximation of the energy and the wave function of a system composed of five particles interacting via two-body forces.

The thesis ends with a general conclusion.

Chapter 1

Schrödinger equation

In physics, specifically quantum mechanics, the Schrödinger equation, formulated in 1926 by Austrian physicist Erwin Schrodinger, is an equation that describes the time-evolution of a quantum system. It is as central to quantum mechanics as Newton's laws are to classical mechanics.

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi \quad . \tag{1.1}$$

In the standard interpretation of quantum mechanics, the quantum state, also called a wave function or state vector, is the most complete description that can be given to a physical system. Solution to Schrödinger's equation describe not only molecular, atomic and subatomic systems, but also macroscopic systems, possibly even the whole universe [8].

The most general form is the time-dependent Schrödinger equation, which gives a description of system evolving with time. For systems in a stationary state, the time-independent Schrödinger equation is suffisent. Approximate solutions to the time-independent Schrödinger equation are commonly used to calculate the energy levels and other properties of atoms and molecules.

Schrödinger's equation can be mathematically transformed into Werner Heisenberg's matrix mechanics, and into Richard Feynman's path integral formulation. The following section presents the Schrödinger equation for the general case and for the simple case encountered in many textbooks.

1.1 General quantum system

For a general quantum system [9].

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi \quad , \tag{1.2}$$

where

- Ψ is a wave function: the probability amplitude for different configurations of the system at different times.
- $i\hbar\frac{\partial}{\partial t}$ is the energy operator (i is the imaginary unit and $\hbar$ is the reduced Planck constant).
- $\hat{H}$ is the Hamiltonian operator.

1.2 Single particle in a potential

For a single particle with potential energy V in position space, the Schrödinger equation takes the form [10].

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) &= \hat{H}\Psi \ , \\ &= \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\Psi(\vec{r},t). \end{aligned} \tag{1.3}$$

where

- $\frac{-\hbar^2}{2m}\nabla^2$ is the kinetic energy operator, where m is the mass of the particle.
- $\nabla^2 = \Delta$ is the laplace operator. In three dimensions, the laplace operator is

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \ . \tag{1.4}$$

  where x, y and z are the cartesian coordinates of space.
- $V(\vec{r},t)$ is the time-independent potential energy at the position $\vec{r}$.
- $\Psi(\vec{r},t)$ is the probability amplitudefor the paticle to be found at position $\vec{r}$ at time t.
- $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)$ is the hamiltonian operator for a single particle in a potential.

1.3 Time independent or stationary equation

When the potential energy is constant in time ($V(\vec{r},t) = V(\vec{r})$) we can simplify the wave equation. We assume that the spatial and time dependencies of the solution can be separated:

$$\Psi(\vec{r},t) = \psi(\vec{r})e^{-i\frac{E}{\hbar}t}$$

The time independent equation, again for a single particle with potential energy V takes the form [11].

$$E\psi(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}), \tag{1.5}$$

This equation describes the standing wave solutions of the time-dependent equation, which are the states with definite energy. The time-independent Schrodinger equation is used for a number of practical problems. Systems with bound states are related to the quantum mechanical "particle in a box", barrier penetration is important in radioactive decay, and the quantum mechanical oscillator is applicable to molecular vibrational modes.

1.3.1 Derivation

Schrödinger's equation can be derived in the following short heuristic way. It should be noted that Schrödinger's wave equation was a result of the ingenious mathematical intuition of Erwin Schrodinger, and cannot be derived independently.

Assumption

1. The total energy E of a particle is

$$E = T + V = \frac{p^2}{2m} + V \ , \tag{1.6}$$

2. Einstein's ligth quanta hypothesis,

$$E = h\upsilon \ . \tag{1.7}$$

3. The de Broglie hypothesis ,

$$p = \frac{h}{\lambda} = \hbar k \ . \tag{1.8}$$

Expressing p and k as vectors, we have

$$\vec{p} = \hbar\vec{k} \ , \tag{1.9}$$

1.3.2 Wave function

The solutions of the Schrödinger equation of a quantum system are called wave functions, they can be considered as a quantum postulate which describes the quantum state of a particle and contains all the information one wants to know about the system [13]. This wave has a probabilistic interpretation [14], the square of the wave function defines the probability dP of finding the quantum object at the desired time in a given place characterized by an elementary volume $d^3\overrightarrow{r}$:

$$dP = |\Psi(\overrightarrow{r}, t)|^2 \, d^3\overrightarrow{r} \ . \tag{1.10}$$

As we have seen that the Schrödinger equation is a partial differential equation of the first order with respect to time and of the second order with respect to spatial coordinates, it is therfore a difficult equation to solve for most quantum systems.

1.3.3 Case of central forces

The central force problems are a generic class of three-dimensional physical systems. They are systems that have a central potential, i.e. a potential energy that depends only on the distance, $r = ||\overrightarrow{r}||$, from the origin: $V(\overrightarrow{r}) = V(r)$. If we use spherical coordinates to parametrize our three-dimensional space, a central potential does not depend on the angular variables θ and φ.

We consider a particle of mass m and at position vector $\overrightarrow{r}$ in a central potential $V(r)$, In quantum mechanics, it is about finding solutions to the eigenvalue equation

$$H\psi = E\psi.$$

H is the hamiltonian operator,

$$H = -\frac{\hbar^2}{2m}\Delta + V(r) \ , \tag{1.11}$$

associated to the energy E of the particle.

Because of the central potential, the spherical coordinates are more adapted: radial coordinate, $r \in [0, \infty]$ and two angular coordinates $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$.

The laplacien Δ is written in the spherical coordinates:

$$\Delta = \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) - \frac{L^2}{\hbar^2 r^2} \right) , \tag{1.12}$$

with

$$L^2 = \hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} (\sin\theta \frac{\partial}{\partial \theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right] . \tag{1.13}$$

L represents the operator of cinematic orbital momentum. The Hamiltonian is written as

$$H = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{L^2}{2mr^2} + V(r) . \tag{1.14}$$

So in spherical coordinates the Schrödinger equation takes the form:

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{L^2}{2mr^2} + V(r) \right] \Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi) . \tag{1.15}$$

1.3.4 Separation of variables

The expression eq. (1.14) shows that all the dependence in θ and ϕ is inclused in the operator L^2 and:

$$\left[H, L^2 \right] = 0 \text{ and } [H, L_z] = 0 . \tag{1.16}$$

The obsarvables H, L^2 and L_z constitute a complete set of commuting observables [15], thus we get:

$$\begin{aligned} H\Psi(r, \theta, \phi) &= E\Psi(r, \theta, \phi) , \\ L^2\Psi(r, \theta, \phi) &= l(l+1)\hbar^2\Psi(r, \theta, \phi) , \\ L_z\Psi(r, \theta, \phi) &= m\hbar\Psi(r, \theta, \phi) . \end{aligned} \tag{1.17}$$

The common eigenfunctions L^2 and L_z which correspond to fixed values l and m are the spherical harmonics $Y_m^l(\theta, \phi)$ the function $\Psi(r, \theta, \phi)$ will be the product of radial function $R(r)$

and the spherical harmonics $Y_m^l(\theta,\phi)$:

$$\Psi(r,\theta,\phi) = R(r)Y_m^l(\theta,\phi)\ . \tag{1.18}$$

By using the fact that:

$$\begin{aligned} L^2\Psi(r,\theta,\phi) &= L^2R(r)Y_m^l(r,\theta,\phi)\ , \\ &= l(l+1)\hbar^2R(r)Y_m^l(\theta,\phi)\ , \end{aligned} \tag{1.19}$$

We end to the radial equation:

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]R(r) = ER(r) \tag{1.20}$$

or

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2m}{\hbar^2}(E - V(r)) - \frac{l(l+1)\hbar^2}{2mr^2}\right]R(r) = 0\ . \tag{1.21}$$

In literature, the solution of the radial Schrödinger equation was found in some physical systems as hydrogen atom (colombian potential), harmonic oscillator,..., while the most different types of potentials will be solved by numerical methods (Euler method, Hann...) or by approximate methods (method of the perturbation and variationnal) [16].

1.4 Two body problem

It is one of the most important samples in physics because it is related to the conversation of energy, moreover to be able to analytically solve the equations of motion of non-relativistic two particles system of respectively masses m_1 and m_2 with designated position by position vectors $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$ of components x_1, y_1, z_1 and x_2, y_2, z_2 respectively we define the relative position $\overrightarrow{r}$,

$$\overrightarrow{r} = \overrightarrow{r}_1 - \overrightarrow{r}_2\ , \tag{1.22}$$

of which the component are:

$$\begin{aligned} x &= x_1 - x_2 \quad , \\ y &= y_1 - y_2 \quad , \\ z &= z_1 - z_2 \quad . \end{aligned} \tag{1.23}$$

Suppose that the two particles interact via the potential $V(r)$ which only depends on the distance, $r = \|\overrightarrow{r}\|$, between them.

The kinetic energy T is

$$T = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_1}\Delta_2 \quad , \tag{1.24}$$

where Δ_1 and Δ_2 are the laplacians with respective coordinates of each particle.

The Hamiltonian operator of this system is then written as

$$\hat{H} = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_1}\Delta_2 + V(r) \ . \tag{1.25}$$

Let's introduce the center of mass vector $\overrightarrow{R}$ defined by:

$$(m_1 + m_2)\overrightarrow{R} = m_1 \overrightarrow{r}_1 + m_2 \overrightarrow{r}_2 \quad . \tag{1.26}$$

The components of $\overrightarrow{R}$ are:

$$\begin{aligned} X &= \frac{m_1}{m_1 + m_2}x_1 + \frac{m_2}{m_1 + m_2}x_2 \ , \\ Y &= \frac{m_1}{m_1 + m_2}y_1 + \frac{m_2}{m_1 + m_2}y_2 \ , \\ Z &= \frac{m_1}{m_1 + m_2}z_1 + \frac{m_2}{m_1 + m_2}z_2 \ . \end{aligned} \tag{1.27}$$

Let us now try to express the Laplacians which appear in the hamiltonian eq. (1.25) in terms of the new variables x, y, z eq. (1.23) and X, Y, Z eq. (1.27).

Let f be a function of two variables $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$ (in fact it is a six-variable function, one for each component of the vectors), and let a second function g of the variables $\overrightarrow{r}$ and $\overrightarrow{R}$ describing the same physical quantity A :

$$A = f(\overrightarrow{r}_1, \overrightarrow{r}_2) = g(\overrightarrow{r}, \overrightarrow{R}) \ . \tag{1.28}$$

The differential of A is written as:

$$dA = df(r_1, r_2) = \frac{df}{dx_1}dx_1 + \frac{df}{dy_1}dy_1 + \frac{df}{dz_1}dz_1 + \frac{df}{dx_2}dx_2 + \frac{df}{dy_2}dy_2 + \frac{df}{dz_2}dz_2 \ , \tag{1.29}$$

if we adopt as variables the vectors $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$, and

$$dA = dg(r, R) = \frac{dg}{dx}dx + \frac{dg}{dy}dy + \frac{dg}{dz}dz + \frac{df}{dX}dX + \frac{df}{dY}dY + \frac{df}{dZ}dZ \ , \tag{1.30}$$

with the variables $\overrightarrow{r}$ and $\overrightarrow{R}$. Using the fact that:

$$\begin{aligned} dx &= x_1 - x_2 \ , \\ dy &= y_1 - y_2 \ , \\ dz &= z_1 - z_2 \ , \end{aligned} \tag{1.31}$$

and

$$\begin{aligned} dX &= \frac{m_1}{m_1+m_2}dx_1 + \frac{m_2}{m_1+m_2}dx_2 \ , \\ dY &= \frac{m_1}{m_1+m_2}dy_1 + \frac{m_2}{m_1+m_2}dy_2 \ , \\ dZ &= \frac{m_1}{m_1+m_2}dz_1 + \frac{m_2}{m_1+m_2}dz_2 \ , \end{aligned} \tag{1.32}$$

one can derive the components of Nabla vectors $\vec{\nabla}_1$ and $\vec{\nabla}_2$ as function of partial derivatives with respect to the components of the relative vector $\overrightarrow{r}$ and those of the center of mass vector $\overrightarrow{R}$:

$$\begin{aligned} \frac{\partial}{\partial x_1} &= \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X} + \frac{\partial}{\partial x}, & \frac{\partial}{\partial x_2} &= \frac{m_2}{m_1+m_2}\frac{\partial}{\partial X} - \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y_1} &= \frac{m_1}{m_1+m_2}\frac{\partial}{\partial Y} + \frac{\partial}{\partial y}, & \frac{\partial}{\partial y_2} &= \frac{m_2}{m_1+m_2}\frac{\partial}{\partial Y} - \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z_1} &= \frac{m_1}{m_1+m_2}\frac{\partial}{\partial Z} + \frac{\partial}{\partial z}, & \frac{\partial}{\partial z_2} &= \frac{m_2}{m_1+m_2}\frac{\partial}{\partial Z} - \frac{\partial}{\partial z}. \end{aligned}$$

The second derivatives are easly deducted:

$$\begin{aligned} \frac{\partial^2}{\partial x_1^2} &= \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x^2} + \frac{2m_1}{m_1+m_2}\frac{\partial}{\partial x}\frac{\partial}{\partial X} \quad , \quad \frac{\partial^2}{\partial x_2^2} = \left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x^2} - \frac{2m_2}{m_1+m_2}\frac{\partial}{\partial x}\frac{\partial}{\partial X} \\ \frac{\partial^2}{\partial y_1^2} &= \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial y^2} + \frac{2m_1}{m_1+m_2}\frac{\partial}{\partial y}\frac{\partial}{\partial Y} \quad , \quad \frac{\partial^2}{\partial y_2^2} = \left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial y^2} - \frac{2m_2}{m_1+m_2}\frac{\partial}{\partial y}\frac{\partial}{\partial Y} \\ \frac{\partial^2}{\partial z_1^2} &= \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial Z^2} + \frac{\partial^2}{\partial z^2} + \frac{2m_1}{m_1+m_2}\frac{\partial}{\partial z}\frac{\partial}{\partial Z} \quad , \quad \frac{\partial^2}{\partial z_2^2} = \left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial Z^2} + \frac{\partial^2}{\partial z^2} - \frac{2m_2}{m_1+m_2}\frac{\partial}{\partial z}\frac{\partial}{\partial Z}, \end{aligned}$$

where we have used the fact that: $\frac{\partial}{\partial\alpha}\frac{\partial}{\partial\beta} = \frac{\partial}{\partial\beta}\frac{\partial}{\partial\alpha}$. The expressions of the Laplacian Δ_1 and Δ_2 can be simplified as follows:

$$\begin{aligned}
\Delta_1 = &\ \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2}, \\
= &\ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + \left(\frac{m_1}{m_1+m_2}\right)^2 \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right) \\
&+\frac{2m_1}{m_1+m_2}\left(\frac{\partial}{\partial x}\frac{\partial}{\partial X} + \frac{\partial}{\partial y}\frac{\partial}{\partial Y} + \frac{\partial}{\partial z}\frac{\partial}{\partial Z}\right), \\
\Delta_2 = &\ \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}, \\
= &\ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + \left(\frac{m_2}{m_1+m_2}\right)^2 \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right) \\
&-\frac{2m_2}{m_1+m_2}\left(\frac{\partial}{\partial x}\frac{\partial}{\partial X} + \frac{\partial}{\partial y}\frac{\partial}{\partial Y} + \frac{\partial}{\partial z}\frac{\partial}{\partial Z}\right).
\end{aligned} \tag{1.33}$$

Finally the kinetic part T of the hamiltonian of the system reduces to:

$$T = \frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{-\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right), \tag{1.34}$$

with $\mu = m_1 m_2/(m_1+m_2)$ and $M = m_1 + m_2$ are respectively the reduced mass and the total mass of the system.

If we adopt the following notation:

$$\begin{aligned}
\Delta_r &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \\
\Delta_R &= \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2},
\end{aligned} \tag{1.35}$$

the hamiltonian can be written in terms of the new variables r and R as follows:

$$H = \frac{-\hbar^2}{2\mu}\Delta_r + \frac{-\hbar^2}{2M}\Delta_R + V(r). \tag{1.36}$$

With the new hamiltonian expression eq. (1.36), Schrodinger's equation takes the form

$$\left(\frac{-\hbar^2}{2\mu}\Delta_r + \frac{-\hbar^2}{2M}\Delta_R + V(r)\right)\psi(\overrightarrow{r}, \overrightarrow{R}) = E\psi(\overrightarrow{r}, \overrightarrow{R}), \tag{1.37}$$

where ψ depends now on the new variables $(\overrightarrow{r}, \overrightarrow{R})$; $\psi(\overrightarrow{r}, \overrightarrow{R}) = \psi(x, y, z, X, Y, Z)$.

Separation of variables

As the potential energy $V(r)$ depends only on the variables x, y and z through the variable r, the equation eq. (1.37) can be simplified by the separation of variables method. Let's find solution under the form:

$$\psi(\overrightarrow{r}, \overrightarrow{R}) = \varphi(\overrightarrow{r})\phi(\overrightarrow{R}) \ . \tag{1.38}$$

Substituted the expression eq. (1.38) in the equation (1.37) we obtain by separation of variables:

$$\begin{aligned} \left(-\frac{\hbar^2}{2\mu}\Delta_r + V(\overrightarrow{r})\right)\varphi(\overrightarrow{r}) &= E_r\varphi(\overrightarrow{r}) \ , \\ -\frac{\hbar^2}{2M}\Delta_R &= E_R\phi(\overrightarrow{R}) \ , \end{aligned} \tag{1.39}$$

with:

$$E = E_r + E_R \ . \tag{1.40}$$

The operator,

$$H_r = -\frac{\hbar^2}{2\mu}\Delta_r + V(\overrightarrow{r}) \ , \tag{1.41}$$

is usually called the relative hamiltonien.

Chapter 2

Exact solvable systems: the harmonic oscillator

In this chapter, we focuses with detailed study on an exactly solvable quantum problem. It's about the simple harmonic oscillator. The concept of the simple harmonic oscillaor plays a major role in different (many) applications in quatum physics. The simple harmonic oscillator corresponds in its simple form, in the movement of a particule of mass m submitted to quadratic potential. However, the importance of this system goes far beyond this, as it can be used to describe the behaviour of a physical system around a stable equilibrium position. The treatment of this model in a quantum formalism is therefore of obvious importance. In addition, nit concerns a system to which many experimental acheevments exist such as trapped particles in the wells where elctromagnetic field exitations. It is also a system for which there are many experimental realisations; for example, particles trapped in well potentials or electromagnetic field excitations,.... The purpose of this chapter will therefore be to the study of a harmonic oscillator in the framework of quantum mechanics in order to determine the energy spectrum and the corresponding quantum states. The classical hamiltonian of one dimentional harmonic oscillator is given by:

$$\hat{H} = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 \ . \tag{2.1}$$

m and ω are respectively the mass and the pulse of the oscillator [16].

2.1 Harmonic approximation

Generally, let us consider a potential $V(x)$ which presents a minimum in a point of space that we take as origin of the displacements. The Taylor series expansion of $V(x)$ in the neighborhood of $x = 0$ reduces, at second order, to

$$\begin{aligned} V(x) &= V(0) + \frac{dV(x)}{dx} \mid_{x=0} x + \frac{1}{2}\frac{d^2V(x)}{dx^2} \mid_{x=0} x^2 + ... \ , \\ &= V(0) + \frac{1}{2}kx^2 + ... \ , \end{aligned} \tag{2.2}$$

As $V(x)$ has a minimum at $x = 0$, which corresponds to a position of stable equilibrium, the coefficient $k = d^2V(x)/dx^2\big|_{x=0}$ is positive and the quantity $dV(x)/dx|_{x=0}$ is zero. When the displacements around the equilibrium point are small enough, one can neglect terms of order greater than two in the expansion. The potential $V(x)$ can be assumed to be zero at the equilibrium point. We then obtain a potential corresponding to that of a harmonic oscillator given by the equation eq. (2.1).

2.2 The one-dimensional harmonic oscillator

Harmonic oscillators have a double importance in quantum physics. The first aspect concerns the possibility of describing in first approximation a bound system by a harmonic oscillator. This provides precious informations about the energy levels, their spacing and their degeneracy. This is the idea used to describe the shell model of atomic nuclei. The second aspect concerns the formalism based on the definition of the creation and annhilation operators. Let us consider a particle of mass m in harmonic potential, i.e. described by the hamiltonian:

$$\hat{H} = \frac{p_x^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2 \ , \tag{2.3}$$

or ω is own pulse of the oscillator. The equation of Schrödinger in this case takes the form as follows:

$$\psi'' + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2x^2\right)\psi = 0 \ , \tag{2.4}$$

As indicated above, since the potential tends to infinity for $|x| \longrightarrow \infty$, there are no diffusion states in this problem. We are only interested in the values of the energy E for which the solutions are square summable, that is to say, relative to the stationary states. It is more convenient to work with dimensionless quantities:

$$\begin{aligned} \varepsilon &:= \tfrac{2E}{\hbar\omega}, \\ y &:= \sqrt{\tfrac{m\omega}{\hbar}}x \ . \end{aligned} \tag{2.5}$$

The energy E is therefore measured in units of $(h\omega)$.

The equation (2.4) is reduced to:

$$\psi'' + \left(\varepsilon - y^2\right)\psi = 0. \tag{2.6}$$

For a given value of the energy E or of ε, this latter (ε) can be neglected in front of y when it goes to infinity, which allows us to write:

$$\psi'' - y^2\psi = 0 \quad \text{when} \ \ \varepsilon \ll y^2 \ . \tag{2.7}$$

This last equation admits solutions of the form:

$$\psi(y) \sim A\exp\left(-y^2/2\right) \ . \tag{2.8}$$

It should be noted that this solution only describes the asymptotic behaviour at infinity of the general solution, which always remains unknown. To determine the general solution of eq. (2.6) one can proceed by the method of variation of the constant $A: \ A = h(y)$. The general solution of the equation (2.6) will therefore be of the form:

$$\psi\left(y\right) = h(y)\exp\left(-y^2/2\right) \ , \tag{2.9}$$

By substituting the expression (2.9) of ψ in the equation (2.6) we obtain the differential equation for the function $h(y)$:

$$h'' - 2yh' + (\varepsilon - 1)h = 0, \tag{2.10}$$

This last equation can be solved by the power series expansion method. By writing:

$$h(y) = \sum_{m=0}^{\infty} a_m y^m = a_0 + a_1 y + a_2 y^2 + a_3 y^3 + ... \tag{2.11}$$

The first and second derivatives of $h(y)$ will be given respectively by:

$$\begin{aligned} h'(y) = &\quad a_1 + 2a_2 y^1 + 3a_3 y^2 ... &&= \sum_{m=0}^{\infty} m a_m y^{m-1}, \\ h''(y) = &\quad (2\times 1)\times a_2 + (3\times 2)\times a_3 y^1 ... &&= \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} y^n, \end{aligned} \tag{2.12}$$

Substituting eq. (2.11) and eq. (2.12) in eq. (2.10) we obtain:

$$\begin{aligned} \left[\sum_{m=0}^{\infty} (n+2)(n+1) a_{n+2} y^n\right] - 2y\left[\sum_{m=0}^{\infty} m a_m y^{m-1}\right] + (\varepsilon - 1)\left[\sum_{m=0}^{\infty} a_m y^m\right] &= 0, \\ \sum_{n=0}^{\infty} \left[(n+2)(n+1) a_{n+2} + (\varepsilon - 1 - 2n) a_n\right] y^n &= 0, \end{aligned}$$

This last equation can only be satisfied when the coefficients of all powers of y are zero, that is:

$$(n+2)(n+1) a_{n+2} + (\varepsilon - 1 - 2n) a_n = 0 \ . \tag{2.13}$$

We therefore obtain a recurrence relation between the coefficients a_n of the expansion:

$$a_{n+2} = \frac{-(\varepsilon - 1 - 2n)}{(n+2)(n+1)} a_n \ . \tag{2.14}$$

Two types of solutions are to be distinguished: The even series and the odd series. Indeed, if we know a_0 we can determine a_2, a_4, ..., a_{2i}, ... i.e. all the even coefficients. Similarly, when a_1 is given we can determine a_3, a_5, ..., a_{2i+1}, ... i.e. all the odd coefficients. We therefore obtain two separate series, one for the solutions corresponding to the even coefficients a_{2i} and the other for the odd coefficients a_{2i+1}.

On the other hand, it is easy to show that the series eq. (2.11) converges. Indeed, for higher

order terms ($m \gg 1$), the equation (2.14) reduces to:

$$a_{m+2} \sim \frac{2}{m} a_m \quad \text{for} \quad m \gg 1 \ , \tag{2.15}$$

or

$$\frac{a_{m+1}}{a_m} \sim \frac{2}{m} < 1 \quad \text{for} \quad m \gg 1. \tag{2.16}$$

So, according to d'Alembert's criterion, the series of the general term a_n is convergent.

Now we try to find the expression of the function $h(y)$. The ratio between two consecutive terms of the expansion (2.11) reduces to:

$$\frac{a_{m+2} y^{m+2}}{a_m y^m} = \frac{2m + 1 - \varepsilon}{(m+2)(m+1)} y^2 \sim \frac{2y^2}{m} \ , \tag{2.17}$$

for large values of $m \gg 1$.

Now, if we examine the series expansion for the function $\exp(x)$,

$$\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + ... \ , \tag{2.18}$$

which gives for the function $\exp(x^2)$:

$$\exp\left(x^2\right) = \sum_{m=0}^{\infty} \frac{\left(x^2\right)^n}{n!} = \sum_{m=0,2,4...}^{\infty} \frac{x^m}{(m/2)!}. \tag{2.19}$$

The ratio between two consecutive terms simplifies to:

$$\frac{\frac{x^{m+2}}{(m/2+1)!}}{\frac{x^m}{(m/2)!}} = \frac{(m/2)!}{(m/2+1)!} x^2 \sim \frac{2x^2}{m}, \tag{2.20}$$

which is equivalent to that obtained for the function $h(y)$ eq.(2.17). So, for large values of m, the function $h(y)$ has the same behavior as the function $\exp(y^2)$:

$$h(y) = \sum_{m=0}^{\infty} a_m y^m \sim e^{y^2} \text{ for } \quad m \gg 1 \ . \tag{2.21}$$

Consequently, the wave function eq. (2.9) reduces to:

$$\begin{aligned} \psi(y) = &\quad h(y)\exp\left(-y^2/2\right) &&\sim \exp\left(-y^2/2\right)\sum_{m=0}^{\infty} a_m y^m, \\ \simeq &\quad \exp\left(-y^2/2\right)\exp\left(y^2\right) &&= \exp\left(y^2/2\right) \qquad for \quad m >> 1, \end{aligned} \tag{2.22}$$

which diverges when $y \to \infty$ and is therefore physically unacceptable. This problem can only be solved if we consider series that are limited to an order n that is well determined. In other words, above a certain order n, all coefficients a_m vanish; $a_m = 0$ for $m > n$ (a_n is not necessarily zero: it is the last non-zero coefficient). From the equation (2.14) we should have:

$$2n + 1 - \varepsilon = 0, \qquad n = 0, 1, 2, \ldots \ . \tag{2.23}$$

replacing ε by its expression as a function of energy we obtain:

$$\varepsilon = 2n + 1 = \frac{2E}{\hbar\omega} \ , \qquad n = 0, 1, 2, \ldots \ , \tag{2.24}$$

or

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \ , \qquad n = 0, 1, 2, \ldots \ , \tag{2.25}$$

which represents the energy quantization for the one-dimensional harmonic oscillator.

Now let's look at the wave function. For each value of n we have a well-determined energy E_n, given by the relation eq. (2.25) and also a particular series $h_n(y)$ for $h(y)$,

$$h_n(y) = \sum_{m=0}^{n} a_m y^m \ , \tag{2.26}$$

and hence different wave functions for different values of n:

$$\psi_n(y) = h_n(y)\exp(-y^2/2) \ = \exp(-y^2/2)\sum_{m=0}^{n} a_m y^m \ . \tag{2.27}$$

The recurrence relation eq. (2.14) becomes:

$$a_{m+2}^{(n)} = \frac{-2(m-n)}{(m+2)(m+1)} a_m^{(n)} \ , \tag{2.28}$$

in which we have replaced ε by its value eq. (2.24).

Two different recurrence relations are to be distinguished, one for even values of m or n and the other for odd values.

For $n = 0$, which corresponds to the ground state, we have

$$h_0(y) = a_0 \ . \tag{2.29}$$

So,

$$\psi_0(y) = a_0 \exp(-y^2/2) \ . \tag{2.30}$$

This is the ground state wave function. The parameter a_0 is a normalization constante.

For $n = 1$ which corresponds to the first exsited state, we have $a_0 = 0$ (which leads to zero values for all the even coefficients a_2, a_4, ...) and:

$$h_1(y) = a_1 y \ . \tag{2.31}$$

Thus, the wave function associated to the first excited state will be given by:

$$\psi_1(y) = a_1 y \exp(-y^2/2) \ . \tag{2.32}$$

Here again, the first parameter a_1 is a normalization one. For $n = 2$, all odd coefficients are zero and

$$h_2(y) = a_0 + a_2 y^2 \ , \tag{2.33}$$

where the parameter a_2 will be determined by the recurrence relation eq. (2.28):

$$a_2 = \frac{-2(0-2)}{(0+2)\,(0+1)} a_0 = 2a_0 \ . \tag{2.34}$$

So

$$h_2(y) = a_0(1 - 2y^2) \ . \tag{2.35}$$

Then

$$\psi_2(y) = a_0(1-2y^2)\exp(-y^2/2)\ . \tag{2.36}$$

The wave functions for the different values of n can be determined by following the same procedure. We obtain for $n=3$ and $n=4$:

$$\begin{aligned} h_3(y) &= a_1 y + a_3 y^3\ , \\ h_4(y) &= a_0 + a_2 y^2 + a_4 y^4\ . \end{aligned} \tag{2.37}$$

We can check that the functions $h_n(y)$ are related to the well-known Hermite polynomials $H_n(y)$:

$$\begin{aligned} H_0 &= 1\ , \\ H_1 &= 2y\ , \\ H_2 &= 4y^2 - 2\ , \\ H_3 &= 8y^3 - 12y\ , \\ H_4 &= 16y^4 - 48y^2 + 12\ , \\ \vdots &= \vdots\ . \end{aligned} \tag{2.38}$$

In terms of the Hermite polynomials, we can express the wave functions of the stationary states of the one-dimensional harmonic oscillator:

$$\psi_n(x) = A_n H_n\left(\sqrt{m\omega/\hbar}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\ , \tag{2.39}$$

where A_n are the normalization constants with values:

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}. \tag{2.40}$$

2.3 The three dimensions harmonic oscillator

Let's consider a particle submitted to a three-dimensional harmonic potential $V(x, y, z)$ with pulsations ω_x, ω_y and ω_z for the different directions O_x, O_y and O_z respectively:

$$V(x, y, z) = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2 + \frac{1}{2}m\omega_z^2 z^2 \ . \tag{2.41}$$

If this oscillator is isotropic, which implies equal pulsations ($\omega_x = \omega_y = \omega_z = \omega$), the potential eq. (2.41) reduces to a function of the single radial variable r, ($r = \sqrt{x^2 + y^2 + z^2}$):

$$V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = \frac{1}{2}m\omega^2 r^2 \ , \tag{2.42}$$

In this case, we have a central field problem, which is often referred to as the spherical harmonic oscillator. The radial Schrödinger equation for the spherical harmonic oscillator can be written as:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{1}{2}m\omega^2 r^2 - E\right)U(r) = 0 \ , \tag{2.43}$$

We will solve this equation by examining the asymptotic behavior of the solutions.

When $r \to 0$, the two terms $(m\omega^2 r^2/2)$ and E will be neglected compared to the centrifugal term $\hbar^2 l(l+1)/(2mr^2)$. The equation (2.43) becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}U(r) = 0 \ , \tag{2.44}$$

which admits solutions of the form $U(r) \sim r^{(l+1)}$.

When $r \to \infty$, the two terms $\hbar^2 l(l+1)/(2mr^2)$ and E will be neglected compared to $(m\omega^2 r^2/2)$. The equation (2.43) becomes in this case:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{1}{2}m\omega^2 r^2\right)U(r) = 0 \ , \tag{2.45}$$

which admits solutions of the form $U(r) \sim \exp\left[-m\omega^2 r^2/2\hbar\right]$.

By combining the two equations (2.44) and eq. (2.45) we can write the solution of the

equation (2.43) under the form:

$$U(r) = f(r) r^{(l+1)} \exp\left(-\frac{m\omega^2 r^2}{2\hbar}\right) \ , \tag{2.46}$$

where $f(r)$ is a function of r. Substituting this expression in eq. (2.43) we obtain an equation for the function $f(r)$:

$$\frac{d^2}{dr^2} f(r) + 2\left(\frac{l+1)}{r} - \frac{m\omega}{\hbar} r\right) \frac{d}{dr} f(r) + \left[\frac{2mE}{\hbar^2} - (2l+3)\frac{m\omega}{\hbar}\right] f(r) = 0 \ . \tag{2.47}$$

We are now looking for solutions for eq. (2.47) in the form of a power series:

$$f(r) = \sum_{n=0}^{\infty} a_n r^n = a_{0+} a_1 r + a_2 r^2 + ... + a_n r^n + ... \ . \tag{2.48}$$

Substituting this expression of $f(r)$ in the equation (2.47), we obtain:

$$\sum_{n=0}^{\infty} \left[n(n-1) a_n r^{n-2} + 2\left(\frac{l+1}{r} - \frac{m\omega}{\hbar} r\right) n a_n r^{n-1} + \left(\frac{2mE}{\hbar^2} - (2l+3)\frac{m\omega}{\hbar}\right) a_n r^n \right] = 0 \ ,$$

which reduces to:

$$\sum_{n=0}^{\infty} \left[n(n-1+2l) a_n r^{n-2} + \left(\frac{2mE}{\hbar^2} - \frac{2m\omega}{\hbar} n - (2l+3)\frac{m\omega}{\hbar}\right) a_n r^n \right] = 0 \ . \tag{2.49}$$

For this equation to be satisfied independently of r, all the coefficients of the different powers of r must be cancelled out separately. We end up with the following recurrence relation:

$$a_{n+2} = \frac{m}{\hbar^2} \frac{\hbar\omega(2n+3l+3) - 2E}{(n+2)(n+2l+3)} a_n \ , \tag{2.50}$$

for $n \geq 2$.

For $n = 0$ and $n = 1$, the equation (2.49) leads to:

$$\begin{aligned} 0 \times (2l+1) a_0 &= 0 \ , \\ 1 \times (2l+2) a_1 &= 0 \ . \end{aligned} \tag{2.51}$$

This implies that a_0 is not necessarily zero and that a_1 is necessarily zero since l is a positive

or zero integer. Therefore, the function $f(r)$ must contain only even powers:

$$f(r) = \sum_{i=0,2,4,...}^{\infty} a_i r^i = \sum_{n=0}^{\infty} a_{2n} r^{2n} \ , \tag{2.52}$$

where all the coeficients a_{2n} are proportional to a_0.

Note that when $n \to \infty$ the function $f(r)$ diverges with an asymptotic behavior like $\exp(r^2)$. The series must be stopped at a certain maximum power $r^{n'}$, it is a polynomial degree n'. The coeficient $a_{n'+2}$ must therefore be null. The equation (2.50) gives :

$$\hbar\omega(2n' + 3l + 3) - 2E = 0 \ , \tag{2.53}$$

where n' is an even number. If we introduce the integer number $N = n'/2 \ \ (N = 1, 2, 3, ...)$ we end up with the energy quantization formula:

$$E_{N,l} = \hbar\omega(2N + l + 3/2) = \hbar\omega(n + 3/2) \ , \tag{2.54}$$

with $n = 2N + l$.

The ground state corresponds to $n = 0$, ($N = 0$ and $l = 0$) and has an energy value of $E_{0,0} = 3\hbar\omega/2$. The associated radial wave function will be:

$$U_{0,0}(r) = a_0 r \exp\left(-\frac{m\omega}{2\hbar}\vec{r}^2\right), \tag{2.55}$$

or

$$R_{0,0}(r) = a_0 \exp\left(-\frac{m\omega}{2\hbar}\vec{r}^2\right) \ , \tag{2.56}$$

which is of gaussian type. The parameter a_0 will be determined by imposing the normalization condition. The wave function ψ will to be of the form:

$$\begin{aligned} \psi_0(r) = & \ \psi_{0,0}(r, \theta, \varphi) = a_0 r \exp\left(-\tfrac{m\omega}{2\hbar}\vec{r}^2\right) Y_0^0(\theta, \varphi), \\ \propto & \ \exp\left(-\tfrac{m\omega}{2\hbar}\vec{r}^2\right). \end{aligned} \tag{2.57}$$

Because $Y_0^0(\theta,\varphi)$ is a constant ($Y_0^0(\theta,\varphi) = 1/\sqrt{4\pi}$).

For an hamiltonian of the form:

$$\hat{H} = ap_x^2 + kx^2 \ , \tag{2.58}$$

the energy spectrum is given by

$$E_n = \hbar\sqrt{ak}(2n+3) \tag{2.59}$$

and the ground state energy equals:

$$E_0 = 3\hbar\sqrt{ak} \ , \tag{2.60}$$

which is none other than $3\hbar\omega/2$ and the wave function:

$$\begin{aligned} \psi_0\left(\vec{r}\right) &\propto \exp\left(-\tfrac{m\omega}{2\hbar}\vec{r}^2\right), \\ &\propto \exp\left(-\tfrac{1}{2\hbar}\sqrt{\tfrac{k}{a}}\vec{r}^2\right). \end{aligned} \tag{2.61}$$

The first excited state corresponds to $n = 1$, ($N = 0$ and $l = 1$), has for energy the value $E_{0,1} = 5\hbar\omega/2$. The associated wave function takes the form:

$$U_{0,1}(\overrightarrow{r}) = a_0 r^3 \exp(-\frac{m\omega}{2\hbar}\overrightarrow{r}^2) \ , \tag{2.62}$$

The second excited state corresponds to $n = 2$, ($N = 1$ and $l = 0$) or ($N = 0$ and $l = 2$) has for energy the value $E_{1,0} = E_{0,2} = 7\hbar\omega/2$. The associated wave function is:

$$U\left(\vec{r}\right) = \left(a_0 + a_2 r^2\right) r \exp\left(-\frac{m\omega}{2\hbar}\vec{r}^2\right) = a_0\left(1 - \frac{2}{3}\frac{m\omega}{\hbar}r^2\right) r \exp\left(-\frac{m\omega}{2\hbar}\vec{r}^2\right), \tag{2.63}$$

This state can be considered as the first excited of s states. It is to say of zero orbital moment ($l = 0$) [16].

2.4 The two-body harmonic oscillator

The potential of two particles in interacting via harmonic forces is of the form:

$$V^{(2)} = k(\overrightarrow{r}_1 - \overrightarrow{r}_2)^2 = k\overrightarrow{r}^2 \ , \tag{2.64}$$

and the hamiltonian of relative motion is:

$$\hat{H}_r^{(2)} = \frac{1}{2\mu_r}\overrightarrow{p}_r^2 + k\overrightarrow{r}^2 \ . \tag{2.65}$$

The problem is therefore reduced to a problem of a three-dimensional space particle in a central potential of harmonic type. The energy spectrum is therefore obtained by the equation (2.61) which becomes in a system of units where $\hbar = 1$:

$$E_n^{(2)} = (2n+3)\sqrt{\frac{k}{2\mu}} \ , \tag{2.66}$$

and the ground state energy reduces to:

$$E_0^{(2)} = 3\sqrt{\frac{k}{2\mu}} \ . \tag{2.67}$$

Chapter 3

Five-body Harmonic Oscillator

In this chapter, we will focus on the system of few bodies interacting via two-body forces that derive from harmonic potentials. This type of systems is often called "N-body Harmonic Oscillator".

Let's consider a system of five bodies with two-body harmonic iteraction depending only on the relative distance between them.

$$V(\overrightarrow{r_i}, \overrightarrow{r_j}) = V(|\overrightarrow{r_i} - \overrightarrow{r_j}|) = k_{ij}(\overrightarrow{r_i} - \overrightarrow{r_j})^2 \ . \tag{3.1}$$

Let us suppose that the only way the particles are distinguished is by their masses. So, the coupling constant k_{ij} of the harmonic interaction between two particles depends only on the masses of the involved particles. This can be formulated as

$$k_{\alpha\beta} = k_{\alpha\gamma} \qquad \text{if} \quad m_\beta = m_\gamma \ , \quad \forall\alpha \tag{3.2}$$

The hamiltonian of the system is then written as:

$$\begin{aligned}\hat{H}^{(5)} &= \frac{\overrightarrow{p}_1^2}{2m_1}+\frac{\overrightarrow{p}_2^2}{2m_2}+\frac{\overrightarrow{p}_3^2}{2m_3}+\frac{\overrightarrow{p}_4^2}{2m_4}+\frac{\overrightarrow{p}_5^2}{2m_5} \\ &+k_{12}(\overrightarrow{r_1}-\overrightarrow{r_2})^2+k_{13}(\overrightarrow{r_1}-\overrightarrow{r_3})^2+k_{14}(\overrightarrow{r_1}-\overrightarrow{r_4})^2+k_{15}(\overrightarrow{r_1}-\overrightarrow{r_5})^2 \\ &+k_{23}(\overrightarrow{r_2}-\overrightarrow{r_3})^2+k_{24}(\overrightarrow{r_2}-\overrightarrow{r_4})^2+k_{25}(\overrightarrow{r_2}-\overrightarrow{r_5})^2 \\ &+k_{34}(\overrightarrow{r_3}-\overrightarrow{r_4})^2+k_{35}(\overrightarrow{r_3}-\overrightarrow{r_5})^2+k_{45}(\overrightarrow{r_4}-\overrightarrow{r_5})^2 \ ,\end{aligned} \tag{3.3}$$

Let us consider some mass configurations:

- The equal masse problem: configuration that we will note (m, m, m, m, m).

- Two different masses: configurations that we will noted (m, m, m, m, M) and (m, m, m, M, M).

- Three different masses: We have chosen a single configuration to be treated (m, m, M, M, m_5).

3.1 Jacobi coordinates

To study a system with a small number of bodies, one can introduce the so-called Jacobi coordinates to separate the motion of the center of mass from the relative motion. For a two-body system, it is familiar to replace the individual coordinates $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$ with the relative coordinate $\overrightarrow{r}$:

$$\overrightarrow{r} = \overrightarrow{r}_1 - \overrightarrow{r}_2 \ , \tag{3.4}$$

and the center of mass coordinate $\overrightarrow{R}$:

$$\overrightarrow{R} = \frac{1}{m_1+m_2}\left(m_1\overrightarrow{r}_1 - m_2\overrightarrow{r}_2\right) \ . \tag{3.5}$$

Consider now a system of N particles of masses m_i and of positions $\overrightarrow{r}$ $(i = 1, ..., N)$. So $M = m_1 + ... + m_N$ is the total mass of the system and $\overrightarrow{R}$ the center of mass coordinate:

$$\overrightarrow{R} = \frac{1}{M}\sum_{i=1}^{N} m_i\overrightarrow{r_i} \ , \tag{3.6}$$

We define the j-th coordinate of Jacobi as the vector connecting the $(j+1)$-th particle and

the center of mass of the first j particles:

$$\vec{\rho}_j = -\vec{r}_{j+1} + \frac{1}{\sum_{i=1}^{j} m_i} \sum_{i=1}^{j} m_i \vec{r}_i \ , \qquad j = 1, ..., N-1.. \tag{3.7}$$

We obtain then $N-1$ Jacobi coordinates. So, instead of working with the coordinates system of the idividual particles$\{\overrightarrow{r}_1, ..., \overrightarrow{r_N}\}$, we use another system of coordinates formed by the Jacobi coordinates with the center of mass vector $\{\overrightarrow{\rho}_1, ..., \overrightarrow{\rho}_{N-1}, \overrightarrow{R}\}$.

3.2 The equal mass problem: Configuration (m, m, m, m, m)

We have to choose four $(4 = 5 - 1)$ Jacobi coordinates; The reltive coordinates of the two particles that we will note $\overrightarrow{\rho}_1$, the vector $\overrightarrow{\rho}_2$ joining the 3^{rd} particle and the mass center of the first two particles (G_{12}), $\overrightarrow{\rho}_3$ vector joining the 4^{th} particle and the mass center of the first three particles (G_{123}) and $\overrightarrow{\rho}_4$ the vector that joins the 5^{th} particle to the mass center of the first four particles (G_{1234}) and :

$$\begin{aligned}
\overrightarrow{\rho}_1 &= -\overrightarrow{r}_2 + \overrightarrow{r}_1, \\
\overrightarrow{\rho}_2 &= -\overrightarrow{r}_3 + \tfrac{1}{2}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2\right), \\
\overrightarrow{\rho}_3 &= -\overrightarrow{r}_4 + \tfrac{1}{3}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2 + \overrightarrow{r}_3\right), \\
\overrightarrow{\rho}_4 &= -\overrightarrow{r}_5 + \tfrac{1}{4}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2 + \overrightarrow{r}_3 + \overrightarrow{r}_4\right) \ .
\end{aligned} \tag{3.8}$$

The vector of the center mass of the system $\overrightarrow{R}$ is defined by:

$$\overrightarrow{R} = \frac{1}{5}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2 + \overrightarrow{r}_3 + \overrightarrow{r}_4 + \overrightarrow{r}_5\right) \ . \tag{3.9}$$

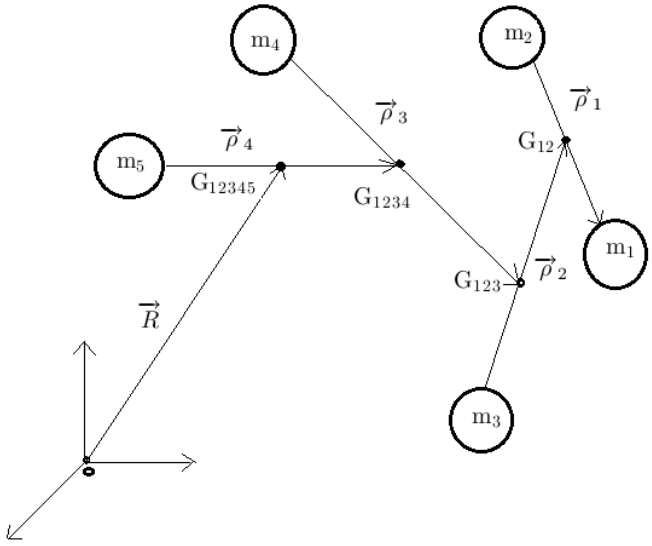

figure 1: Jacobi coordinates for the configuration (m, m, m, m, m) of a five-body system.

We have a system of five equations (3.8) and eq. (3.9). This system can be inverted to obtain the expressions of the individual particles coordinates $\overrightarrow{r}_1$, $\overrightarrow{r}_2$, $\overrightarrow{r}_3$, $\overrightarrow{r}_4$ and $\overrightarrow{r}_5$ in terms of the Jacobi coordinates $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_4$ and the center of mass coordinate $\overrightarrow{R}$. We get:

$$\begin{aligned}
\overrightarrow{r}_1 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{1}{5}\overrightarrow{\rho}_4 \\
\overrightarrow{r}_2 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{1}{5}\overrightarrow{\rho}_4 \\
\overrightarrow{r}_3 &= \overrightarrow{R} - \tfrac{2}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{1}{5}\overrightarrow{\rho}_4 \\
\overrightarrow{r}_4 &= \overrightarrow{R} - \tfrac{3}{4}\overrightarrow{\rho}_3 + \tfrac{1}{5}\overrightarrow{\rho}_4 \\
\overrightarrow{r}_5 &= \overrightarrow{R} - \tfrac{4}{5}\overrightarrow{\rho}_4 \ .
\end{aligned} \tag{3.10}$$

In terms of velocities:

$$\dot{\overrightarrow{r}}_1 = \frac{d\overrightarrow{r}_1}{dt}, \dot{\overrightarrow{r}}_2 = \frac{d\overrightarrow{r}_2}{dt}, \dot{\overrightarrow{r}}_3 = \frac{d\overrightarrow{r}_3}{dt}, \dot{\overrightarrow{r}}_4 = \frac{d\overrightarrow{r}_4}{dt} \text{ and } \dot{\overrightarrow{r}}_5 = \frac{d\overrightarrow{r}_5}{dt} \ , \tag{3.11}$$

the expression of the kinetic energy of the system,

$$
\begin{aligned}
T^{(5)} &= \frac{\overrightarrow{p}_1^{\,2}}{2m} + \frac{\overrightarrow{p}_2^{\,2}}{2m} + \frac{\overrightarrow{p}_3^{\,2}}{2m} + \frac{\overrightarrow{p}_4^{\,2}}{2m} + \frac{\overrightarrow{p}_5^{\,2}}{2m} \ , \\
&= \frac{1}{2}m\,\dot{\overrightarrow{r}}_1^{\,2} + \frac{1}{2}m\,\dot{\overrightarrow{r}}_2^{\,2} + \frac{1}{2}m\,\dot{\overrightarrow{r}}_3^{\,2} + \frac{1}{2}m\,\dot{\overrightarrow{r}}_4^{\,2} + \frac{1}{2}m\,\dot{\overrightarrow{r}}_5^{\,2} \ ,
\end{aligned} \tag{3.12}
$$

reduces, according to the velocities relative to the Jacobi coordinates:

$$
\dot{\overrightarrow{\rho}}_1 = \frac{d\overrightarrow{\rho}_1}{dt},\ \dot{\overrightarrow{\rho}}_2 = \frac{d\overrightarrow{\rho}_2}{dt},\ \dot{\overrightarrow{\rho}}_3 = \frac{d\overrightarrow{\rho}_3}{dt} \quad \text{and} \quad \dot{\overrightarrow{\rho}}_4 = \frac{d\overrightarrow{\rho}_4}{dt} \ , \tag{3.13}
$$

to

$$
T^{(5)} = \frac{1}{2}(5m)\dot{\overrightarrow{R}}^{\,2} + \frac{1}{2}(\frac{m}{2})\dot{\overrightarrow{\rho}}_1^{\,2} + \frac{1}{2}(\frac{2m}{3})\dot{\overrightarrow{\rho}}_2^{\,2} + \frac{1}{2}(\frac{3m}{4})\dot{\overrightarrow{\rho}}_3^{\,2} + \frac{1}{2}(\frac{4m}{5})\dot{\overrightarrow{\rho}}_4^{\,2} \ , \tag{3.14}
$$

where $\dot{\overrightarrow{R}} = d\overrightarrow{R}/dt$ is the velocity of the mass center of the sytem. The masses:

$$
\mu_{\rho_1} = \frac{m}{2}, \quad \mu_{\rho_2} = \frac{2m}{3}, \quad \mu_{\rho_3} = \frac{3m}{4}, \quad \mu_{\rho_4} = \frac{4m}{5} \quad \text{and} \quad \mu_R = 5m \tag{3.15}
$$

are considered as fictive or reduced masses related respectively to the coordinates $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_4$ and $\overrightarrow{R}$. Its obvious that the fictive mass related to the coordinate of the mass of center can only be that of the total mass of the system, $\mathbf{M} = 5m$. In terms of conjugate momenta $\overrightarrow{p}_{\rho_1}$, $\overrightarrow{p}_{\rho_2}$, $\overrightarrow{p}_{\rho_3}$, $\overrightarrow{p}_{\rho_4}$ and $\overrightarrow{P}_R$ the kinetic energy is written:

$$
T^{(5)} = \frac{1}{2\mathbf{M}}\overrightarrow{P}_R + \frac{1}{2(m/2)}\overrightarrow{p}_{\rho_1} + \frac{1}{2(2m/3)}\overrightarrow{P}_{\rho_2} + \frac{1}{2(3m/4)}\overrightarrow{P}_{\rho_3} + \frac{1}{2(4m/5)}\overrightarrow{P}_{\rho_4} \ , \tag{3.16}
$$

The expression of the potential energy $V^{(5)}$:

$$
\begin{aligned}
V^{(5)} &= k\,(\overrightarrow{r}_1 - \overrightarrow{r}_2)^2 + k\,(\overrightarrow{r}_1 - \overrightarrow{r}_3)^2 + k\,(\overrightarrow{r}_1 - \overrightarrow{r}_4)^2 + k\,(\overrightarrow{r}_1 - \overrightarrow{r}_5)^2 + k\,(\overrightarrow{r}_2 - \overrightarrow{r}_3)^2 \\
&\quad + k\,(\overrightarrow{r}_2 - \overrightarrow{r}_4)^2 + k\,(\overrightarrow{r}_2 - \overrightarrow{r}_5)^2 + k\,(\overrightarrow{r}_3 - \overrightarrow{r}_4)^2 + k\,(\overrightarrow{r}_3 - \overrightarrow{r}_5)^2 \\
&\quad + k\,(\overrightarrow{r}_4 - \overrightarrow{r}_5)^2 \ ,
\end{aligned} \tag{3.17}
$$

in the conditions eq. (3.2), that's to say, the coupling constants are all equal: k_{ij}=k,

$(i<j = 1, ..., 5)$, reduces in terms of Jacobi coordinates to:

$$V^{(5)} = \frac{5}{2}k\overrightarrow{\rho}_1^2 + \frac{10}{3}k\overrightarrow{\rho}_2^2 + \frac{15}{4}k\overrightarrow{\rho}_3^2 + 4k\overrightarrow{\rho}_4^2 \ . \tag{3.18}$$

Then, the hamiltonian eq. (3.3) simplifies to:

$$\hat{H}^{(5)} = \frac{\overrightarrow{P}_R}{2\mathbf{M}} + \left(\frac{\overrightarrow{p}_{\rho_1}^2}{2\mu_{\rho_1}} + \frac{5}{2}k\overrightarrow{\rho}_1^2\right) + \left(\frac{\overrightarrow{p}_{\rho_2}^2}{2\mu_{\rho_2}} + \frac{10}{3}k\overrightarrow{\rho}_2^2\right) + \left(\frac{\overrightarrow{p}_{\rho_3}^2}{2\mu_{\rho_3}} + \frac{15}{4}k\overrightarrow{\rho}_3^2\right) + \left(\frac{\overrightarrow{p}_{\rho_4}^2}{2\mu_{\rho_4}} + 4k\overrightarrow{\rho}_4^2\right) \ . \tag{3.19}$$

Substracting the kinetic energy of the center of mass from the hamiltonian eq. (3.3), we get the so called "*relative hamiltonian*" :

$$\hat{H}_r^{(5)} = \left(\frac{\overrightarrow{p}_{\rho_1}^2}{2\mu_{\rho_1}} + \frac{5}{2}k\overrightarrow{\rho}_1^2\right) + \left(\frac{\overrightarrow{p}_{\rho_2}^2}{2\mu_{\rho_2}} + \frac{10}{3}k\overrightarrow{\rho}_2^2\right) + \left(\frac{\overrightarrow{p}_{\rho_3}^2}{2\mu_{\rho_3}} + \frac{15}{4}k\overrightarrow{\rho}_3^2\right) + \left(\frac{\overrightarrow{p}_{\rho_4}^2}{2\mu_{\rho_4}} + 4k\overrightarrow{\rho}_4^2\right), \tag{3.20}$$

which describes the relative motion of the particles. It is clear that $\hat{H}_r^{(5)}$ is none other than the hamiltonian of a system composed of four decoupled harmonic oscillators. The system's energy $E^{(5)}$ is the sum of these four oscillators' energies. Using the result eq. (2.60), we get:

$$\begin{aligned} E^{(5)} &= (2n_1+3)\sqrt{\frac{\frac{5}{2}k}{2\mu_{\rho_1}}} + (2n_2+3)\sqrt{\frac{\frac{10}{3}k}{2\mu_{\rho_2}}} + (2n_3+3)\sqrt{\frac{\frac{15}{4}k}{2\mu_{\rho_3}}} + (2n_4+3)\sqrt{\frac{4k}{2\mu_{\rho_4}}} \\ &= 2\left(n_1+n_2+n_3+n_4+6\right)\sqrt{5\frac{k}{2m}} \\ &= 2\left(n+6\right)\sqrt{5\frac{k}{2m}} \end{aligned}$$

where n_1, n_2, n_3, n_4 and n are positive or zero integers.

The ground state:

The energy of the ground state $E_0^{(5)}$ of the five-body system with all equal masses correspond then to: $n_1 = n_2 = n_3 = n_4 = 0$. we have:

$$E_0^{(5)} = 12\sqrt{\frac{5k}{2m}} \ . \tag{3.21}$$

For example, if we assign the unit value of the constants: k and m $(k = 1\ ,\ m = 1)$ we the following numerical value for the ground state enrgy of

$$E_0^{(5)} = 12\sqrt{\frac{5}{2}} = 18.97367 \ . \tag{3.22}$$

The wave function associated to the ground state is the product of the wave functions of the involved four oscillators. So it looks like a simple gaussian:

$$\psi_0(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) \propto \exp \frac{-1}{2} \left(\sqrt{\frac{5m}{2}k}\overrightarrow{\rho}_1^2 + \sqrt{\frac{40m}{9}k}\overrightarrow{\rho}_2^2 + \sqrt{\frac{45m}{8}k}\overrightarrow{\rho}_3^2 + \sqrt{\frac{32m}{5}k}\overrightarrow{\rho}_4^2 \right) \tag{3.23}$$

if we assign the unit value of the constants $(k = 1\ ,\ m = 1)$, we get:

$$\begin{aligned} \psi_0(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) &\propto \exp \frac{-1}{2} \left(\sqrt{\frac{5}{2}}\overrightarrow{\rho}_1^2 + \sqrt{\frac{40}{9}}\overrightarrow{\rho}_2^2 + \sqrt{\frac{45}{8}}\overrightarrow{\rho}_3^2 + \sqrt{\frac{32}{5}}\overrightarrow{\rho}_4^2 \right) \\ &\propto e^{-\frac{1}{2}\left(1.581\overrightarrow{\rho}_1^2 + 2.108\overrightarrow{\rho}_2^2 + 2.372\overrightarrow{\rho}_3^2 + 2.530\overrightarrow{\rho}_4^2\right)} \end{aligned} \tag{3.24}$$

3.3 System having two different masses

There are two possible configurations to be considered: (m, m, m, M, M) and (m, m, m, m, M).

3.3.1 Configuration (m, m, m, m, M)

The system considered here is formed of four particles with equal masses $m_1 = m_2 = m_3 = m_4 = m$ and the fifth particle with mass $m_5 = M$ (m and M are in general, different but not necessarly). The Jacobi coordinates $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$ and $\overrightarrow{\rho}_4$ are defined in the same way as in the case of the equal mass problem eqs. (3.8) while, the center of mass coordinate takes the new following expression

$$\overrightarrow{R} = \frac{1}{4m + M} \left(m\overrightarrow{r}_1 + m\overrightarrow{r}_2 + m\overrightarrow{r}_3 + m\overrightarrow{r}_4 + M\overrightarrow{r}_5 \right). \tag{3.25}$$

We are going to proceed in the same way as we did with the previous configurations. By inverting the system of the equations (3.8,3.25) we obtain the individual particle coordinates $\overrightarrow{r}_1$, $\overrightarrow{r}_2$, $\overrightarrow{r}_3$, $\overrightarrow{r}_4$ and $\overrightarrow{r}_5$ in terms of the Jacobi coordinates $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_4$ and the coordinate

of the center of mass $\overrightarrow{R}$ with the result:

$$\begin{aligned}
\overrightarrow{r}_1 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{M}{M+4m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_2 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{M}{M+4m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_3 &= \overrightarrow{R} - \tfrac{2}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \tfrac{M}{M+4m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_4 &= \overrightarrow{R} - \tfrac{3}{4}\overrightarrow{\rho}_3 + \tfrac{M}{M+4m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_5 &= \overrightarrow{R} - \tfrac{4m}{M+4m}\overrightarrow{\rho}_4 \ .
\end{aligned} \tag{3.26}$$

The kinetic energy

$$\begin{aligned}
T^{(5)} &= \frac{\overrightarrow{p}_1^{\,2}}{2m} + \frac{\overrightarrow{p}_2^{\,2}}{2m} + \frac{\overrightarrow{p}_3^{\,2}}{2m} + \frac{\overrightarrow{p}_4^{\,2}}{2m} + \frac{\overrightarrow{p}_5^{\,2}}{2M} \ , \\
&= \frac{1}{2}m\dot{\overrightarrow{r}}_1^{\,2} + \frac{1}{2}m\dot{\overrightarrow{r}}_2^{\,2} + \frac{1}{2}m\dot{\overrightarrow{r}}_3^{\,2} + \frac{1}{2}m\dot{\overrightarrow{r}}_4^{\,2} + \frac{1}{2}M\dot{\overrightarrow{r}}_5^{\,2} \ ,
\end{aligned} \tag{3.27}$$

reduces to:

$$T^{(5)} = \frac{1}{2}\left(M+4m\right)\dot{\overrightarrow{R}}^{\,2} + \frac{1}{2}(2m)\dot{\overrightarrow{\rho}}_1^{\,2} + \frac{1}{2}(\frac{2m}{3})\dot{\overrightarrow{\rho}}_2^{\,2} + \frac{1}{2}(\frac{3m}{4})\dot{\overrightarrow{\rho}}_3^{\,2} + \frac{1}{2}(\frac{2Mm}{M+4m})\dot{\overrightarrow{\rho}}_4^{\,2} \ . \tag{3.28}$$

New expressions for the reduced masses relative to the Jacobi coordinates emerge:

$$\mu_{\rho_1} = \frac{m}{2}, \quad \mu_{\rho_2} = \frac{2m}{3}, \quad \mu_{\rho_3} = \frac{3m}{4}, \quad \mu_{\rho_4} = \frac{4Mm}{M+4m} \quad \text{and} \quad \mu_R = M+4m. \tag{3.29}$$

In terms of conjugated momenta $\overrightarrow{p}_{\rho_1}$, $\overrightarrow{p}_{\rho_2}$, $\overrightarrow{p}_{\rho_3}$, $\overrightarrow{p}_{\rho_4}$ and $\overrightarrow{p}_R$ the kinetic energy is written:

$$T^{(5)} = \frac{\overrightarrow{p}_{\rho_1}}{2\mu_{\rho_1}} + \frac{\overrightarrow{p}_{\rho_2}}{2\mu_{\rho_2}} + \frac{\overrightarrow{p}_{\rho_3}}{2\mu_{\rho_3}} + \frac{\overrightarrow{p}_{\rho_4}}{2\mu_{\rho_4}} + \frac{\overrightarrow{p}_R}{2\mu_R} \ . \tag{3.30}$$

For the potential energy $V^{(5)}$ we found:

$$\begin{aligned}
V^{(5)} &= k\left(\overrightarrow{r}_1 - \overrightarrow{r}_2\right)^2 + k\left(\overrightarrow{r}_1 - \overrightarrow{r}_3\right)^2 + k\left(\overrightarrow{r}_1 - \overrightarrow{r}_4\right)^2 + K\left(\overrightarrow{r}_1 - \overrightarrow{r}_5\right)^2 + k\left(\overrightarrow{r}_2 - \overrightarrow{r}_3\right)^2 \\
&\quad + k\left(\overrightarrow{r}_2 - \overrightarrow{r}_4\right)^2 + K\left(\overrightarrow{r}_5 - \overrightarrow{r}_2\right)^2 + k\left(\overrightarrow{r}_3 - \overrightarrow{r}_4\right)^2 + K\left(\overrightarrow{r}_3 - \overrightarrow{r}_5\right)^2 + K(\overrightarrow{r}_4 - \overrightarrow{r}_5)^2 \ , \\
&= \frac{1}{2}\left(4k+K\right)\overrightarrow{\rho}_1^2 + \frac{2}{3}\left(4k+K\right)\overrightarrow{\rho}_2^2 + \frac{3}{4}\left(4k+K\right)\overrightarrow{\rho}_3^2 + 4K\overrightarrow{\rho}_4^2 \ ,
\end{aligned} \tag{3.31}$$

where we have used the fact that

$$\begin{aligned} k_{12} = \quad & k_{13} = k_{14} = k_{23} = k_{24} = k_{34} = k, \\ k_{15} = \quad & k_{25} = k_{35} = k_{45} = K \ , \end{aligned} \tag{3.32}$$

which arises from the symmetry of the problem ($m_1 = m_2 = m_3$ and $m_4 = m_5$) according to the condition eq. (3.2).

The hamiltonian of the system simplifies to:

$$H^{(5)} = \frac{\overrightarrow{p}_R}{2\mu_R} + H_r^{(5)}, \tag{3.33}$$

where $H_r^{(5)}$ is the relative hamiltonian given by

$$\begin{aligned} H_r^{(5)} \quad = \quad & \left[\frac{\overrightarrow{p}_{\rho_1}}{2\mu_{\rho_1}} + \frac{1}{2}(4k+K)\,\overrightarrow{\rho}_1^2\right] + \left[\frac{\overrightarrow{p}_{\rho_2}}{2\mu_{\rho_2}} + \frac{2}{3}(4k+K)\,\overrightarrow{\rho}_2^2\right] \\ + \quad & \left[\frac{\overrightarrow{p}_{\rho_3}}{2\mu_{\rho_3}} + \frac{3}{4}(4k+K)\,\overrightarrow{\rho}_3^2\right] + \left[\frac{\overrightarrow{p}_{\rho_4}}{2\mu_{\rho_4}} + 4K\overrightarrow{\rho}_4^2\right]. \end{aligned} \tag{3.34}$$

Her again the hamiltonian relative motion $H_r^{(5)}$ is the sum of four decoupled harmonic oscillators. The energy spectrum is generated by the following expression

$$E = (2n_1{+}3)\sqrt{\frac{(4k_{12}{+}K)}{2m}}{+}(2n_2{+}3)\sqrt{\frac{(4k_{12}{+}K)}{2m}}{+}(2n_3{+}3)\sqrt{\frac{(4k{+}K)}{2m}}{+}(2n_4{+}3)\sqrt{\frac{(M{+}4m)K}{2Mm}}\ , \tag{3.35}$$

The ground state

The energy $E_0^{(5)}$ of the ground state of the system in the configuration (m, m, m, m, M) corresponds then to $n_1 = n_2 = n_3 = n_4 = 0$. We have:

$$E_0^{(5)} = 3\left[\sqrt{\frac{1}{2Mm}(MK + 4mK)} + 3\sqrt{\frac{1}{2m}(4k+K)}\right] \ .$$

And the wave function associated to $E_0^{(5)}$ is a simple gaussian:

$$\begin{aligned}\Psi_0(\overrightarrow{\rho}_1,\overrightarrow{\rho}_2,\overrightarrow{\rho}_3,\overrightarrow{\rho}_4) &= A\exp\left(-\frac{1}{2}\sqrt{m\frac{1}{2}(4k+K)}\overrightarrow{\rho}_1^2\right)\exp\left(-\frac{1}{2}\sqrt{2\frac{2m}{3}\frac{2}{3}(4k+K)}\overrightarrow{\rho}_2^2\right)\\ &\exp\left(-\frac{1}{2}\sqrt{2\frac{3m}{4}\frac{3}{4}(4k+K)}\overrightarrow{\rho}_3^2\right)\exp\left(-\frac{1}{2}\sqrt{2\frac{4Mm}{M+4m}4K}\overrightarrow{\rho}_4^2\right)\ ,\end{aligned}$$

Note that we must find the same result as for the equal mass problem when $k=K=1$ and $m=M=1$:

$$E_0^{(5)} = 12\sqrt{\frac{5}{2}} = 18.97376\ , \tag{3.36}$$

and also for the wave function associated eq. (3.24).

3.3.2 Configuration (m,m,m,M,M) : Standard choice of Jacobi coordinates

The considered system here is formed of five particles whose three first particles as having equal masses $m_1=m_2=m_3=m$ and the two last particles with equal masses $m_4=m_5=M$. For this mass configuration, the coordinate of the center of mass of the system has the following expression:

$$\overrightarrow{R} = \frac{1}{3m+2M}\left(m(\overrightarrow{r}_1+\overrightarrow{r}_2+\overrightarrow{r}_3)+M(\overrightarrow{r}_4+\overrightarrow{r}_5)\right)\ . \tag{3.37}$$

We will make the same choice for the Jacobi coordinates, eq. (3.7), as for the mass configuration (m,m,m,m,m) adapted for this configuration (m,m,m,M,M). We have:

$$\begin{aligned}\overrightarrow{\rho}_1 &= -\overrightarrow{r}_2+\overrightarrow{r}_1,\\ \overrightarrow{\rho}_2 &= -\overrightarrow{r}_3+\tfrac{1}{2}(\overrightarrow{r}_1+\overrightarrow{r}_2),\\ \overrightarrow{\rho}_3 &= -\overrightarrow{r}_4+\tfrac{1}{3}(\overrightarrow{r}_1+\overrightarrow{r}_2+\overrightarrow{r}_3),\\ \overrightarrow{\rho}_4 &= -\overrightarrow{r}_5+\tfrac{1}{3m+M}(m\overrightarrow{r}_1+m\overrightarrow{r}_2+m\overrightarrow{r}_3+M\overrightarrow{r}_4)\ .\end{aligned} \tag{3.38}$$

We can draw the expressions of the individual particles coordinates $\overrightarrow{r}_1$, $\overrightarrow{r}_2$, $\overrightarrow{r}_3$, $\overrightarrow{r}_4$ and $\overrightarrow{r}_5$ in terms of Jacobi coordinates $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_4$ and the center of mass coordinate $\overrightarrow{R}$ by

inverting the equations system eq. (3.8) and eq. (3.37). We obtain:

$$\begin{aligned}
r_1 &= R + \tfrac{1}{2}\rho_1 + \tfrac{1}{3}\rho_2 + \tfrac{M}{M+3m}\rho_3 + \tfrac{M}{2M+3m}\rho_4, \\
r_2 &= R + \tfrac{1}{3}\rho_2 - \tfrac{1}{2}\rho_1 + \tfrac{M}{M+3m}\rho_3 + \tfrac{M}{2M+3m}\rho_4, \\
r_3 &= R - \tfrac{2}{3}\rho_2 + \tfrac{M}{M+3m}\rho_3 + \tfrac{M}{2M+3m}\rho_4, \\
r_4 &= R - \tfrac{3m}{M+3m}\rho_3 + \tfrac{M}{2M+3m}\rho_4, \\
r_5 &= R - \tfrac{M}{2M+3m}\rho_4 - \tfrac{3m}{2M+3m}\rho_4.
\end{aligned} \tag{3.39}$$

In terms of the Jacobi coordinates the kinetic energy of the system reduces to

$$\begin{aligned}
T^{(5)} &= \frac{\overrightarrow{p}_1^{\,2}}{2m} + \frac{\overrightarrow{p}_2^{\,2}}{2m} + \frac{\overrightarrow{p}_3^{\,2}}{2m} + \frac{\overrightarrow{p}_4^{\,2}}{2M} + \frac{\overrightarrow{p}_5^{\,2}}{2M} \\
&= \frac{1}{2\mathbf{M}}\overrightarrow{P}_R^{\,2} + \frac{1}{2\mu_{\rho_1}}\overrightarrow{p}_{\rho_1}^{\,2} + \frac{1}{2\mu_{\rho_2}}\overrightarrow{P}_{\rho_2}^{\,2} + \frac{1}{2\mu_{\rho_3}}\overrightarrow{P}_{\rho_3}^{\,2} + \frac{1}{2\mu_{\rho_4}}\overrightarrow{P}_{\rho_4}^{\,2}
\end{aligned} \tag{3.40}$$

where the reduced masses take the new following expressions

$$\mu_{\rho_1} = \frac{m}{2}, \quad \mu_{\rho_2} = \frac{2m}{3}, \quad \mu_{\rho_3} = \frac{3Mm}{M+3m} \quad \text{and} \quad \mu_{\rho_4} = M\frac{M+3m}{2M+3m}\ . \tag{3.41}$$

$\mu_R = 2M + 3m = \mathbf{M}$ is the total mass of the system.

Using the fact that,

$$\begin{aligned}
k_{12} &= \quad k_{13} = k_{23} = k, \\
k_{14} &= \quad k_{15} = k_{24} = k_{25} = k_{34} = k_{35} = k_{45} = K\ ,
\end{aligned} \tag{3.42}$$

which arises from the symmetry of the problem ($m_1 = m_2 = m_3$ and $m_4 = m_5$) according to the condition eq. (3.2), then, we obtain for the potential energy $V^{(5)}$ the result:

$$\begin{aligned}
V^{(5)} &= k\,(\overrightarrow{r}_1 - \overrightarrow{r}_2)^2 + k\,(\overrightarrow{r}_1 - \overrightarrow{r}_3)^2 + K\,(\overrightarrow{r}_1 - \overrightarrow{r}_4)^2 + K\,(\overrightarrow{r}_1 - \overrightarrow{r}_5)^2 + k\,(\overrightarrow{r}_2 - \overrightarrow{r}_3)^2 \\
&\quad + K\,(\overrightarrow{r}_2 - \overrightarrow{r}_4)^2 + K\,(\overrightarrow{r}_5 - \overrightarrow{r}_2)^2 + K\,(\overrightarrow{r}_3 - \overrightarrow{r}_4)^2 + K\,(\overrightarrow{r}_3 - \overrightarrow{r}_5)^2 + k_{45}(\overrightarrow{r}_4 - \overrightarrow{r}_5)^2\ , \\
&= \left(K + \frac{3}{2}k\right)\vec{\rho}_1^{\,2} + \left(\frac{4}{3}K + 2k\right)\vec{\rho}_2^{\,2} + 3\frac{2KM^2 + 9Km^2 + 3m^2k_{45} + 6KMm}{(M+3m)^2}\vec{\rho}_3^{\,2} \\
&\quad + (3K + k_{45})\,\vec{\rho}_4^{\,2} + 6\frac{KM - mk_{45}}{M+3m}\vec{\rho}_3.\vec{\rho}_4\ .
\end{aligned} \tag{3.43}$$

Therefore, the hamiltonian of the system will be expressed as the sum of four oscillators

which are not decoupled because of the crossed term $\vec{\rho}_3.\vec{\rho}_4$. So the energies of the system and the associated wave functions can not be deduced directly. To solve this problem we procced by changing the variables in order to diagonalize the hamiltonian. Therefore the wave function of the ground state will be a correlated gaussian

$$\psi_0(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) \propto \exp\left(-\alpha_1 \overrightarrow{\rho}_1^2 - \alpha_2 \overrightarrow{\rho}_2^2 - \alpha_3 \overrightarrow{\rho}_3^2 - \alpha_4 \overrightarrow{\rho}_4^2 - \beta \overrightarrow{\rho}_3.\overrightarrow{\rho}_4\right) \tag{3.44}$$

with $\alpha_1, \alpha_2, \alpha_3, \alpha_4 > 0$.

We can get around this problem by making a new modified choice of the Jacobi coordinates.

3.3.3 Configuration (m, m, m, M, M) : Modified choice of Jacobi coordinates

The new choice of the Jacobi coordinates consists in taking the standard Jacobi coordinates eq. (3.7) for the first three particles, the relative coordinate of the last two particles and the vector connecting the center of mass of the first three particles to the center of mass of the last two particles

$$\begin{aligned}
\overrightarrow{\rho}_1 &= -\overrightarrow{r}_2 + \overrightarrow{r}_1, \\
\overrightarrow{\rho}_2 &= -\overrightarrow{r}_3 + \tfrac{1}{2}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2\right), \\
\overrightarrow{\rho}_3 &= -\overrightarrow{r}_5 + \overrightarrow{r}_4 \\
\overrightarrow{\rho}_4 &= -\tfrac{1}{2}\left(\overrightarrow{r}_4 + \overrightarrow{r}_5\right) + \tfrac{1}{3}\left(\overrightarrow{r}_1 + \overrightarrow{r}_2 + \overrightarrow{r}_3\right).
\end{aligned} \tag{3.45}$$

The coordinate of the mass center $\overrightarrow{R}$ is always defined by eq. (3.37)

$$\overrightarrow{R} = \frac{1}{3m + 2M}\left(m(\overrightarrow{r}_1 + \overrightarrow{r}_2 + \overrightarrow{r}_3) + M(\overrightarrow{r}_4 + \overrightarrow{r}_5)\right) \tag{3.46}$$

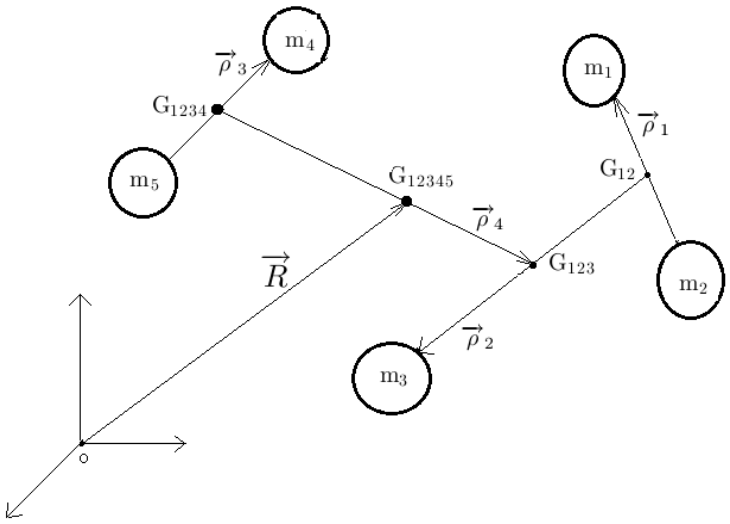

figure 2: Modified choice of Jacobi coordinates
for of a five-body system, configuration (m, m, m, M, M).

After inverting the system of equations (3.7,3.37) we found

$$\begin{aligned}
\overrightarrow{r}_1 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{2M}{2M+3m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_2 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{2M}{2M+3m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_3 &= \overrightarrow{R} - \tfrac{2}{3}\overrightarrow{\rho}_2 + \tfrac{2M}{2M+3m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_4 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_3 - \tfrac{3m}{2M+3m}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_5 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_3 - \tfrac{3m}{2M+3m}\overrightarrow{\rho}_4 \ .
\end{aligned} \tag{3.47}$$

In terms of the velocities relative to the Jacobi coordinates $\dot{\overrightarrow{\rho}}_i$, the kinetic energy of the system reduces to the equation (3.40) but with new expressions for the reduced masses:

$$\mu_{\rho_1} = \frac{m}{2}, \quad \mu_{\rho_2} = \frac{2m}{3}, \quad \mu_{\rho_3} = \frac{M}{2}, \quad \mu_{\rho_4} = \frac{6Mm}{2M+3m} \quad . \tag{3.48}$$

Now, the potential part $V^{(5)}$ eq. (3.43), takes the form

$$V^{(5)} = \frac{1}{2}(3k+2K)\,\overrightarrow{\rho}_1^2 + \frac{2}{3}(3k+2K)\,\overrightarrow{\rho}_2^2 + \frac{1}{2}(3k+2K)\,\overrightarrow{\rho}_1^2 + \frac{2}{3}(3k+2K)\,\overrightarrow{\rho}_2^2 \ , \tag{3.49}$$

where we can see the disappearance of all of the cross terms. Therefore, the relative hamiltonian $H_r^{(5)}$ reduced into a sum of four decoupled harmonic oscillators:

$$\begin{aligned} H_r^{(5)} &= \left[\frac{p_{\rho_1}^2}{2\mu_{\rho_1}} + \frac{1}{2}(3k+2K)\,\overrightarrow{\rho}_1^{\,2}\right] + \left[\frac{p_{\rho_2}^2}{2\mu_{\rho_2}} + \frac{2}{3}(3k+2K)\,\overrightarrow{\rho}_2^{\,2}\right] \\ &\quad + \left[\frac{p_{\rho_3}^2}{2\mu_{\rho_3}} + \frac{1}{2}(3K+2k_{45})\,\overrightarrow{\rho}_3^{\,2}\right] + \left[\frac{p_{\rho_4}^2}{2\mu_{\rho_4}} + 6K\overrightarrow{\rho}_4^{\,2}\right] . \end{aligned} \tag{3.50}$$

The energy spectrum is obtained by summing the energies of the four harmonic oscillators:

$$\begin{aligned} E^{(5)} &= (2n_1+3)\sqrt{\frac{3k+2K}{2m}} + (2n_2+3)\sqrt{\frac{3k+2K}{2m}} \\ &\quad + (2n_3+3)\sqrt{\frac{3K+2k_{45}}{2M}} + (2n_4+3)\sqrt{\frac{(2M+3m)K}{2Mm}} , \end{aligned} \tag{3.51}$$

where n_1, n_2, n_3, and n_4 are positive or zero integers.

The ground state

The energy $E_0^{(5)}$ of the ground state of the system in the configuration (m, m, m, M, M) corresponds then to $n_1 = n_2 = n_3 = n_4 = 0$. We have:

$$E_0^{(5)} = 3\left[\sqrt{\frac{3k+2K}{2m}} + \sqrt{\frac{3k+2K}{2m}} + \sqrt{\frac{3K+2k_{45}}{2M}} + \sqrt{\frac{(2M+3m)K}{2Mm}}\right] , \tag{3.52}$$

3.4 System having three different masses

We have two configurations (m, m, m, M, m_5) and (m, m, M, M, m_5) but we will just study the last one.

Based on the discussion presented in the previous section, we can show that the standard choice of the Jacobi coordinates leads to a diagonal form of the kinetic part of the hamiltonian but a non diagonal form of the potential part with more crossed terms; $(\vec{\rho}_2.\vec{\rho}_3)$, $(\vec{\rho}_2.\vec{\rho}_4)$ and $(\vec{\rho}_3.\vec{\rho}_4)$. So, the wave function that is associated to the ground state contains more parameters $\alpha_1, \alpha_2, ..., \beta_3$, which will be treated as variational parameters

$$\psi_0(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) \propto \exp\left(-\alpha_1 \overrightarrow{\rho}_1^{\,2} - \alpha_2 \overrightarrow{\rho}_2^{\,2} - \alpha_3 \overrightarrow{\rho}_3^{\,2} - \alpha_4 \overrightarrow{\rho}_4^{\,2} - \beta_1 \overrightarrow{\rho}_2.\overrightarrow{\rho}_3 - \beta_2 \overrightarrow{\rho}_2.\overrightarrow{\rho}_4 - \beta_3 \overrightarrow{\rho}_3.\overrightarrow{\rho}_4\right) . \tag{3.53}$$

Consequently, we have to look for a new choice of the Jacobi coordinates that leads to an hamiltonian note necessary diagonal but at least with minimum number of crossed terms leading to a correlated gaussian with minimum number of parameters as the exact wave of ground state.

3.4.1 Configuration (m, m, M, M, m_5) : Modified choice of Jacobi coordinates

The considered system here is formed of five particles whose two first particles are of equal masses $m_1 = m_2 = m$, the third and the fourth particles also have equal masses $m_3 = m_4 = M$ and the last particle with mass m_5.

Our new choice for the Jacobi coordinates are as follows:

The first Jacobi coordinate $\overrightarrow{\rho}_1$ is defined as the relative coordinate between the 1^{st} and 2^{nd} particle. The 2^{nd} Jacobi coordinate $\overrightarrow{\rho}_2$ is defined as the relative coordinate between the 3^{rd} and 4^{th} particule. The 3^{nd} Jacobi coordinate $\overrightarrow{\rho}_3$ is defined as the the vector that connects the center of mass of the 1^{st} and the 2^{nd} particles to the center of mass of 3^{nd} and the 4^{th} particule. The last Jacobi coordinate $\overrightarrow{\rho}_4$ is defined as the relative coordinate between the mass center of the system (m_1, m_2, m_3, m_4) and the last particle m_5. More precisely

$$\begin{aligned}
\overrightarrow{\rho}_1 &= -\overrightarrow{r}_2 + \overrightarrow{r}_1 \\
\overrightarrow{\rho}_2 &= -\overrightarrow{r}_4 + \overrightarrow{r}_3 \\
\overrightarrow{\rho}_3 &= \tfrac{1}{2}\left(-(\overrightarrow{r}_3 + \overrightarrow{r}_4) + (\overrightarrow{r}_1 + \overrightarrow{r}_2)\right) \\
\overrightarrow{\rho}_4 &= \overrightarrow{r}_5 - \tfrac{1}{2m+2M}\left(m(\overrightarrow{r}_1 + \overrightarrow{r}_2) + M(\overrightarrow{r}_3 + \overrightarrow{r}_4)\right).
\end{aligned} \tag{3.54}$$

The coordinate of the center of mass of the system is

$$\overrightarrow{R} = \frac{1}{2m + 2M + m_5}\left(m(\overrightarrow{r}_1 + \overrightarrow{r}_2) + M(\overrightarrow{r}_3 + \overrightarrow{r}_4) + m_5\overrightarrow{r}_5\right). \tag{3.55}$$

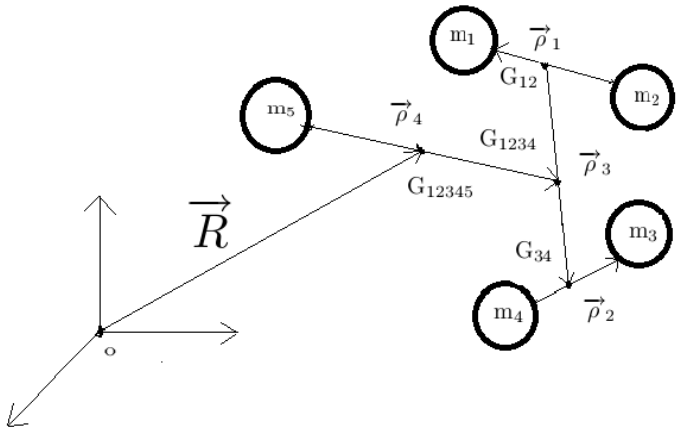

figure 3: Modified choice of Jacobi coordinates
for of a five-body system, configuration (m, m, M, M, m_5).

We can express the coordinates of each particle $\overrightarrow{r}_1$, $\overrightarrow{r}_2$, $\overrightarrow{r}_3$, $\overrightarrow{r}_4$ and $\overrightarrow{r}_5$ in terms of Jacobi $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_4$ and the coordinates of the mass center $\overrightarrow{R}$ by using the system of equations (3.54,3.55). We obtain:

$$\begin{aligned}
\overrightarrow{r}_1 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{M}{M+m}\overrightarrow{\rho}_3 + \tfrac{m_5}{2M+2m+m_5}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_2 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{M}{M+m}\overrightarrow{\rho}_3 + \tfrac{m_5}{2M+2m+m_5}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_3 &= \overrightarrow{R} + \tfrac{1}{2}\overrightarrow{\rho}_2 - \tfrac{m}{M+m}\overrightarrow{\rho}_3 + \tfrac{m_5}{2M+2m+m_5}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_4 &= \overrightarrow{R} - \tfrac{1}{2}\overrightarrow{\rho}_2 - \tfrac{m}{M+m}\overrightarrow{\rho}_3 + \tfrac{m_5}{2M+2m+m_5}\overrightarrow{\rho}_4 \ , \\
\overrightarrow{r}_5 &= \overrightarrow{R} - \tfrac{2M+2m}{2M+2m+m_5}\overrightarrow{\rho}_4 \ .
\end{aligned} \tag{3.56}$$

The kinetic energy

$$T^{(5)} = \frac{1}{2}m\dot{\overrightarrow{r}}_1^{\,2} + \frac{1}{2}m\dot{\overrightarrow{r}}_2^{\,2} + \frac{1}{2}M\dot{\overrightarrow{r}}_3^{\,2} + \frac{1}{2}M\dot{\overrightarrow{r}}_4^{\,2} + \frac{1}{2}m_5\dot{\overrightarrow{r}}_5^{\,2},$$

can then be reduced in terms of the velocities relative to the Jacobi coordinates as:

$$T^{(5)} = \frac{1}{2}\left(2M + 2m + m_5\right)\dot{\overrightarrow{R}}^{\,2} + \frac{1}{4}m\dot{\overrightarrow{\rho}}_1^{\,2} + \frac{1}{4}M\dot{\overrightarrow{\rho}}_2^{\,2} + \frac{Mm}{M+m}\dot{\overrightarrow{\rho}}_3^{\,2} + m_5\frac{M+m}{2M+2m+m_5}\dot{\overrightarrow{\rho}}_4^{\,2}$$

or in terms of conjugate momenta eq. (3.54) with the folowing reduced masses

$$\mu_{\rho_1} = \frac{m}{2},\ \mu_{\rho_2} = \frac{M}{2},\ \mu_{\rho_3} = 2\frac{Mm}{M+m},\ \mu_{\rho_4} = 2m_5\frac{M+m}{2M+2m+m_5}. \tag{3.57}$$

Of course, $\mu_R = 2M + 2m + m_5 = \mathbf{M}$, total mass of the system is the reduced mass relative to the center of mass.

The expression of the potential energy $V^{(5)}$ simplifies to:

$$\begin{aligned} V^{(5)} = \quad & k_{12}(\overrightarrow{r}_1 - \overrightarrow{r}_2)^2 + k_{13}(\overrightarrow{r}_1 - \overrightarrow{r}_3)^2 + k_{13}(\overrightarrow{r}_1 - \overrightarrow{r}_4)^2 + k_{15}(\overrightarrow{r}_1 - \overrightarrow{r}_5)^2 \\ & + k_{13}(\overrightarrow{r}_2 - \overrightarrow{r}_3)^2 + k_{13}(\overrightarrow{r}_2 - \overrightarrow{r}_4)^2 + k_{15}(\overrightarrow{r}_2 - \overrightarrow{r}_5)^2 \\ & + k_{34}(\overrightarrow{r}_3 - \overrightarrow{r}_4)^2 + k_{35}(\overrightarrow{r}_3 - \overrightarrow{r}_5)^2 \\ & + k_{35}(\overrightarrow{r}_4 - \overrightarrow{r}_5)^2 \ , \\ = \quad & \tfrac{1}{2}\left(2k_{12} + 2k_{13} + k_{15}\right)_1^2 \overrightarrow{\rho} + \tfrac{1}{2}\left(2k_{13} + 2k_{34} + k_{35}\right)\overrightarrow{\rho}_2^2 \\ & + 2\tfrac{2M^2k_{13} + M^2k_{15} + 2m^2k_{13} + m^2k_{35} + 4Mmk_{13}}{(M+m)^2}\overrightarrow{\rho}_3^2 + 2\left(k_{15} + k_{35}\right)\overrightarrow{\rho}_4^2 + 4\tfrac{Mk_{15} - mk_{35}}{M+m}\overrightarrow{\rho}_3.\overrightarrow{\rho}_4 \ , \end{aligned} \tag{3.58}$$

where we have taken into account the symmetry of the problem, which gives rise to the folowing constraints

$$\begin{aligned} k_{13} = \quad & k_{14} = k_{23} = k_{24} \ , \\ k_{15} = \quad & k_{25} \ , \\ k_{35} = \quad & k_{45} \ . \end{aligned} \tag{3.59}$$

The potential term eq. (3.58) appears in a quadratic form in the variables $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$ and $\overrightarrow{\rho}_4$ with only one non diagonal term $(\overrightarrow{\rho}_3.\overrightarrow{\rho}_4)$. The hamiltonian takes also a non diagonal form describing two decoupled harmonic oscillators (relative to $\overrightarrow{\rho}_1$ and $\overrightarrow{\rho}_2$) and two coupled harmonic oscillators (relative to $\overrightarrow{\rho}_3$ and $\overrightarrow{\rho}_4$). So without going through the derivation of the hamiltonian, it is clear that the ground state will be described by a correlated gaussian with a single cross term $(\overrightarrow{\rho}_3.\overrightarrow{\rho}_4)$. That is to say

$$\psi_0(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) \propto \quad \exp\left(-\alpha_1\overrightarrow{\rho}_1^2 - \alpha_2\overrightarrow{\rho}_2^2 - \alpha_3\overrightarrow{\rho}_3^2 - \alpha_4\overrightarrow{\rho}_4^2 + \beta_1\overrightarrow{\rho}_3.\overrightarrow{\rho}_4\right) \quad . \tag{3.60}$$

Chapter 4

Expansion over correlated gaussians

In this chapter we will present in detail the method of expansion on correlated gaussians applied to five-body systems. We will then apply the method to solve approximately the Schrödinger equation by approximately determining the wave function.

4.1 Ritz variational theorem

The method of variations known as the Ritz method is a method widely used to approximate the ground state of a stationary system. [17].

Let us consider a system described by a time-independent hamiltonian H whose solutions are not known a priori. However, we know that this hamiltonian has eigenvectors which form a complete basis of the state space. To simplify the writing we will admit that the spectrum of H is discrete (only certain frequencies appear) and not degenerate. It comes:

$$H\left|u_n\right\rangle = E\left|u_n\right\rangle \ , \tag{4.1}$$

with $n = 0, 1, 2, ...$ and:

$$E_0 \leq E_1 \leq ... \leq E_n \leq ... \ . \tag{4.2}$$

Each vector $|\psi\rangle$ of the state space may be developed on the base of eign-vectors of H.

$$\left|\psi\right\rangle = \sum_n c_n \left|u_n\right\rangle , \tag{4.3}$$

where the c_n are coefficients of the development. The mean value of the system energy in the state $|\psi\rangle$ is:

$$\begin{aligned}\langle E\rangle &= \frac{\langle\psi|\, H\,|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_m \left(c_m^* \langle u_m|\right) \sum_n H\left(c_n\,|u_n\rangle\right)}{\sum_m \langle u_m|\, c_m^* \sum_n c_n\,|u_n\rangle}, \\ &= \frac{\sum_{m,n} c_m^* c_n E_n \langle u_m|u_n\rangle}{\sum_{m,n} c_m^* c_n E_n \langle u_m|u_n\rangle}.\end{aligned} \tag{4.4}$$

Knowing that $\langle u_m|u_n\rangle = \delta_{m,n}$, it comes that:

$$\langle E\rangle = \frac{\sum_n |c_n|^2 E_n}{\sum_n |c_n|^2}.$$

Under the assumption eq. (4.2) we can deduce that:

$$\langle E\rangle = \frac{\langle\psi|\, H\,|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0. \tag{4.5}$$

The formule eq. (4.5) is the master equation of the variations theorem. It stipulates that the average value of H for any state $|\psi\rangle$ constitutes on approximate value by the excess of the ground state energy E_0. There is a strict equality when the state $|\psi\rangle$ is eignvector of H associated to the energy E_0. In other words, the mean value of the hamiltonian in any state $|\psi\rangle$ is always greater than the ground state energy.

4.2 Variational method

The variational method is a very useful approximation technique. It is based on the Ritz variational principle [18]. The result eq. (4.5) lies at the origin of the variational method. A possible use of this result consists in taking a wave function, depending on a certain number n of parameters $\lambda_1, \lambda_2, ..., \lambda_n$, called *trial wave function*, to evluate the mean value of the hamiltonian for this trial wave function. Then, we get a family of upper bounds for the ground state energy E_0, an upper bound $E(\lambda_1, ..., \lambda_n)$, for each set of parameters $\lambda_1, ..., \lambda_n$. The set of parameters $\lambda_1^0, ..., \lambda_n^0$ as:

$$E(\lambda_1^0, ..., \lambda_n^0) = \min_{\lambda_1,....,\lambda_n} \frac{\langle\psi|\, H\,|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{4.6}$$

leads to a value that is closest to E_0, i.e. the best approximation for the ground state energy. $E(\lambda_1^0, ..., \lambda_n^0)$ is called variational approximation of E_0. Of course $E(\lambda_1^0, ..., \lambda_n^0)$ stills always above E_0 [14].

$$E_0 \leq \frac{\left\langle \psi\left(\lambda_1^0, ..., \lambda_n^0\right) \right| H \left| \psi\left(\lambda_1^0, ..., \lambda_n^0\right) \right\rangle}{\left\langle \psi\left(\lambda_1^0, ..., \lambda_n^0\right) \right| \left. \psi\left(\lambda_1^0, ..., \lambda_n^0\right) \right\rangle} \ , \tag{4.7}$$

4.2.1 Choice of the trial wave function

Given a system of N particles of masses $m_1, m_2, ..., m_N$ interacting by forces depending only on the distance between these bodies, the hamiltonian of the system is written:

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m_i} + \sum_{i<j=1}^{N} V^{(ij)}\left(r_{ij}\right) \ . \tag{4.8}$$

By making a choice of Jacobi coordinates $\{\vec{\rho}_k\}$, the relative hamiltonian can be put in the form:

$$H_r = \sum_{i=1}^{N-1} \frac{\vec{p}_{\rho_i}^2}{2\mu_i} + \sum_{i<j=1}^{N} V^{(ij)}\left(r_{ij}\left\{\vec{\rho}_k\right\}\right), \tag{4.9}$$

where $\overrightarrow{p}_{\rho_i}$ denotes the conjucated momentum of the i^{rd} Jacobi's coordinates $\overrightarrow{\rho}_i$ and μ_i is a reduced mass relative to that coordinate. The potential $V^{(ij)}(r_{ij}\{\vec{\rho}_k\})$ must be considered as function of the Jacobi coordinates $\vec{\rho}_k$:

$$\overrightarrow{r}_{ij} = \sum_{k=1}^{N-1} d_{ij}^k \overrightarrow{\rho}_k \ . \tag{4.10}$$

The d_{ij}^k which are the development coefficients of $\overrightarrow{r}_{ij}$ on the $\overrightarrow{x}_k$ can be eventually considered as column matrix elements $(N-1) \times 1$, noted d_{ij}.

On the base of the obtained results in the previous chapter, it is obvious that the wave function associated to the ground state of the N-body harmonic oscillator must be in general a correlated gaussian. Therefore, the choice of a gaussian as a trial wave function seems to be a suitable to cover the exact result of the N-body harmonic oscillator case (We are always talking about the ground state).

The method of systematic expansion on correlated Gaussians, which is one of the most used methods for the approximate resolution of the Schrödinger equation for systems with a small number of bodies, consists in adopting:

$$\psi\left(\vec{\rho}_1...\vec{\rho}_{N-1}\right) = \sum_{n=1}^{g} c_n \exp\left(\frac{-1}{2}\sum_{i,j=1}^{N-1} A_{ij}^{(n)}\vec{\rho}_i.\vec{\rho}_j\right), \tag{4.11}$$

as a trial wave function. The range parameters $A_{ij}^{(n)}$ can be considered as elements of a is a real, symmetric and positive definite square matrix $A^{(n)}$ of order $(N-1)$. g is called the number of generations of gaussians. The weight parameters c_n and the range parameters $A_{ij}^{(n)}$ will be determined by a variational procedure. If we adopt the following notation:

$$\left\langle\vec{\rho}_1...\vec{\rho}_{N-1}|m\right\rangle \equiv \exp\left(\frac{-1}{2}\sum_{i,j=1}^{N-1} A_{ij}^{(n)}\vec{\rho}_i.\vec{\rho}_j\right). \tag{4.12}$$

The state vector may be put under the form:

$$|\psi\rangle = \sum_{m=1}^{g} c_m |m\rangle . \tag{4.13}$$

The mean value of any observable Λ evaluated in the state $|\psi\rangle$, eq. (4.13), will be given by the expression:

$$\langle\Lambda\rangle_\psi = \frac{\sum_{m,n=1}^{g} c_n^* c_m \ \langle n|\Lambda|m\rangle}{\sum_{m,n=1}^{g} c_n^* c_m \ \langle n|m\rangle}. \tag{4.14}$$

Therefore, the calculation of the average value of an observable is reduced to that of the matrix elements of the observable in question between two correlated Gaussians $\langle n|\Lambda|m\rangle$ and to the evaluation of the overlaps of Gaussians $\langle n|m\rangle$.

4.2.2 The hamiltonian

The calculation of the hamiltonian matrix elements of the system between two correlated gaussians $\langle n|H|m\rangle$, leads to the calculation of the matrix elements of the kinetic and potential

energy terms between two correlated gaussians:

$$\langle n|\,\frac{\overrightarrow{p}^{\,2}_{\rho_i}}{2\mu_i}\,|m\rangle \qquad i{=}1,2,...,N-1 \qquad \text{et} \qquad \langle n|\,V_{ij}\left(r_{ij}\{\overrightarrow{\rho}_k\}\right)|m\rangle \quad i{<}j{=}1,2,...,N. \tag{4.15}$$

Consider successively the potential energy terms and the kinetic one.

4.2.3 The potential energy

Our problem leads to the calculation of the matrix element of any function $f(\overrightarrow{r}_{ij})$ of variable $\overrightarrow{r}_{ij}$ $i{<}j{=}1,2,...,N$ between two correlated gaussian $\langle n|\,f\left(\overrightarrow{r}_{ij}\right)|m\rangle$. We have:

$$\langle n|\,f\left(\overrightarrow{r}_{ij}\right)|m\rangle = \int\cdots\int d^3\overrightarrow{\rho}_1...d^3\overrightarrow{\rho}_{N-1} f\left(\overrightarrow{r}_{ij}\right)\exp\left(-\tfrac{1}{2}\textstyle\sum_{k,l=1}^{N-1}\left(A^{(n)}_{kl}+A^{(m)}_{kl}\right)\overrightarrow{\rho}_k.\overrightarrow{\rho}_l\right). \tag{4.16}$$

If we pose

$$A_{kl} = \frac{1}{2}(A^{(n)}_{kl}+A^{(m)}_{kl})\ , \tag{4.17}$$

the previous expression may be put under the form:

$$\langle n|\,f\left(\overrightarrow{r}_{ij}\right)|m\rangle = \int\cdots\int d^3\overrightarrow{\rho}_1...d^3\overrightarrow{\rho}_{N-1} f\left(\overrightarrow{r}_{ij}\right)\exp\left(-\sum_{k,l=1}^{N-1}A_{kl}\overrightarrow{\rho}_k.\overrightarrow{\rho}_l\right). \tag{4.18}$$

By doing an orthogonal transformation R :

$$R^TR = RR^T = I\ , \tag{4.19}$$

on A and let us choose it in such a way as to reduce A into its diagonal form, which we will denote by $\tilde{A}$

$$RAR^T = \tilde{A}\ . \tag{4.20}$$

We can also express A in function of $\tilde{A}$:

$$A = R^T\tilde{A}R\ . \tag{4.21}$$

The argument of the exponential occurring in the expression of $\langle n|\,f\left(\overrightarrow{r}_{ij}\right)|m\rangle$ can then be

put in the form:

$$\sum_{k,l=1}^{N-1} A_{kl}\,\overrightarrow{\rho}_k.\overrightarrow{\rho}_l = \sum_{k,l,n,m=1}^{N-1} R^T_{km}\widetilde{A}_{mn}R_{nl}\,\overrightarrow{\rho}_k.\overrightarrow{\rho}_l = \sum_{n,m=1}^{N-1}\widetilde{A}_{mn}\,\overrightarrow{y}_m.\overrightarrow{y}_n = \sum_{n=1}^{N-1}\widetilde{A}_{nn}\,\overrightarrow{y}^2_n, \quad (4.22)$$

where we introduce a new Jacobi coodinates $\{\overrightarrow{y}_k\}$ linked to the old ones $\{\overrightarrow{\rho}_k\}$ by the relations:

$$\overrightarrow{y}_k = \sum_{l=1}^{N-1} R_{kl}\,\overrightarrow{\rho}_l\ , \quad (4.23)$$

that's to say that the $\{\overrightarrow{\rho}_k\}$ and $\{\overrightarrow{y}_k\}$ are related by an orthogonal transformation, the one that reduced A to its diagonal form $\tilde{A}$. To obtain eq. (4.22), we also used the fact that $\tilde{A}$ is a diagonal matrix.

On the other hand, we can notice that the integration element $d^3\overrightarrow{\rho}_1...d^3\overrightarrow{\rho}_{N-1}$ is an invariant under an orthogonal transformation. So,

$$d^3\overrightarrow{\rho}_1...d^3\overrightarrow{\rho}_{N-1} = d^3\overrightarrow{y}_1...d^3\overrightarrow{y}_{N-1} \quad (4.24)$$

and $\langle n|\,f\,(\overrightarrow{r}_{ij})\,|m\rangle$ can be put in the form:

$$\langle n|\,f\,(\overrightarrow{r}_{ij})\,|m\rangle = \int\cdots\int d^3\overrightarrow{y}_1...d^3\overrightarrow{y}_{N-1} f(\overrightarrow{r}_{ij})\exp\left(-\sum_{k=1}^{N-1}\widetilde{A}_{kk}\,\overrightarrow{y}^2_k\right), \quad (4.25)$$

where $\overrightarrow{r}_{ij}$ must now be considered as a function of $\overrightarrow{y}_k$.

By inversing eqs. (4.23) we get the $\overrightarrow{\rho}_k$ in terms of $\overrightarrow{y}_l$.

$$\overrightarrow{\rho}_k = \sum_{l=1}^{N-1} R^T_{kl}\,\overrightarrow{y}_l\ , \quad (4.26)$$

Then, by reporting in eq. (4.10), we get:

$$\overrightarrow{r}_{ij} = \sum_{l=1}^{N-1}\left(\sum_{k=1}^{N-1} d^k_{ij}\,R^T_{kl}\right)\overrightarrow{y}_l\ . \quad (4.27)$$

Now, let's do a scale transformation on the $\{\overrightarrow{y}_l\}$:

$$\overrightarrow{Z} = \left(\tilde{A}_{ll}\right)^{1/2}\overrightarrow{y}_l\ . \quad (4.28)$$

We have

$$\exp\left(-\sum_{k=1}^{N-1}\tilde{A}_{kk}\,\overrightarrow{y}_k^2\right)=\exp\left(-\sum_{k=1}^{N-1}\overrightarrow{Z}_k^2\right)\ , \tag{4.29}$$

and

$$\begin{aligned} d^3\overrightarrow{y}_1...d^3\overrightarrow{y}_{N-1} &= \left(\tilde{A}_{11}\right)^{-3/2}d^3\overrightarrow{Z}_1...\left(\tilde{A}_{N-1,N-1}\right)^{-3/2}d^3\overrightarrow{Z}_{N-1}\ , \\ &= (\Delta)^{-3/2}\,d^3\overrightarrow{Z}_1...d^3\overrightarrow{Z}_{N-1}\ . \end{aligned}$$

The matrix element $\langle n\mid f(\overrightarrow{r}_{ij})\mid m\rangle$ is put then under the form:

$$\langle n|\,f\,(\overrightarrow{r}_{ij})\,|m\rangle=(\Delta)^{-3/2}\int\cdots\int d^3\overrightarrow{Z}_1...d^3\overrightarrow{Z}_{N-1}f(\overrightarrow{r}_{ij})\exp\left(-\sum_{k=1}^{N-1}\overrightarrow{Z}_k^2\right), \tag{4.30}$$

where Δ designates the determinant of the matrix A. It should be noted that $\overrightarrow{r}_{ij}$ in the previous expression must now be considered as a function of the $\overrightarrow{Z}_k$

$$\overrightarrow{r}_{ij}=\sum_{l=1}^{N-1}\left(\sum_{k=1}^{N-1}d_{ij}^k R_{kl}^T\right)(\widetilde{A}_{ll})^{-1/2}\overrightarrow{Z}_l\ . \tag{4.31}$$

It is always possible to perform an orthogonal transformation on the $\overrightarrow{Z}_k$ ($\{\overrightarrow{Z}_k\}\rightarrow\{\overrightarrow{W}_k\}$) such that $\overrightarrow{r}_{ij}$ is proportional to $\overrightarrow{W}_1$. It is clear that, taking into account the fact that:

$$A^{-1}=R^T\tilde{A}^{-1}R\ , \tag{4.32}$$

the proportionality factor is:

$$\begin{aligned} \left[\sum_{k,n=1}^{N-1}\sum_{l,m=1}^{N-1}(d_{ij}^kR_{kl}^T(\widetilde{A}_{ll})^{\frac{-1}{2}})(d_{ij}^nR_{nm}^T(\widetilde{A}_{mm})^{\frac{-1}{2}})\delta_{l,m}\right]^{\frac{1}{2}} &= \left[\sum_{k,n=1}^{N-1}\sum_{l=1}^{N-1}d_{ij}^kR_{kl}^T(\widetilde{A}_{ll})^{-1}R_{ln}d_{ij}^n\right]^{\frac{1}{2}} \\ &= \left[d_{ij}^TA^{-1}d_{ij}\right]^{\frac{1}{2}}. \end{aligned}$$

As $d^3\overrightarrow{Z}_1...d^3\overrightarrow{Z}_{N-1}$ and $\sum_{k=1}^{N-1}\overrightarrow{Z}_k^2$ are invariants under any orthogonal transformation:

$$\langle n|\,f\,(\overrightarrow{r}_{ij})\,|m\rangle=(\Delta)^{-3/2}\int...\int d^3\overrightarrow{W}_1...d^3\overrightarrow{W}_{N-1}f\left(\sqrt{d_{ij}^TA^{-1}d_{ij}}\overrightarrow{W}_1\right)\exp\left(-\sum_{k=1}^{N-1}\overrightarrow{W}_k^2\right).$$

If we use the result

$$\int \exp\left(-\overrightarrow{r}^2\right) d^3\overrightarrow{r} = \pi^{3/2}, \tag{4.33}$$

the integration on $\overrightarrow{W}_2, \overrightarrow{W}_3, ..., \overrightarrow{W}_{N-1}$ is immediate. It follows that:

$$\langle n| f\left(\overrightarrow{r}_{ij}\right)|m\rangle = (\Delta)^{-3/2}(\pi)^{3(N-2)/2}\int d^3\overrightarrow{W}_1 f\left(\left(d_{ij}^T A^{-1} d_{ij}\right)^{1/2}\overrightarrow{W}_1\right)\exp\left(-\overrightarrow{W}_1^2\right). \tag{4.34}$$

If we make the change of variable

$$\overrightarrow{W}_1' = \left(d_{ij}^T A^{-1} d_{ij}\right)^{1/2}\overrightarrow{W}_1\ , \tag{4.35}$$

$\langle n| f\left(\overrightarrow{r}_{ij}\right)|m\rangle$ can be rewriten under the form:

$$\begin{aligned}\langle n| f\left(\overrightarrow{r}_{ij}\right)|m\rangle &= (\Delta)^{-3/2}(\pi)^{3(N-2)/2}\left(d_{ij}^T A^{-1} d_{ij}\right)^{-3/2} \\ &\times\int d^3\overrightarrow{W}_1' f\left(\overrightarrow{W}_1'\right)\exp\left(-\left(d_{ij}^T A^{-1} d_{ij}\right)^{-1}\overrightarrow{W}_1'^2\right).\end{aligned} \tag{4.36}$$

From eq. (4.34), we can deduce the overlap of two gaussians by setting $f(\overrightarrow{r}_{ij}) = 1$. We get:

$$\langle n|\, m\rangle = \left(\pi^{N-1}/\Delta\right)^{3/2}. \tag{4.37}$$

We can use this expression of $\langle n|\, m\rangle$ to rewrite $\langle n| f\left(\overrightarrow{r}_{ij}\right)|m\rangle$ under the following form:

$$\langle n| f\left(\overrightarrow{r}_{ij}\right)|m\rangle = \langle n|\, m\rangle\pi^{-3/2}\int d^3\overrightarrow{W}_1 f\left(\left(d_{ij}^T A^{-1} d_{ij}\right)^{1/2}\overrightarrow{W}_1\right)\exp\left(-\overrightarrow{W}_1^2\right). \tag{4.38}$$

Suppose now that the interactions between the particles of the system are described by power law potentials:

$$V(\overrightarrow{r}_{ij}) = \lambda_{ij} r_{ij}^{\nu_{ij}}\ . \tag{4.39}$$

The expression eq. (4.38) reduces to:

$$\langle n|\,\lambda_{ij} r_{ij}^{\nu_{ij}}\,|m\rangle = \langle n|\, m\rangle\pi^{-3/2}\lambda_{ij}\left(d_{ij}^T A^{-1} d_{ij}\right)^{\nu_{ij}/2}\int d^3\overrightarrow{W}_1 W_1^{\nu_{ij}}\exp\left(-\overrightarrow{W}_1^2\right). \tag{4.40}$$

By using the result

$$\int d^3\overrightarrow{W}_1 W_1^{\nu_{ij}} e^{-\overrightarrow{W}_1^2} = 4\pi \int_0^\infty dW_1 W_1^{\nu_{ij}+2} e^{-W_1^2} = 2\pi\Gamma\left(\frac{\nu_{ij}+3}{2}\right) \quad \text{pour} \quad \nu_{ij} > -3, \tag{4.41}$$

We finally get

$$\langle n|\, \lambda_{ij} r_{ij}^{\nu_{ij}}\, |m\rangle = \langle n|\, m\rangle \frac{2\lambda_{ij}}{\sqrt{\pi}} \left(d_{ij}^T A^{-1} d_{ij}\right)^{\nu_{ij}/2} \Gamma\left(\frac{\nu_{ij}+3}{2}\right), \tag{4.42}$$

which can be rewriten as

$$\langle n|\, \lambda_{ij} r_{ij}^{\nu_{ij}}\, |m\rangle = \langle n|\, m\rangle \frac{2\lambda_{ij}}{\sqrt{\pi}} \Gamma\left(\frac{\nu_{ij}+3}{2}\right) \gamma_{ij,ij}^{\nu_{ij}/2}\ , \tag{4.43}$$

if we introduce the notation

$$\gamma_{ij,kl} = d_{ij}^T A^{-1} d_{kl}. \tag{4.44}$$

4.2.4 The kinetic energy

Let's calculate the matrix element $\langle n|\, \overrightarrow{p}_k^2/\left(2\mu_k\right) |m\rangle$. We have

$$\langle n|\, \frac{\overrightarrow{p}_k^2}{2\mu_k}\, |m\rangle = \frac{1}{2\mu_k} \left(\langle n|\, \overrightarrow{p}_k\right) \left(\overrightarrow{p}_k\, |m\rangle\right). \tag{4.45}$$

Using the relationship that defines the correlated gaussians eq. (4.12), we get

$$\overrightarrow{p}_k\, |m\rangle = i\hbar \sum_{p=1}^{N-1} A_{kp}^m \overrightarrow{\rho}_p\, |m\rangle\,. \tag{4.46}$$

It is follows that

$$\langle n|\, \frac{\overrightarrow{p}_k^2}{2\mu_k}\, |m\rangle = \frac{\hbar^2}{2\mu_k} \sum_{q,p=1}^{N-1} A_{kq}^n A_{kp}^m \langle n|\, \overrightarrow{\rho}_q.\overrightarrow{\rho}_p\, |m\rangle\,. \tag{4.47}$$

So, this leads us to calculate the matrix elements of $\overrightarrow{\rho}_q.\overrightarrow{\rho}_p$. We have:

$$\langle n|\, \overrightarrow{\rho}_q.\overrightarrow{\rho}_p\, |m\rangle = \int\cdots\int d^3\overrightarrow{x}_1 ... d^3\overrightarrow{x}_{N-1} \left(\overrightarrow{\rho}_q.\overrightarrow{\rho}_p\right) \exp\left(-\sum_{i,j=1}^{N-1} A_{ij}\overrightarrow{\rho}_i.\overrightarrow{\rho}_j\right). \tag{4.48}$$

In terms of $\overrightarrow{y}_k$, eq. (4.27) takes the following form:

$$\langle n|\,\overrightarrow{\rho}_q.\overrightarrow{\rho}_p\,|m\rangle = \sum_{i,j=1}^{N-1} R^{-1}_{qi}R^{-1}_{pj}\int\cdots\int d^3\overrightarrow{y}_1...d^3\overrightarrow{y}_{N-1}\,(\overrightarrow{y}_i.\overrightarrow{y}_j)\exp\left(-\sum_{k=1}^{N-1}\widetilde{A}_{kk}\,\overrightarrow{y}^2_k\right). \quad (4.49)$$

The integral appearing in the right-hand side of the previous expression is zero for $i \neq j$, because we have to integrate an odd function of $\overrightarrow{y}_i$ (and of $\overrightarrow{y}_j$). So

$$\langle n|\,\overrightarrow{\rho}_q.\overrightarrow{\rho}_p\,|m\rangle = \sum_{j=1}^{N-1} R^{T}_{qj}R_{jp}\int\cdots\int d^3\overrightarrow{y}_1...d^3\overrightarrow{y}_{N-1}\,\overrightarrow{y}^2_j\exp\left(-\sum_{k=1}^{N-1}\widetilde{A}_{kk}\,\overrightarrow{y}^2_k\right). \quad (4.50)$$

By using the result

$$\int_{-\infty}^{\infty}\overrightarrow{r}^2\exp(-a\,\overrightarrow{r}^2)d^3\overrightarrow{r} = \frac{3}{2a}\left(\frac{\pi}{a}\right)^{3/2}\ , \quad (4.51)$$

valid for $a > 0$, we end up with

$$\begin{aligned}\langle n|\,\overrightarrow{\rho}_q.\overrightarrow{\rho}_p\,|m\rangle &= \frac{3}{2}\left(\frac{\pi}{\Delta}\right)^{3/2}\pi^{\frac{3(N-2)}{2}}\sum_{j=1}^{N-1}R^{T}_{qj}\widetilde{A}^{-1}_{jj}R_{jp}\\ &= \frac{3}{2}\left(\frac{\pi}{\Delta}\right)^{3/2}\pi^{\frac{3(N-2)}{2}}A^{-1}_{qp}\\ &= \frac{3}{2}\langle n|\,m\rangle A^{-1}_{qp}. \end{aligned} \quad (4.52)$$

Finally, by reporting in the expression eq. (4.47), we obtain:

$$\begin{aligned}\langle n|\,\frac{\overrightarrow{p}^2_k}{2\mu_k}\,|m\rangle &= \frac{3}{2}\langle n|\,m\rangle\frac{\hbar^2}{2\mu_k}\sum_{q,p=1}^{N-1}A^n_{kq}A^{-1}_{qp}A^m_{kp},\\ &= \frac{3}{2}\langle n|\,m\rangle\frac{\hbar^2}{2\mu_k}\left(A^nA^{-1}A^m\right)_{kk}\ . \end{aligned} \quad (4.53)$$

This leads to the expression for the kinetic energy matrix element between two correlated Gaussians

$$\langle n|\,T\,|m\rangle = \frac{3}{2}\langle n|\,m\rangle\sum_{k=1}^{N-1}\frac{\hbar^2}{2\mu_k}\left(A^nA^{-1}A^m\right)_{kk}. \quad (4.54)$$

The matrix element of the hamiltonian between two correlated gaussians in the case of power law potentials eq. (4.39) therefore reduces to:

$$\langle n|\, H\, |m\rangle = \langle n|\, m\rangle \left[\frac{3}{2}\sum_{k=1}^{N-1}\frac{\hbar^2}{2\mu_k}\left(A^n A^{-1} A^m\right)_{kk} + \frac{2\lambda_{ij}}{\sqrt{\pi}}\Gamma\left(\tfrac{\nu_{ij}+3}{2}\right)\gamma_{ij,ij}^{\nu_{ij}/2}\right]. \tag{4.55}$$

Let us give as an example the mean value of the hamiltonian for a single generation of gaussians $|1\rangle$ in the case of a power law potential eq. (4.39). We get:

$$\frac{\langle 1|\, H\, |1\rangle}{\langle 1|\, 1\rangle} = \frac{3}{2}\sum_{k=1}^{N-1}\frac{\hbar^2}{2\mu_k}A_{kk} + \frac{2}{\sqrt{\pi}}\sum_{i<j=1}^{N}\Gamma\left(\tfrac{\nu_{ij}+3}{2}\right)\lambda_{ij}\gamma_{ij,ij}^{\nu_{ij}/2}. \tag{4.56}$$

The variational approximation $E_{0var}^{5)}$ for the ground state energy will be obtained by minimization of $\langle 1|\, H\, |1\rangle \,/\, \langle 1|\, 1\rangle$ with respect to the parameters A_{ij}.

$$E_{0var}^{(5)} = \min_{\{A_{ij}\}}\frac{\langle 1|\, H\, |1\rangle}{\langle 1|\, 1\rangle} = \frac{3}{2}\sum_{k=1}^{N-1}\frac{\hbar^2}{2\mu_k}A_{kk} + \frac{2}{\sqrt{\pi}}\sum_{i<j=1}^{N}\Gamma\left(\tfrac{\nu_{ij}+3}{2}\right)\lambda_{ij}\gamma_{ij,ij}^{\nu_{ij}/2}. \tag{4.57}$$

4.3 Application to the five-body problem

Knowing that the treatment of the N-body problem requires the introduction of a set of $N-1$ Jacobi coordinates, four Jacobi coordinates are required to treat the five-body problems. That is: $\overrightarrow{\rho}_1$, $\overrightarrow{\rho}_2$, $\overrightarrow{\rho}_3$ and $\overrightarrow{\rho}_4$. The trial wave function is therefore chosen as a series of correlated gaussians eq. (4.11) with $N = 5$:

$$\begin{aligned}
\langle \vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \overrightarrow{\rho}_4|\psi\rangle \equiv & \sum_{n=1}^{g} c_n \exp(\tfrac{-1}{2}\sum_{i,j=1}^{5} A_{ij}^{(n)}\vec{\rho}_i.\vec{\rho}_j), \\
= & \sum_{n=1}^{g} c_n \exp\Big[\tfrac{-1}{2}(A_{11}^{(n)}\vec{\rho}_1^{\,2} + A_{22}^{(n)}\vec{\rho}_2^{\,2} + A_{33}^{(n)}\vec{\rho}_3^{\,2} + A_{44}^{(n)}\vec{\rho}_4^{\,2} \\
& + 2A_{12}^{(n)}\vec{\rho}_1.\vec{\rho}_2 + 2A_{13}^{(n)}\vec{\rho}_1.\vec{\rho}_3 + 2A_{14}^{(n)}\vec{\rho}_1.\vec{\rho}_4), \\
& + 2A_{23}^{(n)}\vec{\rho}_2.\vec{\rho}_3 + 2A_{24}^{(n)}\vec{\rho}_2.\vec{\rho}_4 + 2A_{34}^{(n)}\vec{\rho}_3.\vec{\rho}_4\Big] \ ,
\end{aligned} \tag{4.58}$$

where the parameters of weight c_n and the range parameters $A_{11}^{(n)}$, $A_{22}^{(n)}$, $A_{33}^{(n)}$, $A_{44}^{(n)}$, $A_{12}^{(n)}$, $A_{13}^{(n)}$, $A_{14}^{(n)}$, $A_{23}^{(n)}$, $A_{24}^{(n)}$ and $A_{34}^{(n)}$ are considered as variationals parameters.

The range parameters for each correlated gaussian can be considered as elements of a sym-

metric matrix of order 4:

$$A^{(n)} = \begin{pmatrix} A_{11}^{(n)} & A_{12}^{(n)} & A_{13}^{(n)} & A_{14}^{(n)} \\ A_{12}^{(n)} & A_{22}^{(n)} & A_{23}^{(n)} & A_{24}^{(n)} \\ A_{13}^{(n)} & A_{23}^{(n)} & A_{33}^{(n)} & A_{34}^{(n)} \\ A_{14}^{(n)} & A_{24}^{(n)} & A_{34}^{(n)} & A_{44}^{(n)} \end{pmatrix} . \tag{4.59}$$

The matrix element of the hamiltonian between two gaussians reduces to:

$$\begin{aligned} \frac{\langle n| H |m\rangle}{\langle n|m\rangle} = & \frac{3}{4}\Big[\frac{1}{\mu_1}(A^{(n)}A^{-1}A^{(m)})_{11}+\frac{1}{\mu_2}(A^{(n)}A^{-1}A^{(m)})_{22}+\frac{1}{\mu_3}(A^{(n)}A^{-1}A^{(m)})_{33}+\frac{1}{\mu_4}(A^{(n)}A^{-1}A^{(m)})_{44}\Big] \\ & +\frac{2}{\sqrt{\pi}}\Gamma(\tfrac{\nu+3}{2})\left[\lambda_{12}\gamma_{12,12}^{\nu/2}+\lambda_{13}\gamma_{13,13}^{\nu/2}+\lambda_{14}\gamma_{14,14}^{\nu/2}+\lambda_{15}\gamma_{15,15}^{\nu/2}+\lambda_{23}\gamma_{23,23}^{\nu/2}\right] \\ & +\frac{2}{\sqrt{\pi}}\Gamma(\tfrac{\nu+3}{2})\left[\lambda_{24}\gamma_{24,24}^{\nu/2}+\lambda_{25}\gamma_{25,25}^{\nu/2}+\lambda_{34}\gamma_{34,34}^{\nu/2}+\lambda_{35}\gamma_{35,35}^{\nu/2}+\lambda_{45}\gamma_{45,45}^{\nu/2}\right], \end{aligned} \tag{4.60}$$

where A^{-1} is the inverse of the folowing diagonal matrix:

$$A = \begin{pmatrix} \frac{1}{2}(A_{11}^{(n)}+A_{11}^{(m)}) & \frac{1}{2}(A_{12}^{(n)}+A_{12}^{(m)}) & \frac{1}{2}(A_{13}^{(n)}+A_{13}^{(m)}) & \frac{1}{2}(A_{14}^{(n)}+A_{14}^{(m)}) \\ \frac{1}{2}(A_{12}^{(n)}+A_{12}^{(m)}) & \frac{1}{2}(A_{22}^{(n)}+A_{22}^{(m)}) & \frac{1}{2}(A_{23}^{(n)}+A_{23}^{(m)}) & \frac{1}{2}(A_{24}^{(n)}+A_{24}^{(m)}) \\ \frac{1}{2}(A_{13}^{(n)}+A_{13}^{(m)}) & \frac{1}{2}(A_{23}^{(n)}+A_{23}^{(m)}) & \frac{1}{2}(A_{33}^{(n)}+A_{33}^{(m)}) & \frac{1}{2}(A_{34}^{(n)}+A_{34}^{(m)}) \\ \frac{1}{2}(A_{14}^{(n)}+A_{14}^{(m)}) & \frac{1}{2}(A_{24}^{(n)}+A_{24}^{(m)}) & \frac{1}{2}(A_{34}^{(n)}+A_{34}^{(m)}) & \frac{1}{2}(A_{44}^{(n)}+A_{44}^{(m)}) \end{pmatrix} . \tag{4.61}$$

The reduced masses $\mu_1 = \mu_{\rho_1}$, $\mu_2 = \mu_{\rho_2}$, $\mu_3 = \mu_{\rho_3}$ and $\mu_4 = \mu_{\rho_4}$ relative to Jacobi coordinates must be taken according to the choice made for these coordinates. We have assumed that all pairs of particles interact via the same power law, $\nu_{ij} = \nu$. The elements $\gamma_{12,12}$, $\gamma_{13,13}$, $\gamma_{14,14}$, $\gamma_{15,15}$, $\gamma_{23,23}$, $\gamma_{24,24}$, $\gamma_{25,25}$, $\gamma_{34,34}$, $\gamma_{35,35}$ and $\gamma_{45,45}$ are the diagonal elements of the matrix $\gamma = d^T A^{-1} d$ eq. (4.44). Therefore, we must find the expression of the matrix d, eq. (4.10), which relates the relative vectors $\overrightarrow{r}_{ij}$ for each pair of particles to the Jacobi coordinates.

4.3.1 Choice of Jacobi coordinates

In our study, we will limit ourselves to systems of five particles whose diversity goes up to three different masses.

It is well known that the complexity of the numerical computations carried out to solve all variational problems increases with the number of variational parameters, in our case the

weight parameters $c^{(n)}$ and the range parameters $A_{ij}^{(n)}$. So, in order to reduce the numerical computations as much as possible, the number of variational parameters involved has to be smaller. On the basis of the discussions carried out in the previous sections (3.2, 3.3 and 3.4), we have established that to recover the exact solution of the five-body harmonic oscillator it is necessary to choose a trial wave function in the form of a correlated gaussian with the same number of parameters. Note that if we consider more parameters, we end up with the same results but with more numerical computations, while we get zero values for the additional parameters.

For this reason, we have to consider:

- the standard choice of Jacobi coordinates eq. (3.8,3.25) to treat the configurations (m, m, m, m, m) and (m, m, m, m, M)
- the modified choice of Jacobi coordinates eq. (3.45,3.46) to treat the configuration (m, m, m, M, M).
- the modified choice of Jacobi coordinates eqs. (3.54,3.55) to treatm the configuration (m, m, M, M, m_5)

Configurations (m, m, m, m, m) **and** (m, m, m, m, M)

To treat the configuration (m, m, m, m, m) and (m, m, m, m, M) we will adopt the standard choice of the Jacobi coordinates eq. (3.8).

We start by the derivation of the matrix d eq. (4.10). We must first express the relative vector $\overrightarrow{r}_{ij}, (\overrightarrow{r}_{ij} = \overrightarrow{r}_1 - \overrightarrow{r}_2)$ for each pair of particles using eqs. (3.26). The calculation results in

$$
\begin{aligned}
\overrightarrow{r}_1 - \overrightarrow{r}_2 &= \overrightarrow{\rho}_1 \\
\overrightarrow{r}_1 - \overrightarrow{r}_3 &= \tfrac{1}{2}\overrightarrow{\rho}_1 + \overrightarrow{\rho}_2 \\
\overrightarrow{r}_1 - \overrightarrow{r}_4 &= \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \\
\overrightarrow{r}_1 - \overrightarrow{r}_5 &= \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \\
\overrightarrow{r}_2 - \overrightarrow{r}_3 &= -\tfrac{1}{2}\overrightarrow{\rho}_1 + \overrightarrow{\rho}_2 \\
\overrightarrow{r}_2 - \overrightarrow{r}_4 &= -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \\
\overrightarrow{r}_2 - \overrightarrow{r}_5 &= -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \\
\overrightarrow{r}_3 - \overrightarrow{r}_4 &= -\tfrac{2}{3}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \\
\overrightarrow{r}_3 - \overrightarrow{r}_5 &= -\tfrac{2}{3}\overrightarrow{\rho}_2 + \tfrac{1}{4}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \\
\overrightarrow{r}_4 - \overrightarrow{r}_5 &= -\tfrac{3}{4}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4
\end{aligned}
\tag{4.62}
$$

or in matrix form

$$
\begin{pmatrix}
\overrightarrow{r}_1 - \overrightarrow{r}_2 \\
\overrightarrow{r}_1 - \overrightarrow{r}_3 \\
\overrightarrow{r}_1 - \overrightarrow{r}_4 \\
\overrightarrow{r}_1 - \overrightarrow{r}_5 \\
\overrightarrow{r}_2 - \overrightarrow{r}_3 \\
\overrightarrow{r}_2 - \overrightarrow{r}_4 \\
\overrightarrow{r}_2 - \overrightarrow{r}_5 \\
\overrightarrow{r}_3 - \overrightarrow{r}_4 \\
\overrightarrow{r}_3 - \overrightarrow{r}_5 \\
\overrightarrow{r}_4 - \overrightarrow{r}_5
\end{pmatrix}
= d^T
\begin{pmatrix}
\overrightarrow{\rho}_1 \\
\overrightarrow{\rho}_2 \\
\overrightarrow{\rho}_3 \\
\overrightarrow{\rho}_4
\end{pmatrix}
\ , \tag{4.63}
$$

with

$$
d = \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\
0 & 1 & \frac{1}{3} & \frac{1}{3} & 1 & \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} & 0 \\
0 & 0 & 1 & \frac{1}{4} & 0 & 1 & \frac{1}{4} & 1 & \frac{1}{4} & -\frac{3}{4} \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1
\end{pmatrix}
\ . \tag{4.64}
$$

The matrix γ eq. (4.44) can be calculated directly from this last expression of the matrix d and its transpose d^T.

Notice that the configuration (m, m, m, m, m) considered as particular cas of te configuration (m, m, m, m, M) with $m = M$. So, we limit ourselves to the calculations relating to this last configuration.

The reduced masses are taken to be as follows

$$\mu_1 = \frac{m}{2}, \qquad \mu_2 = \frac{2m}{3}, \quad \mu_3 = \frac{3m}{4}, \qquad \mu_4 = \frac{4Mm}{M+4m} \quad . \tag{4.65}$$

According to the results of the previous chapter, the standard choice of the Jacobi coordinates allow us to deduce directly the exact wave function and the energy of the ground state of the configurations (m, m, m, m, m) and (m, m, m, m, M) of five-body harmonic oscillator; the exact wave functions are non correlated gaussian.

The gaussian function that will be used for the variational calculation of the configuration (m, m, m, m, M) also for the problems of nonharmonic forces is of the form

$$\left\langle \vec{\rho}_1 ... \vec{\rho}_{N-1} | n \right\rangle \equiv \exp \frac{-1}{2} \left[A_{11}^{(n)} \vec{\rho}_1^{\,2} + A_{22}^{(n)} \vec{\rho}_2^{\,2} + A_{33}^{(n)} \vec{\rho}_3^{\,2} + A_{44}^{(n)} \vec{\rho}_4^{\,2} \right] \tag{4.66}$$

without any term of correlation, i.e.,

$$A_{12}^{(n)} = A_{13}^{(n)} = ... = A_{34}^{(n)} = 0.$$

Configurations (m, m, m, M, M)

To treat this configuration we will adopt the modified choice of the Jacobi coordinates given by eq. (3.26).

The equations (3.26) allow us to express the relative vectors $\overrightarrow{r}_{ij}, (\overrightarrow{r}_{ij} = \overrightarrow{r}_1 - \overrightarrow{r}_2)$ for each

pair of particles in terms of Jacobi coordinates with the following result

$$\begin{aligned}
&\overrightarrow{r}_1 - \overrightarrow{r}_2 = \overrightarrow{\rho}_1 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_3 = \tfrac{1}{2}\overrightarrow{\rho}_1 + \overrightarrow{\rho}_2 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_4 = \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 - \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_5 = \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_3 = -\tfrac{1}{2}\overrightarrow{\rho}_1 + \overrightarrow{\rho}_2 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_4 = -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 - \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_5 = -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{3}\overrightarrow{\rho}_2 + \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_3 - \overrightarrow{r}_4 = -\tfrac{2}{3}\overrightarrow{\rho}_2 - \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_3 - \overrightarrow{r}_5 = -\tfrac{2}{3}\overrightarrow{\rho}_2 + \tfrac{1}{2}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_4 - \overrightarrow{r}_5 = \overrightarrow{\rho}_3 \ .
\end{aligned} \tag{4.67}$$

So, we can derive the following expression for the matrix d:

$$d = \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\
0 & 1 & \frac{1}{3} & \frac{1}{3} & 1 & \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} & 0 \\
0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 1 \\
0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0
\end{pmatrix} . \tag{4.68}$$

The matrix γ is computed directly from this last expression of the matrix d and its transpose d^T.

The reduced masses are taken to be as follows

$$\mu_{\rho_1} = \frac{m}{2}, \quad \mu_{\rho_2} = \frac{2m}{3}, \quad \mu_{\rho_3} = \frac{M}{2}, \quad \mu_{\rho_4} = \frac{6Mm}{2M+3m} \quad . \tag{4.69}$$

We have shown in section 3.3.3 that the modified choice of Jacobi coordinates applied to this configuration (m, m, m, M, M) leads to a diagonal form for the hamiltonian allowing us to deduce directly the exact wave function and the energy of the ground state of five-body harmonic oscillator; the exact wave functions are non correlated gaussian. So, the gaussian function that will be used for the variational calculation of the configuration (m, m, m, M, M)

also for problems of nonharmonic forces is of the form

$$\left\langle \vec{\rho}_1 ... \vec{\rho}_{N-1} | n \right\rangle \equiv \exp\left[\frac{-1}{2} (A_{11}^{(n)} \vec{\rho}_1^2 + A_{22}^{(n)} \vec{\rho}_2^2 + A_{33}^{(n)} \vec{\rho}_3^2 + A_{44}^{(n)} \vec{\rho}_4^2) \right] \tag{4.70}$$

without any term of correlation, i.e.,

$$A_{12}^{(n)} = A_{13}^{(n)} = ... = A_{34}^{(n)} = 0.$$

Configurations (m, m, M, M, m_5)

The modified choice of Jacobi coordinates eq. (3.54) is more appropriate for the treatment of this configuration.

We start by the derivation of the matrix d eq. (4.10). We must first express the relative vector $\overrightarrow{r}_{ij}, (\overrightarrow{r}_{ij} = \overrightarrow{r}_1 - \overrightarrow{r}_2)$ for each pair of particles in terms of Jacobi coordinates eq. (3.54). Using the expressions (3.56) we obtain

$$\begin{aligned}
&\overrightarrow{r}_1 - \overrightarrow{r}_2 = \overrightarrow{\rho}_1 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_3 = \tfrac{1}{2}\overrightarrow{\rho}_1 - \tfrac{1}{2}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_4 = \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{2}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \ , \\
&\overrightarrow{r}_1 - \overrightarrow{r}_5 = \tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{M}{M+m}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_3 = -\tfrac{1}{2}\overrightarrow{\rho}_1 - \tfrac{1}{2}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_4 = -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{1}{2}\overrightarrow{\rho}_2 + \overrightarrow{\rho}_3 \ , \\
&\overrightarrow{r}_2 - \overrightarrow{r}_5 = -\tfrac{1}{2}\overrightarrow{\rho}_1 + \tfrac{M}{M+m}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_3 - \overrightarrow{r}_4 = \overrightarrow{\rho}_2 \ , \\
&\overrightarrow{r}_3 - \overrightarrow{r}_5 = \tfrac{1}{2}\overrightarrow{\rho}_2 - \tfrac{m}{M+m}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ , \\
&\overrightarrow{r}_4 - \overrightarrow{r}_5 = -\tfrac{1}{2}\overrightarrow{\rho}_2 - \tfrac{m}{M+m}\overrightarrow{\rho}_3 + \overrightarrow{\rho}_4 \ ,
\end{aligned} \tag{4.71}$$

which we can rewrite under the matrix form eq. (4.63) with

$$d = \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{2} & 0 & 0 & 0 \\
0 & \frac{-1}{2} & \frac{1}{2} & 0 & \frac{-1}{2} & \frac{1}{2} & 0 & 1 & \frac{1}{2} & \frac{-1}{2} \\
0 & 1 & 1 & \frac{M}{M+m} & 1 & 1 & \frac{M}{M+m} & 0 & \frac{-m}{M+m} & \frac{-m}{M+m} \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1
\end{pmatrix} . \tag{4.72}$$

The matrix γ is computed directly from this last expression of the matrix d and its transpose d^T.

The follows reduced masses are to be taken:

$$\mu_{\rho_1} = \frac{m}{2},\ \mu_{\rho_2} = \frac{M}{2},\ \mu_{\rho_3} = 2\frac{Mm}{M+m},\ \mu_{\rho_4} = 2m_5\frac{M+m}{2M+2m+m_5}. \tag{4.73}$$

According to the results of the section 3.4, the modified choice of the Jacobi coordinates eq. (3.54) allow us to reduce the number of crossed terùs in the hamiltonian. We have only one term $(\overrightarrow{\rho}_3.\overrightarrow{\rho}_4)$. This term should apear in the exponent of the exact wave function of the ground state.

Therefore, to reach the exact solution of the five-body harmonic oscillator by variational calculation we should consider a trial wave function as a correlated gaussian that includes the term $(\overrightarrow{\rho}_3.\overrightarrow{\rho}_4)$. Ins

$$\left\langle \vec{\rho}_1 ... \vec{\rho}_{N-1} | n \right\rangle \equiv \exp\left[\frac{-1}{2} (A_{11}^{(n)} \vec{\rho}_1^2 + A_{22}^{(n)} \vec{\rho}_2^2 + A_{33}^{(n)} \vec{\rho}_3^2 + A_{44}^{(n)} \vec{\rho}_4^2 + 2A_{34}^{(n)} \overrightarrow{\rho}_3.\overrightarrow{\rho}_4) \right] \tag{4.74}$$

instead of eq. (3.53) which contains more terms; $\overrightarrow{\rho}_2.\overrightarrow{\rho}_3$, $\overrightarrow{\rho}_2.\overrightarrow{\rho}_4$ and $\overrightarrow{\rho}_3.\overrightarrow{\rho}_4$.

4.3.2 One generation of correlated gaussians

We will adopt a single correlated gaussian ($g = 1$) to be the trial wave function:

$$\begin{aligned} \psi(\overrightarrow{\rho}_1, \overrightarrow{\rho}_2, \overrightarrow{\rho}_3, \overrightarrow{\rho}_4) &= c_1 \exp(-\frac{1}{2} \sum_{i,j=1}^{4} A_{ij}^{(n)} \overrightarrow{\rho}_i.\overrightarrow{\rho}_j)\ , \\ |1\rangle &= c_1 \exp(-a_1 \overrightarrow{\rho}_1^2 - b_1 \overrightarrow{\rho}_2^2 - w_1 \overrightarrow{\rho}_3^2 - t_1 \overrightarrow{\rho}_4^2 - s_1 \overrightarrow{\rho}_1 \overrightarrow{\rho}_2 \\ &\quad -m_1 \overrightarrow{\rho}_1 \overrightarrow{\rho}_3 - u_1 \overrightarrow{\rho}_1 \overrightarrow{\rho}_4 - l_1 \overrightarrow{\rho}_2 \overrightarrow{\rho}_3 - d_1 \overrightarrow{\rho}_2 \overrightarrow{\rho}_4 - e_1 \overrightarrow{\rho}_3 \overrightarrow{\rho}_4)\ , \end{aligned} \tag{4.75}$$

where are implicated the variationals parameters:

$$\begin{aligned} a_1 &= A_{11}^{(1)}/2,\ b_1 = A_{22}^{(1)}/2,\ w_1 = A_{33}^{(1)}/2,\ t_1 = A_{44}^{(1)}/2,\ s_1 = A_{12}^{(1)}, \\ m_1 &= A_{13}^{(1)},\ u_1 = A_{14}^{(1)},\ l_1 = A_{23}^{(1)},\ d_1 = A_{24}^{(1)},\ e_1 = A_{34}^{(1)}\ . \end{aligned} \tag{4.76}$$

We have to calculate a single matrix element. The hamiltonian average value is simplified in this case:

$$\begin{aligned}\langle H\rangle_\psi = & \frac{\langle 1|\, H\, |1\rangle}{\langle 1|1\rangle} \\ = & \tfrac{3}{4}\left[\tfrac{1}{\mu_1}(A^{(n)}A^{-1}A^{(m)})_{11}+\tfrac{1}{\mu_2}(A^{(n)}A^{-1}A^{(m)})_{22}+\tfrac{1}{\mu_3}(A^{(n)}A^{-1}A^{(m)})_{33}+\tfrac{1}{\mu_4}(A^{(n)}A^{-1}A^{(m)})_{44}\right] \\ & +\tfrac{2}{\sqrt{\pi}}\Gamma(\tfrac{\nu+3}{2})\left[\lambda_{12}\gamma_{12,12}^{\nu/2}+\lambda_{13}\gamma_{13,13}^{\nu/2}+\lambda_{14}\gamma_{14,14}^{\nu/2}+\lambda_{15}\gamma_{15,15}^{\nu/2}+\lambda_{23}\gamma_{23,23}^{\nu/2}\right] \\ & +\tfrac{2}{\sqrt{\pi}}\Gamma(\tfrac{\nu+3}{2})\left[\lambda_{24}\gamma_{24,24}^{\nu/2}+\lambda_{25}\gamma_{25,25}^{\nu/2}+\lambda_{34}\gamma_{34,34}^{\nu/2}+\lambda_{35}\gamma_{35,35}^{\nu/2}+\lambda_{45}\gamma_{45,45}^{\nu/2}\right]\ ,\end{aligned} \tag{4.77}$$

And since the matrix A is none other than the matrix $A^{(1)}$ itself, then: $A^{(1)}A^{-1}A^{(1)} = A^{(1)}$. So the expression (4.77) reduces to:

$$\begin{aligned}\langle H\rangle_\psi = & \frac{3}{4}\left[\frac{1}{\mu_1}A_{11}^{(1)}+\frac{1}{\mu_2}A_{22}^{(1)}+\frac{1}{\mu_3}A_{33}^{(1)}+\frac{1}{\mu_4}A_{44}^{(1)}\right] \\ & +\frac{2}{\sqrt{\pi}}\Gamma(\frac{\nu+3}{2})\left[\lambda_{12}\gamma_{12,12}^{\nu/2}+\lambda_{13}\gamma_{13,13}^{\nu/2}+\lambda_{14}\gamma_{14,14}^{\nu/2}+\lambda_{15}\gamma_{15,15}^{\nu/2}+\lambda_{23}\gamma_{23,23}^{\nu/2}\right] \\ & +\frac{2}{\sqrt{\pi}}\Gamma(\frac{\nu+3}{2})\left[\lambda_{24}\gamma_{24,24}^{\nu/2}+\lambda_{25}\gamma_{25,25}^{\nu/2}+\lambda_{34}\gamma_{34,34}^{\nu/2}+\lambda_{35}\gamma_{35,35}^{\nu/2}+\lambda_{45}\gamma_{45,45}^{\nu/2}\right]\end{aligned} \tag{4.78}$$

This last expression of mean value of the hamiltonian is function of ten free parameters a_1, b_1, w_1, t_1, s_1,m_1, u_1, l_1, d_1 and e_1. According to the variational principle for each set of these parameters we have an upper bound for ground stat energy of the system. The nearest bound to the ground state energy is that of the smallest value. Thus, the best approximation of the ground state energy, noted by $E_{0var}^{(1)} = E_{0var}^{(g=1)}$, will be obtained by the minimisation of $\langle H\rangle_\psi$ over tens parameters:

$$E_{0var}^{(1)} = \min_{a_1,b_1,w_1,t_1,s_1,m_1,u_1,l_1,d_1,e_1} \langle H\rangle_\psi\ , \tag{4.79}$$

It should be noted that the parameter c_1 disappears from this formula (this normalisation parameter does not play a role when working with a single gaussian).

4.3.3 Two generations of correlated gaussians

If we use two generations gaussians $|1\rangle$ and $|2\rangle$ as the test wave function:

$$|\psi\rangle = c_1 |1\rangle \ + c_2 |2\rangle \ , \tag{4.80}$$

with

$$\begin{aligned}
|1\rangle \ &\equiv \ c_1 \exp \frac{-1}{2} \Big[A_{11}^{(1)} \vec{\rho}_1^{\,2} + A_{22}^{(1)} \vec{\rho}_2^{\,2} + A_{33}^{(1)} \vec{\rho}_3^{\,2} + A_{44}^{(1)} \vec{\rho}_4^{\,2} \\
&\quad +2(A_{12}^{(1)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_2 + A_{13}^{(1)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_3 + A_{14}^{(1)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_4 + A_{23}^{(1)} \overrightarrow{\rho}_2 . \overrightarrow{\rho}_3 + A_{24}^{(1)} \overrightarrow{\rho}_2 . \overrightarrow{\rho}_4 + A_{34}^{(1)} \overrightarrow{\rho}_3 . \overrightarrow{\rho}_4) \Big] , \\
&\equiv \ c_1 \exp \big[-a_1 \overrightarrow{\rho}_1^{\,2} - b_1 \overrightarrow{\rho}_2^{\,2} - w_1 \overrightarrow{\rho}_3^{\,2} - t_1 \overrightarrow{\rho}_4^{\,2} \\
&\quad -s_1 \overrightarrow{\rho}_1 . \overrightarrow{\rho}_2 - m_1 . \overrightarrow{\rho}_1 \overrightarrow{\rho}_3 - u_1 \overrightarrow{\rho}_1 . \overrightarrow{\rho}_4 - l_1 \overrightarrow{\rho}_2 . \overrightarrow{\rho}_3 - d_1 \overrightarrow{\rho}_2 . \overrightarrow{\rho}_4 - e_1 \overrightarrow{\rho}_3 . \overrightarrow{\rho}_4)]
\end{aligned} \tag{4.81}$$

and

$$\begin{aligned}
|2\rangle \ &\equiv \ c_2 \exp \frac{-1}{2} \Big[A_{11}^{(2)} \vec{\rho}_1^{\,2} + A_{22}^{(2)} \vec{\rho}_2^{\,2} + A_{33}^{(2)} \vec{\rho}_3^{\,2} + A_{44}^{(2)} \vec{\rho}_4^{\,2} \\
&\quad +2(A_{12}^{(2)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_2 + A_{13}^{(2)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_3 + A_{14}^{(2)} \overrightarrow{\rho}_1 . \overrightarrow{\rho}_4 + A_{23}^{(2)} \overrightarrow{\rho}_2 . \overrightarrow{\rho}_3 + A_{24}^{(2)} \overrightarrow{\rho}_2 . \overrightarrow{\rho}_4 + A_{34}^{(2)} \overrightarrow{\rho}_3 . \overrightarrow{\rho}_4) \Big] , \\
&\equiv \ c_1 \exp \big[-a_2 \overrightarrow{\rho}_1^{\,2} - b_2 \overrightarrow{\rho}_2^{\,2} - w_2 \overrightarrow{\rho}_3^{\,2} - t_2 \overrightarrow{\rho}_4^{\,2} \\
&\quad -s_2 \overrightarrow{\rho}_1 . \overrightarrow{\rho}_2 - m_2 \overrightarrow{\rho}_1 . \overrightarrow{\rho}_3 - u_2 \overrightarrow{\rho}_1 . \overrightarrow{\rho}_4 - l_2 \overrightarrow{\rho}_2 . \overrightarrow{\rho}_3 - d_2 \overrightarrow{\rho}_2 . \overrightarrow{\rho}_4 - e_2 \overrightarrow{\rho}_3 . \overrightarrow{\rho}_4] \ .
\end{aligned} \tag{4.82}$$

Then, we got twenty-two variational parameters a_1, b_1, w_1, t_1, s_1, m_1, u_1, l_1, d_1, e_1, a_2, b_2, w_2, t_2, s_2,m_2, u_2, l_2, d_2, e_2, c_1, and c_2.

The best approximation of the ground state using two generations of gaussianns eq. (4.80), noted by $E_{0var}^{(2)} = E_{0var}^{(g=2)}$ will be obtained by the minimisation of $\langle H \rangle_\psi$ compared to twentytwo parameters:

$$E_{0var}^{(2)} = \min_{c_1, c_2, a_1, a_2, \ldots, e_1, e_2} \langle H \rangle_\psi \tag{4.83}$$

with

$$\langle H \rangle_\psi = \frac{c_1^2 \langle 1| H |1\rangle + 2c_1 c_2 \langle 1| H |2\rangle + c_2^2 \langle 2| H |2\rangle}{c_1^2 \langle 1|1\rangle + 2c_1 c_2 \langle 1|2\rangle + c_2^2 \langle 2|2\rangle}, \tag{4.84}$$

where $\langle 1| H |1\rangle$, $\langle 1| H |2\rangle$ and $\langle 2| H |2\rangle$ are given by the equation (4.60). The overlap of the gaussian functions $\langle 1|1\rangle$, $\langle 1|2\rangle$ et $\langle 2|2\rangle$ will be calculated by the equation (4.37) which is reduced

in our case to:

$$\langle 1|1\rangle = \pi^6 \left\| \begin{array}{cccc} A^1_{11} & A^1_{12} & A^1_{13} & A^1_{14} \\ A^1_{21} & A^1_{22} & A^1_{23} & A^1_{24} \\ A^1_{31} & A^1_{32} & A^1_{33} & A^1_{34} \\ A^1_{41} & A^1_{42} & A^1_{43} & A^1_{44} \end{array} \right\|^{-3/2} , \tag{4.85}$$

$$\langle 2|2\rangle = \pi^6 \left\| \begin{array}{cccc} A^2_{11} & A^2_{12} & A^2_{13} & A^2_{14} \\ A^2_{21} & A^2_{22} & A^2_{23} & A^2_{24} \\ A^2_{31} & A^2_{32} & A^2_{33} & A^2_{34} \\ A^2_{41} & A^2_{42} & A^2_{43} & A^2_{44} \end{array} \right\|^{-3/2} ,$$

and

$$\langle 1|2\rangle = \pi^6 \left\| \begin{array}{cccc} \frac{1}{2}(A^1_{11}+A^2_{11}) & \frac{1}{2}(A^1_{12}+A^2_{1}) & \frac{1}{2}(A^1_{13}+A^2_{13}) & \frac{1}{2}(A^1_{14}+A^2_{14}) \\ \frac{1}{2}(A^1_{21}+A^2_{21}) & \frac{1}{2}(A^1_{22}+A^2_{22}) & \frac{1}{2}(A^1_{23}+A^2_{23}) & \frac{1}{2}(A^1_{24}+A^2_{24}) \\ \frac{1}{2}(A^1_{31}+A^2_{31}) & \frac{1}{2}(A^1_{32}+A^2_{32}) & \frac{1}{2}(A^1_{33}+A^2_{33}) & \frac{1}{2}(A^1_{34}+A^2_{34}) \\ \frac{1}{2}(A^1_{41}+A^2_{41}) & \frac{1}{2}(A^1_{42}+A^2_{42}) & \frac{1}{2}(A^1_{43}+A^2_{43}) & \frac{1}{2}(A^1_{44}+A^2_{44}) \end{array} \right\|^{-3/2} . \tag{4.86}$$

4.3.4 Numerical results

In the following tables, we reported the approximative values of the fundamentals states of energies $E^{(g)}_{0var}$ (g=1, 2) of five-body systems in interaction by using g correlated gaussians as trial wave function. We consider different mass configuration $(m_1, m_2, m_3, m_4, m_5)$. We are limited to the two-body interactions which is derived from power-law potentials of the same type for all pairs of particles.:

$$V^{(ij)}(r_{ij}) = \lambda r^{\nu}_{ij} , \tag{4.87}$$

with $\lambda = sign(\nu)$. That is to say, λ and ν are of the same sign. We considered all configurations of the five-body problem studied in chapter 3 and four representative forms of the power law potential were chosen, namely; the harmonic potential $\upsilon = 2$ (tables 1, 5, 9 and 13), the linear potential $\upsilon = 1$ (tables 2, 6, 10 and 14), the Martin potential $\upsilon = 0.1$ (tables 3, 7, 11 and 15) "widely used in heavy meson spectroscopy" and the colombian potential $\upsilon = -1$ (tables 4, 8,

12 and 16). All the numerical minimization calculations, always in the system of natural units or $\hbar = 1$, were carried out with a special software, the **Mathcad** software.

An example of **Mathcad** numerical calculation is illustrated by a **Mathcad** screen shoot (figure 4) which we have created to calculate the variational approximations of the energy of the ground state of the five-body system using a single gaussian with the standard choice of Jacobi coordinates. we consider the configuration (m, m, M, M, m_5)=$(1, 1, 2, 2, 0.1)$ for a linear potential $\nu = 1$ and $\lambda_{ij} = 1$.

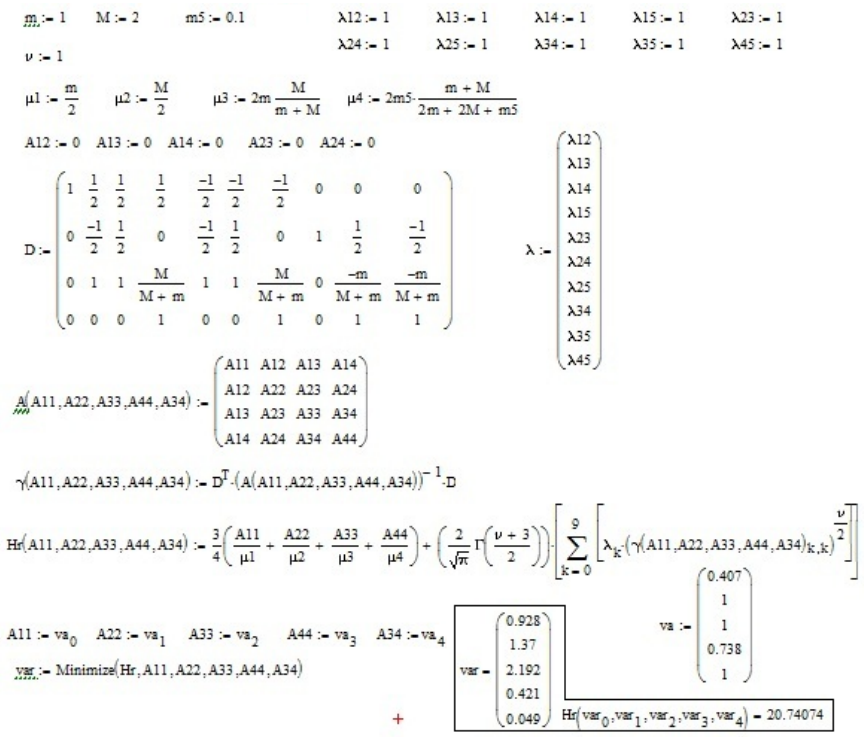

figure 4: Mathcad page for calculating $E^{(1)}_{0var}$ for a five-body system Configuration $(1, 1, 2, 2, 0.1)$ with $\nu = 1$.

To meet the requirements of the software we have redefined some parameters:

- **va** is a five element vector whose elements are the initial values of the variational parameters $A_{11}, .., A_{44}$ and A_{34}.

- **Hr** is the mean value of the hamiltonian, function of variational parameters $A_{11}, .., A_{44}$

and A_{34}. This is the function tahat will be minimized.

- **var** is a five element vector whose elements are the resulting values of the variational parameters $A_{11}, .., A_{44}$ and A_{34} that minimize **Hr.**

At the end of the programme, the results are displayed in a box at the bottom of the page:

$$\mathbf{Hr} = E^{(1)}_{0var} = 20.74074$$

is the value of best approximation of the ground state energy and

$$A_{11} = 0.928, \quad A_{22} = 1.37, \quad A_{33} = 2.192, \; A_{44} = 0.421 \quad \text{and} \quad A_{34} = 0.049$$

are the values of the variational parameters corresponding to $E^{(1)}_{0var}$. So the gaussian function which best approximates the ground state is

$$|1\rangle \equiv c_1 \exp \frac{-1}{2} \left[0.928\vec{\rho}_1^{\,2} + 1.37\vec{\rho}_2^{\,2} + 2.192\vec{\rho}_3^{\,2} + 0.421\vec{\rho}_4^{\,2} + 0.049\vec{\rho}_3.\vec{\rho}_4\right].$$

Noting that applying this method in the case of harmonic forces $\nu = 2$ and $\lambda = 1$ for the configuration $(1, 1, 1, 1, 1)$ one finds identically the exact solution eqs. (3.24,).

We will present in what follows some numerical results for 5-body systems. It is about upper bounds $E^{(1)}_{0var}$ eq. (4.79) and $E^{(2)}_{0var}$ eq. (4.83) obtained by the variational approximation using one or two generations of gaussians. We have also reported the exact values of the ground state energy when it is available (only for harmonic oscillator).

Table 1: E_{exact} and $E^{(1)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m) interacting via a potential, $V_{ij}(r_{ij}) = r^2_{ij}$, with $\nu = 2$, m variable.

m	2.5	2	1.5	1	0.1
E_{exact}	12.000	13.416	15.492	18.974	60.000
$E^{(1)}_{0var}$	12.000	13.416	15.492	18.974	60.000

Table 2: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m) interacting via a potential, $V_{ij}(r_{ij}) = r^{1}_{ij}$, with $\nu = 1,\ m$ variable.

m	2.5	2	1.5	1	0.1
$E^{(1)}_{0var}$	12.729	13.720	15.092	17.276	37.221
$E^{(2)}_{0var}$	12.717	13.699	15.078	17.260	37.187

Table 3: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m) interacting via a potential, $V_{ij}(r_{ij}) = r^{0.1}_{ij}$, with $\nu = 0.1,\ m$ variable.

m	2.5	2	1.5	1	0.1
$E^{(1)}_{0var}$	11.346	11.468	11.626	11.852	12.035
$E^{(2)}_{0var}$	11.340	11.461	11.619	11.845	13.218

Table 4: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m) interacting via a potential, $V_{ij}(r_{ij}) = r^{-1}_{ij}$, with $\nu = -1,\ m$ variable.

m	2.5	2	1.5	1	0.1
$E^{(1)}_{0var}$	-13.263	-10.610	-7.958	-5.305	-0.531
$E^{(2)}_{0var}$	-13.768	-11.014	-8.261	-5.507	-0.530

Table 5: E_{exact} and $E^{(1)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{2}_{ij}$, with $\nu = 2,\ m = 1$, and m_5 variable.

m_5	1000	2	1	0.5	0.1	0.01
E_{exact}	16.356	17.904	18.974	20.594	27.813	56.710
$E^{(1)}_{0var}$	16.356	17.904	18.974	20.594	27.813	56.710

Table 6: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^1_{ij}$, with $\nu = 1,\ m = 1$, and m_5 variable.

m_5	1000	2	1	0.5	0.1	0.01
$E^{(1)}_{0var}$	15.591	16.613	17.276	18.231	21.964	33.257
$E^{(2)}_{0var}$	15.590	16.597	17.260	18.213	21.941	33.202

Table 7: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{0.1}_{ij}$, with $\nu = 0.1,\ m = 1$, and m_5 variable.

m_5	1000	2	1	0.5	0.1	0.01
$E^{(1)}_{0var}$	11.673	11.785	11.852	11.942	12.230	12.778
$E^{(2)}_{0var}$	11.673	11.778	11.845	11.935	12.222	12.768

Table 8: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, m, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{-1}_{ij}$, with $\nu = -1,\ m = 1$, and m_5 variable.

m_5	1000	2	1	0.5	0.1	0.01
$E^{(1)}_{0var}$	-7.439	-5.994	-5.305	-4.557	-3.177	-2.614
$E^{(2)}_{0var}$	-7.438	-6.223	-5.507	-4.731	-3.305	-2.742

Table 9: E_{exact} and $E^{(1)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, M, M) interacting via a potential, $V_{ij}(r_{ij}) = r^2_{ij}$, with $\nu = 2,\ m = 1,\ M = 1$ variable.

m, M	$1, 2$	$1, 1$	$1, 0.5$	$1, 0.1$	$1, 0.01$
E_{exact}	16.810	18.974	22.195	36.487	93.786
$E^{(1)}_{0var}$	16.810	18.974	22.195	36.487	93.786

Table 10: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, M, M) interacting via a potential, $V_{ij}(r_{ij}) = r^{1}_{ij}$, with $\nu = 1,\ m = 1,\ M$ variable.

M	$1, 2$	$1, 1$	$1, 0.5$	$1, 0.1$	$1, 0.01$
$E^{(1)}_{0var}$	15.922	17.276	19.159	26.367	47.894
$E^{(2)}_{0var}$	15.907	17.260	19.141	26.340	47.830

Table 11: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, M, M) interacting via a potential, $V_{ij}(r_{ij}) = r^{0.1}_{ij}$, with $\nu = 0.1,\ m = 1,\ M$ variable.

M	$1, 2$	$1, 1$	$1, 0.5$	$1, 0.1$	$1, 0.01$
$E^{(1)}_{0var}$	11.713	11.853	12.027	12.557	13.533
$E^{(2)}_{0var}$	11.706	11.845	12.019	12.549	13.523

Table 12: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, m, M, M) interacting via a potential, $V_{ij}(r_{ij}) = r^{-1}_{ij}$, with $\nu = -1,\ m = 1,\ M$ variable.

M	$1, 2$	$1, 1$	$1, 0.5$	$1, 0.1$	$1, 0.01$
$E^{(1)}_{0var}$	-6.840	-5.305	-3.935	-1.840	-1.050
$E^{(2)}_{0var}$	-7.100	-5.507	-4.084	-1.912	-1.050

Table 13: E_{exact} and $E^{(1)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, M, M, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{2}_{ij}$, with $\nu = 2,\ m = 1,\ M$ and m_5 variable.

M, m_5	$1, 1000$	$1, 1$	$0.5, 1.5$	$0.5, 1$	$2, 0.1$	$0.1, 0.5$	$0.01, 2$
E_{exact}	16.335	18.974	21.541	22.195	25.744	37.975	92.894
$E^{(1)}_{0var}$	16.335	18.974	21.541	22.195	25.744	37.975	92.894

Table 14: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, M, M, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{1}_{ij}$, with $\nu = 1,\ m = 1,\ M$ and m_5 variable.

M, m_5	$1, 1000$	$1, 1$	$0.5, 1.5$	$0.5, 1$	$2, 0.1$	$0.1, 0.5$	$0.01, 2$
$E^{(1)}_{0var}$	15.590	17.276	18.770	19.159	20.740	27.152	47.449
$E^{(2)}_{0var}$	15.576	17.260	18.763	19.153	20.729	27.211	47.449

Table 15: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, M, M, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{0.1}_{ij}$, with $\nu = 0.1,\ m = 1,\ M$ and m_5 variable.

M, m_5	$1, 1000$	$1, 1$	$0.5, 1.5$	$0.5, 1$	$2, 0.1$	$0.1, 0.5$	$0.01, 2$
$E^{(1)}_{0var}$	11.673	11.852	11.990	12.026	12.115	12.617	13.498
$E^{(2)}_{0var}$	11.666	11.845	11.984	12.020	12.108	12.612	13.488

Table 16: $E^{(1)}_{0var}$ and $E^{(2)}_{0var}$ for the ground state energy of a five-body system in configuration (m, m, M, M, m_5) interacting via a potential, $V_{ij}(r_{ij}) = r^{-1}_{ij}$, with $\nu = -1,\ m = 1,\ M$ and m_5 variable.

M, m_5	$1, 1000$	$1, 1$	$0.5, 1.5$	$0.5, 1$	$2, 0.1$	$0.1, 0.5$	$0.01, 2$
$E^{(1)}_{0var}$	-7.438	-5.305	-4.209	-4.152	-4.153	-1.593	-1.260
$E^{(2)}_{0var}$	-7.726	-5.507	-4.369	-4.084	-4.152	-1.653	-1.316

Conclusion

The work in this thesis is an extension of previous studies that have been carried out on three and four body systems. Thus, in this work we are interested in the approximate solution of the stationary Schrödinger equation for spinless five-body systems.

We started with a brief presentation of Schrödinger's quantum physics. We have emphasized the modifications to be made in order to generalize the study of a one-dimensional problem when this study extends to a three-dimensional problem and in particular for central forces with spherical symmetry. The generalization to three dimensions will be immediate in the case of central forces. For this last case it suffices to consider a spherical wave function instead of a plane wave function.

We then presented a detailed analytical study of an exactly solvable case. This is the harmonic oscillator problem. We have used a purely analytical method, which does not require creation and annihilation operators. Firstly, we have looked at the one-dimensional harmonic oscillator. The energy spectrum and the exact wave functions are derived. For the three-dimensional isotropic harmonic oscillator it is preferable to work in spherical coordinates and apply the results already derived for the central forces problem. We have followed the same approach to analytically determine the expressions of the bound state wave functions and the corresponding eigen-energies.

We have once again taken up the problem of the harmonic oscillator, but this time for a system with five particles. Instead of using the position vectors of the individual particles as variables, we have used the coordinate of the centre of mass of the system with four other coordinates, the so-called *Jacobi coordinates*. In this new coordinate system, we were able to express the hamiltonian of the system as a sum of four decoupled two-body harmonic oscillator

hamiltonians, which allowed us to determine the energy spectrum and the associated wave functions. For some mass configurations the standard choice of Jacobi coordinates leads to a non-diagonal form for the hamiltonian. This hamiltonian therefore describes a system of four coupled harmonic oscillators. Consequently, the solution of the problem can no longer be directly deduced. In order to get around this problem, we have made a new choice for these Jacobi coordinates. In fact, a diagonal form for the hamiltonian is obtained with an appropriate choice of these coordinates and the solution to the problem will be found immediately. We have shown that, in general, the exact wave function associated to the ground state of the five-body harmonic oscillator is no longer a simple gaussian in Jacobi coordinates but a correlated gaussian.

On the other hand, we have focused on approximate solutions of the five-body problem with non-harmonic interactions, where exact solutions can't be obtained in general. For this, we have used the method of expansion on correlated gaussians, which is a method of variational nature based on the Ritz variational principle. This method consists of minimizing the mean value of the hamiltonian over a number of free parameters involved in a wave function called the *trial wave function*.

We have restricted ourselves to problems with five particles interacting with each other through two-body forces that are derived from power-law potentials. The trial wave function is chosen to be a series of correlated gaussians with Jacobi coordinates as variables. We have analytically calculated the matrix elements needed to calculate the mean value of the system's hamiltonian. The method was then applied to five-body problems for different mass configurations. It turns out that the method converges to the exact ground state energy by increasing the number of gaussians, but this requires variational treatment that becomes more and more complicated. It should be taken into account that we are dealing with non-linear optimisation problem with constraints, where the number of variational parameters increases rapidly with the number of gaussians used, and therefore requires considerable numerical calculations.

Finally, some numerical values of our calculations for the ground state energy of five-body systems are presented in tables where we have limited ourselves to two-body interactions derived from power-law potentials of the same type and for different powers.

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Abstract

The content of this thesis is summarized by the interest in the approximate solution to the stationary Schrödinger equation for the five-body system, where we use the expansion on the associated Gaussians to derive the upper limits of the energy of the fundamental case, and adjustments have been made in order to generalize the study of a one-dimensional problem when this study extends to a three-dimensional problem in the case of central forces. The case is considered as a spherical wave function instead of a plane one, where we presented an analytical study of a solvable case and dealt with the problem of the harmonic oscillator for a system consisting of five bodies. The standard Jacobi coordinates were also used, which allows us to determine the energy spectrum and the wave functions associated with it.

Résumé

Le contenu de cette thèse est résumé par l'intérêt de la solution approchée de l'équation de Schrödinger constante pour le système à cinq corps, où l'on utilise le développement sur les gaussiennes associées pour en déduire les bornes supérieures de l'énergie du cas

fondamentale, et des ajustements ont été faites dans le but de généraliser l'étude d'un problème unidimensionnel lorsque cette étude s'étend à un problème tridimensionnel dans le cas des forces centrales, le cas étant considéré comme une fonction d'onde sphérique au lieu d'une fonction d'onde plane, où nous avons présenté une étude analytique d'un cas résoluble et a traité le problème de l'oscillateur harmonique pour un système composé de cinq corps.Les coordonnées standard de Jacobi ont également été utilisées, ce qui permet de déterminer le spectre d'énergie et les fonctions d'onde qui lui sont associées.