République Algérienne Démocratique et Populaire
Ministère de L'Enseignement Supérieur et de la Recherche Scientifique
Université des Sciences et de la Technologie SAAD DAHLEB
Faculté Des Science

Thèse
Présentée pour l'obtention du **diplôme** de **MASTER**
**En :**Physique Moluculaire
**Spécialité : Physique Theorique**
**Par :** ATTABA Alaaeddine

**Sujet**

# The Solution of the Rotational Morse Potential Using the Method of Inverse Contour Representation.

Soutenue publiquement, le 30/06/2024, devant le jury composé de :

| | | | |
|---|---|---|---|
| HADJ-MOUSSA Mohamed | President | MCA | à l'USDB |
| CHERROUD Othmane | Examinateur | MCA | à l'Univ de Medea |
| YAHIAOUI Sid-Ahmed | Encadreur | MCB | à l'USDB |
| BRADJI Okba | Co-Encadreur | MCB | à l'USDB |

# Acknowledgement

First and foremost, I would like to express my deepest gratitude to my supervisor, Dr. Yahiaoui and Dr. Bradji, for their invaluable guidance, encouragement, and unwavering support throughout the development of this thesis. Their expertise and insight have been instrumental in shaping this work and inspiring me to explore new dimensions in the field of molecular physics.

I would also like to extend my heartfelt thanks to the members Dr. Hadji Moussa and Dr. Cheroud for their constructive feedback, fruitful discussions, and generous sharing of knowledge and resources. Their contributions have greatly enriched this research and provided me with valuable perspectives.

Finally, I am deeply grateful to my family and friends for their unwavering support, patience, and encouragement, which provided me with the strength and motivation to complete this work. This accomplishment would not have been possible without their love and understanding.

Thank you all for being an integral part of this journey.

# ملخص

بالنسبة للقيم غير الصفرية للعدد الكمومي $l$ ، نقدم حلاً تحليلياًا للمعادلة الشعاعية لشرودنغر من أجل الجهد الدوراني لموريس باستخدام تقريب بيكيريس في إطار طريقة تمثيل الكنتور العكسي في سياق التحولات التكاملية لكثافة لابلاس لحل مشكلة الحالات المقيدة للمعادلة التفاضلية لشرودنغر في الجهد الدوراني لموريس. الهدف الرئيسي من هذه الطريقة هو دراسة كيفية عمل هذه الطريقة. بشكل عام، يعد تحديد التحويل العكسي للكنتور هو المشكلة الرئيسية في استخدام التحويلات التكاملية، إلا إذا تم تمثيله من خلال دالة معروفة التي تاخذنا مباشرة الى حساب البواقي . من الجدير بالذكر أن هذه الطريقة كانت ناجحة وسهلة نسبياًا، حيث لا توجد اختيار محدد للكنتور الذي يتم التكامل عليه، مما يسمح باستخدام العديد من أنواع الكنتورات غير المحدودة. لقد أظهرنا أن تمثيل الكنتور العكسي يفتح الطريق لعملية اشتقاق جديدة لحالات مقيدة للجهد الدوراني لموريس. في النهاية، سيكون من المثير للاهتمام إكمال نهجنا للأنواع المختلفة من الجهود التي تنتمي إلى معادلة هيبراجوميات التفاضل .تم الحصول على القيم الذاتية للطاقة الخاصة بالحالات المقيدة والدوال الذاتية المقابلة لها. يتم حساب مستويات الطاقة لجميع الحالات المقيدة بسهولة باستخدام هذه الطريقة. تم مقارنة الحسابات العددية لأربع جزيئات ثنائية الذرة نموذجية، $HCl$ و $CO$ و $H_2$ و $LiH$، مع تلك التي تم الحصول عليها بواسطة طرق أخرى مثل الفائض التناظري والطريقة التغيرية. وقد تبين أن النتائج التي تم الحصول عليها بواسطة الطريقة الحالية تتوافق جيداً مع تلك التي تم الحصول عليها بواسطة طرق تقريبية أخرى.

**الكلمات المفتاحية :** الجهد الدوراني لموريس، تقريب بيكيريس، التحويلات التكاملية للا بلاس، التحويل العكسي للكونتور، دالة بيتا اولر، حساب البواقي لكوشي، دوال هيبرجيوميتريك،سطح ريمان ، معادلة شرودينجر

## Abstract

For non-zero  values, we present an analytical solution of the radial Schrodinger equation for the rotating Morse potential using the Pekeris approximation within the framework of the method of inverse contour representation , The bound state energy eigenvalues and the corresponding eigenfunctions are obtained , The energy levels of all the bound states are easily calculated from this approche , The numerical calculations for four typical diatomic molecules HCl, CO ,$H_2$ and LiH are compared with those obtained by other methods such as the super-symmetry, the variational, It is found that the results obtained by the present method are in good agreement with those obtained by other approximate methods.

**Keywords :** Rotational morse potential , Pekeris approximation , Radial Schrodinger equation, Inverse contour representation, Curvilinear laplace transform , Confluent hypergeometric function, Euler Beta function, The riemann surfaces, Residues theorem of cauchy,

## Résumé

Pour des valeurs de non nulles, nous présentons une solution analytique de l'équation de Schrödinger radiale pour le potentiel de Morse rotatif en utilisant l'approximation de Pekeris dans le cadre de la méthode de représentation de contour inverse. Les valeurs propres de l'énergie des états liés et les fonctions propres correspondantes sont obtenues. Les niveaux d'énergie de tous les états liés sont facilement calculés à partir de cette approche. Les calculs numériques pour quatre molécules diatomiques typiques, HCl, CO, $H_2$ et LiH, sont comparés avec ceux obtenus par d'autres méthodes telles que la supersymétrie et la méthode variationnelle. Il a été constaté que les résultats obtenus par la méthode actuelle sont en bon accord avec ceux obtenus par d'autres méthodes approximatives.

**Mots clé :** Potentielle de morse rotationelle, l'approximation de pekerise, représentation de contoure inverse, représentation de laplace curviligne, fonction de euler beta , theoreme de résidus de cauchy , feuilles de riemaan , fonction hypergéomitric ,

# Table des matières

# Table des figures

# Liste des tableaux

# Liste des Algorithmes

# Introduction

The Morse potential [13] is one of the potentials belonging to the Natanzon class [14], which has a finite number of states that can be solved exactly (analytically) through the Schrödinger equation. It was introduced by P. M. Morse in 1929 to describe the vibrational energy of a diatomic molecule and is given by :

$$V_M(r) := V_0 \left( e^{-2\sigma(r-r_e)} - 2e^{-\sigma(r-r_e)} \right), \tag{1}$$

where $V_0$ is the dissociation energy of the molecule, $\sigma$ is a parameter that controls the depth of the potential well, and $r_e$ is associated with the equilibrium internuclear distance between the molecules.

However, it is well known that the case of the radial Morse potential (also referred to as the rotational Morse potential) for an arbitrary state $l$-states ($l \neq 0$), i.e., one that includes a centrifugal term,

$$V_M(r) := V_0 \left( e^{-2\sigma(r-r_e)} - 2e^{-\sigma(r-r_e)} \right) + \frac{\hbar^2 l(l+1)}{2\mu r^2}, \tag{2}$$

where $\mu = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass in the center of mass, and $m_i$ are the masses of the two molecules, cannot be solved analytically and exactly unless certain approximation techniques are employed. Among these methods is the Pekeris approximation [15], where the basic idea is to treat an arbitrary $l$-state as an $s$-state (i.e., $l = 0$) by approximating the centrifugal term to match that of the Morse potential, which is well-known to be exactly solvable through the Schrödinger equation.

The Pekeris approximation for the radial Morse potential has been solved using various methods, including, for example (as referenced below) : quantum mechanical supersymmetry [12], the variational approach [8], the Nikiforov-Uvarov method [4] , the shifted and modified $1/N$ expansion [10], [2], the iterative asymptotic method [3], and the exact quantization rule [16].

In this thesis, the goal is to solve the Schrödinger equation for the radial Morse potential using an alternative approach known as the inverse contour representation [11], formulated within the framework of curvilinear Laplace transforms. We will see that this approach is closely connected to the integral representation of Euler's beta function in the formalism of Cauchy integrals. This method relies on the creation of a barrier, or a branch cut, connecting the points 0 and 1, which represent the integration limits of Euler's beta function.

This thesis consists of two chapters : **the first chapter** is dedicated to the Pekeris approximation and We demonstrated how this approximation is effective in addressing the challenges associated with the centrifugal term . Generalizing the Pekeris approximation and replacing the centrefugal term by specific form.**the second chapter** We showed that by applying the Pekeris approximation to the radial Morse potential, we obtained a new form of the centrifugal term that had previously caused problems. Substituting this into the Schrödinger equation, we derived the new approximate equation. From there, we were able to find the bound states for $l = 0$ and $l > 0$. We solved this using a method called the Inverse Contour Representation, treating the new function as curvilinear Laplace transforms and how it can be applied to the wave equation while incorporating necessary boundary conditions to ensure the resulting wave function is physically meaningful like through the choice of contour and ensures the correct behavior of the wave-function at the boundaries of the system, especially at infinity. By addressing these conditions, we provide a framework for using the CLT to solve quantum mechanical problems in curvilinear coordinates and ensure that the solutions correspond to valid quantum states. and finaly we demonstrates how contour integration can be applied to derive solutions to bound-state problems, particularly for the Morse potential, with emphasis on normalization and the calculation of energy eigenvalues and compare it with another methods to ensure the reliability of this method.

Finally, a general conclusion concludes this work, followed by the references and the Mathematica graph codes.

# Chapitre 1

# The Pekeris approximation, it technique

## 1.1 Introduction

In the last decade a large community of researchers have been involved a search of approximate solutions for wave equations (non-relativistic or relativistic) including the centrifugal term and subject to different potential functions $V(r)$. The main characteristic of these solutions lies in the substitution of the centrifugal term by an approximation, so that one can obtain an equation, normally hypergeometric, which is solvable.

## 1.2 Purpose of the Pekeris Approximation

The primary purpose of the Pekeris approximation is to address the singularities or complexities that arise in the Schrödinger equation when dealing with potentials that have a centrifugal term. In quantum mechanics, the Schrödinger equation describes the behavior of particles, and it contains terms related to both kinetic and potential energy. The centrifugal term can lead to mathematical complexities, especially when solving for bound-state energy levels

## 1.3 General procedure

The Pekeris approximation for the centrifugal term has been successfully applied to the Schrodinger equation with many potentials , So the main objective is to simplifying the centrefugal terme and expand it in powers series where y = f(r) the function that is chosen diffrently according to the potentials we are dealing with but in such way that is suitable for each one of them but we choose it in general , we began with the centrefugal term

$$V_c(\rho) = \frac{h^2 l(l+1)}{2\mu(1+\rho)^2 r_e^2} \tag{1.1}$$

with $r = (1+\rho)r_e$

$$V_c(\rho) = \frac{h^2 l(l+1)}{2\mu r_e^2} \frac{1}{(1+\rho)^2} \tag{1.2}$$

$$V_c(\rho) = \frac{h^2 l(l+1)}{2\mu r_e^2} \left(\frac{r_e}{r}\right)^2 \tag{1.3}$$

Now we consider this expression as the expantion of the centrefugal term

$$F(y) = \left(\frac{r_e}{r}\right)^2 = \left(1 - \frac{f-1(y)}{ar_e}\right)^{-2} \tag{1.4}$$

with the specific function that is suitable for this case

$$y = exp[-a(r-re)] \tag{1.5}$$

then F will be

$$F(y) = \left(\frac{r_e}{r}\right)^2 = \left(1 - \frac{ln(y)}{ar_e}\right)^{-2} \tag{1.6}$$

The Taylor expansion series for F(y) , with specific choise of $\alpha = 1$

$$F(y) = \sum_{n=0}^{\infty} c_n (y-\alpha)^n \tag{1.7}$$

then we consider the first three terms

$$F(y) = \left(\frac{r_e}{r}\right)^2 \approx c_0 + (y-\alpha)c_1 + \frac{c_2}{2!}(y-\alpha)^2 \tag{1.8}$$

we calculate the terms until n=2

$$c_n = \frac{1}{n!} \frac{d^n F(y)}{dy^n}\bigg|_{y=\alpha} \tag{1.9}$$

$$c_0 = 1 \tag{1.10}$$

for the calculation of $c_1$ et $c_2$ we will use this two applications :
$(\mathrm{U}^n)' = n.u'.u^{n-1}$

$(u-v)' = u' - v'$

$$c_1 = \frac{dF(y)}{dy}|_{y=1} = \frac{2ar_e}{y(ar_e)^2}\frac{(ar_e)^3}{(ar_e - ln(y))^3} = \frac{2(ar_e)^2}{(ar_e - ln(y))^3 y}|_{y=1} = \frac{2}{ar_e} \tag{1.11}$$

$$\begin{aligned} c_2 = \frac{1}{2}\frac{d^2F(y)}{dy^2}\bigg|_{y=1} &= -(-3(-\frac{ar_e}{(ar_e)^2 y})(1-\frac{ln(y)}{ar_e})^{-4}(-\frac{ar_e}{(ar_e)^2 y})2+2(-\frac{-(ar_e)^3)}{((ar_e)^2)^2}(1-\frac{ln(y)}{ar_e})^{-3} = \\ &\frac{1}{2}(\frac{-2(ar_e)^3 + (ar_e)^2 2ln(y) + 6(ar_e)^2}{(ar_e - ln(y))^4 y^2})|_{y=1} = -\frac{1}{ar_e} + \frac{3}{(ar_e)^2} \end{aligned} \tag{1.12}$$

now substituting (1.10),(1.11) and (1.12) into (1.8), one obtain

$$\left(\frac{r_e}{r}\right)^2 \approx (1-\frac{3}{\sigma r_e}+\frac{3}{(\sigma r_e)^2})+(\frac{4}{\sigma r_e}-\frac{6}{(\sigma r_e)^2})\exp\left[-\sigma\left(r-r_e\right)\right]+(\frac{3}{(\sigma r_e)^2}-\frac{1}{\sigma r_e})\exp\left[-2\sigma\left(r-r_e\right)\right] \tag{1.13}$$

and then we subtitu (1.13) into the radial shrodinger equqtion and continu the procedure with the new approximation of course where V(r) is arbitrary potential here but we will see in the following chapters this approximation with radial morse potential and what methode we approche to solve it .

# Chapitre 2

# Physical Applications

## 2.1 Part 1 : Pekeris Approximation on the Radial Morse Potential

It is well known that the shrodinger equation cannot be solved analytically because of the centrifugal term in the radial morse potential,

$$V_M(r) := V_0 \left(e^{-2\sigma(r-r_e)} - 2e^{-\sigma(r-r_e)}\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2}, \tag{2}$$

which has problems such as a singularity problem also This term makes the equation even harder to solve analytically, especially for states with nonzero angular momentum (non zero "l").

To obtain an approximate analytical solution, we uses the Pekeris approximation, which is a mathematical technique that allows one to transform a potential function with angular momentum (non zero "l") into an equivalent potential function without angular momentum (l = 0). This is done by approximating the centrifugal term using a function that only depends on the radial coordinate, effectively "eliminating" the angular momentum from the equation not entirely gone but it is hidden in the term $\gamma$.By doing this, we are able to solve the Schrödinger equation for the rotating Morse potential, so firstly via a limited development the centrifugal potential will be :

$$V_c(\rho) = \frac{h^2 l(l+1)}{2\mu(1+\rho)^2 r_e^2} \tag{2.1}$$

$$V_c(\rho) = \frac{\hbar^2 l(l+1)}{2\mu r_e^2}\left(1 - 2\rho + 3\rho^2 - 4\rho^3 + \cdots\right) \tag{2.2}$$

and then we define an equivalent potential with coefficients to be determined :

$$\tilde{V}_c(\rho) \approx \gamma \left(A_0 + A_1 e^{-\alpha\rho} + A_2 e^{-\varepsilon\alpha\rho}\right) \tag{2.3}$$

this expression can be extended :

$$\tilde{V}_c(\rho) \approx \gamma \left(A_1 + A_1 + A_2 - \rho\left(A_1\alpha + 2A_2\alpha\right) + \rho^2\left(A_1\frac{\alpha^2}{2} + 2A_2\alpha^2\right) - \rho^3\left(A_n\frac{\alpha^3}{6} + \frac{4}{3}A_2\alpha^3\right) + \ldots\ldots\right) \tag{2.4}$$

this extension can be replaced by :

$$\frac{1}{(1+\rho)^2} = \left(A_0 + A_1 e^{-\alpha\rho} + A_2 e^{-\varepsilon\alpha\rho}\right) \tag{2.5}$$

then we find the coefficients as follow :

$$A_0 + A_1 + A_2 = 1 \Rightarrow A_0 = 1 - \frac{3}{\alpha} + \frac{3}{\alpha^2} \tag{2.6}$$

$$A_1\alpha + 2A_2\alpha = 2 \Rightarrow A_1 = \frac{4}{\alpha} - \frac{6}{\alpha^2} \tag{2.7}$$

$$A_1\frac{\alpha^2}{2} + 2A_2\alpha^2 = 3 \Rightarrow A_2 = \frac{3}{\alpha^2} - \frac{1}{\alpha} \tag{2.8}$$

$$\gamma = \frac{\hbar^2 l(l+1)}{2\mu r_e^2} \tag{2.9}$$

we can now take $\tilde{V}_{rot}$ instead of the potential $V_{rot}$ , now we are able to solve the Schrödinger equation for non zero "l" , so now we will substitues (2) and (2.3) into the shrodinger equation for the new morse potential

so we begin with shrodinger equation [5] :

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}\left[V(r) - E_{nl}\right]\right] R_{ne}(r) = 0 \tag{2.10}$$

according to this :

$r = (1+\rho)r_e$

$$\frac{d}{dr} = \frac{d\rho}{dr}\frac{d}{d\rho} = \frac{1}{re}\frac{d}{d\rho} \tag{2.11}$$

and to simplify things put $l = 0$ so that the rotational Mvt alone is gone, but there remains the vibration/rotation couple inside the potential of Mouse.

Now, we will insert the new potential into our equation :

$$\left[\frac{1}{r_e^2}\frac{d^2}{d\rho^2} - \frac{2\mu}{\hbar^2}\left[V(r) - E_{n\rho}\right]\right] R_{n\rho}(\rho) = 0 \tag{2.12}$$

$$\left[\frac{d^2}{df^2} - \frac{2\mu}{\hbar^2} r_e^2 \left[V_0\left(e^{-2\sigma(rr_e)} - 2e^{-\sigma(r-r_e)}\right) + \ \gamma\left(A_0 + A_1e^{-\alpha r} + A_2e^{-2\alpha r}\right) - E_n\rho\right]\right] R_{nl}(\rho) = 0 \tag{2.13}$$

of course where $\begin{cases} r - r_e = f_r \\ \\ \sigma r_e = \alpha \end{cases}$

$\left[\frac{d^2}{d\rho^2} - \frac{2\mu}{\hbar^2} r_e^2\left[V_0e^{-2\alpha\rho} + \gamma A_2e^{-2\alpha\rho} - 2V_0e^{-\alpha\rho} + \gamma A_1e^{-\alpha\rho} + \ \gamma A_0 - E_{nl}\right]R_{n\rho}(\rho) = 0(2.14)\right.$

$$\left[\frac{d^2}{d\rho^2} - \frac{2\mu}{\hbar^2} r_e^2 \left[\left(V_0 + \gamma A_2\right)e^{-2\alpha\rho} - \left(2V_0 - \gamma A_1\right)e^{-\alpha\rho} + \ \left(\gamma A_0 - E_{nl}\right)\right]\right] R_{ne}(\rho) = 0 \tag{2.15}$$

$$\left[\frac{d^2}{d\rho^2} - \frac{2\mu}{\hbar^2} r_e^2 \left(V_0 + \gamma A_2\right) e^{-2\alpha\rho} + \frac{2\mu r_e^2}{\hbar^2} \left(eV_0 - \gamma A_1\right) e^{-\alpha\rho} - \frac{2\mu}{\hbar^2} r_e^2 \left(\gamma A_0 - E_{nl}\right)\right] R_{nl}(\rho) = 0 \tag{2.16}$$

we obtain :

$$\left[\frac{d^2}{d\rho^2} - \beta_2^2 e^{-2\alpha\rho} + \beta_1^2 e^{-\alpha\rho} - E_{ne}^2\right] R_{n\rho}(\rho) = 0 \tag{2.17}$$

where :

$$\beta_2^2 = \frac{2\mu r_e^2}{\hbar^2} \left(V_0 + \gamma A_2\right) = \Lambda_0^2 \left(V_0 + \gamma A_2\right) \tag{2.18}$$

$$\beta_1^2 = \frac{2\mu r_e^2}{\hbar^2} \left(2V_0 - \gamma A_1\right) = A_0^2 \left(2V_0 - \gamma A_1\right) \tag{2.19}$$

$$E_{nl}^2 = \frac{2\mu r_e^2}{\hbar^2} \left(\gamma A_0 - E_{nl}\right) = \Lambda_0^2 \left(\gamma A_0 - E_{nl}\right) \tag{2.20}$$

this equation will be solved via the Laplace transform method in the non-zero "l" case, taking into account rotations in addition to vibrations.

$$\left(\frac{d^2}{d\rho^2} - \beta_2^2 e^{-2\alpha\rho} + \beta_1^2 e^{-\alpha\rho} - \epsilon_{ne}^2\right) R_{nl}(\rho) = 0 \tag{2.21}$$

we first define a change of variable because The effect that is the presence of the exponential term in equation , which makes it difficult to solve analytically.

To deal with this issue, we introduce a new variable $\xi$, which is defined as :

$\rightarrow \quad \xi = e^{-\alpha\rho}$

where $\alpha$ is a constant and r is the radial variable.

We have Furthermore :

$$\frac{d}{df} = \frac{d\xi}{df}\frac{d}{d\xi} \tag{2.22}$$

so

$$\frac{d\xi}{d\rho} = -\alpha e^{-\alpha\rho} \overset{z}{=} -\alpha e^{-\alpha\rho}\frac{d}{d\xi} \tag{2.23}$$

$\frac{d}{d\rho} = -\alpha\xi\frac{d}{d\xi}$

then we dudected that :

$$\frac{d^2}{d\rho^2} = \frac{d}{d\rho}\frac{d}{d\rho} = \alpha^2\left(\xi\frac{d}{d\xi}\right)\left(\xi\frac{d}{d\xi}\right) \tag{2.24}$$

$$= \alpha^2\xi\left[\frac{d\xi}{d\xi}\frac{d}{d\xi} + \xi\frac{d}{d\xi}\frac{d}{d\xi}\right] \tag{2.25}$$

$$= \alpha^2\xi^2\frac{d^2}{d\xi^2} + \alpha^2\xi\frac{d}{d\xi} \tag{2.26}$$

so we will insert what we deducted and what we impose into our equation we obtain :

$$\left(\alpha^2\xi^2\frac{d^2}{d\xi^2} + \alpha^2\xi\frac{d}{d\xi} - \beta_2^2\xi^2 + \beta_1^2\xi - \epsilon_{nl}^2\right)R_{nl}\left(\rho\right) = 0 \tag{2.27}$$

$$\left(\xi^2\frac{d^2}{d\xi^2} + \xi\frac{d}{d\xi} - \frac{\beta_2^2}{\alpha^2}\xi^2 + \frac{\beta_1^2}{\alpha^2}\xi - \frac{\epsilon_{nl}^2}{\alpha^2}\right)R_{nl}\left(\rho\right) = 0 \tag{2.28}$$

we take into account this expression where k is constant :

$R_{nl}(\rho) = \xi^k F_{nl}(\xi)$

$$\frac{dR_{nl}(\rho)}{d\xi} = \frac{d}{d\xi}\left(\xi^k F_{nl}(\xi)\right) \tag{2.29}$$

$$= k\xi^{k-1}F_{nl}(\xi) + \xi^k \frac{d}{d\xi}F_{nl}(\xi) \tag{2.30}$$

we have furthermore :

$$\frac{d^2}{d\xi^2}R_{nl}(\rho) = \frac{d}{d\xi}\left[k\xi^{k-1}F_{nl}(\xi) + \xi^k \frac{d}{d\xi}F_{nl}(\xi)\right] \tag{2.31}$$

$$= k(k-1)k^{k-2}F_{nl}(\xi) + k\xi^{k-1}\frac{d}{d\xi}F_{nl}(\xi) + k\xi^{k-1}\frac{dF_{nl}}{d\xi} + \xi^k \frac{d^2}{d\xi^2}F_{nl}(\xi) \tag{2.32}$$

$$\frac{d^2}{d\xi^2}R_{nl}(\xi) = k(k-1)\xi^{k-2}F_{nl}(\xi) + 2k\xi^{k-1}\frac{d}{d\xi}F_{nl}(\xi) + \xi^k \frac{d^2}{d\xi^2}F_{nl}(\xi) \tag{2.33}$$

will become :

$$\xi^2\left[k(k-1)\xi^{k-2}F_{ne}(\xi) + 2k\xi^{k-1}\frac{d}{d\xi}F_{ne}(\xi) + \xi^k\frac{d^2}{d\xi^2}F_{ne}(\xi)\right] + \xi\left[k\xi^{k-1}F_{nl}(\xi) + \xi^k\frac{d}{d\xi}F_{nl}(\xi)\right] - \frac{\beta_2^2}{\alpha^2}\xi^2 R_{nl}(\rho) + \frac{\beta_1^2}{\alpha^2}\xi R_{nl}(\rho) - \frac{\epsilon_{nl}^2}{\alpha^2}R_{nl}(\rho) = 0 \tag{2.34}$$

we will do further manipulation :

$R_{nl}(\rho) = \xi^k F_{nl}(\xi)$

$$\xi^2 \left[k(k-1)\xi^{k-2}F_{ne}(\xi) + 2k\xi^{k-1}\frac{d}{d\xi}F_{ne}(\xi) + \xi^k\frac{d^2}{d\xi^2}F_{ne}(\xi)\right] + \xi\left[k\xi^{k-1}F_{nl}(\xi) + \xi^k\frac{d}{d\xi}F_{nl}(\xi)\right] + \frac{\beta_2^2}{\alpha^2}\xi^2\xi^kF_{nl}(\xi) + \frac{\beta_1^2}{\alpha^2}\xi\xi^kF_{\mathrm{nl}}\,(\xi) - \frac{\epsilon_{nl}^2}{\alpha^2}\xi^kF_{nl}(\xi) = 0 \quad (2.35)$$

$$k(k-1)\xi^kF_{nl}(\xi) + 2k\xi^{k+1}\frac{d}{d\xi}F_{nl}(\xi) + \xi^{k+2}\frac{d^2}{d\xi^2}F_{nl}(\xi) + k\xi^kF_{nl}(\xi) + \xi^{k+1}\frac{d}{d\xi}F_{nl}(\xi) - \frac{\beta_2^2}{\alpha^2}\xi^{k+2}F_{nl}(\xi) + \frac{\beta_1^2}{\alpha^2}\xi^{k+1}F_{nl}(\xi) - \frac{\epsilon_{nl}^2}{\alpha^2}\xi^kF_{nl}(\xi) = 0 \quad (2.36)$$

$$k(k-1)F_{nl}(\xi) + 2k\xi\frac{d}{d\xi}F_{nl}(\xi) + \xi^2\frac{d^2}{d\xi^2}F_{nl}(\xi) + kF_{nl}(\xi) + \xi\frac{d}{d\xi}F_{nl}(\xi) - \frac{\beta_2^2}{\alpha^2}\xi^2F_{nl}(\xi) + \frac{\beta_1^2}{\alpha^2}\xi F_{nl}(\xi) - \frac{\epsilon_{nl}^2}{\alpha^2}F_{nl}(\xi) = 0 \quad (2.37)$$

$$[\xi^2\frac{d^2}{d\xi^2} + k(k-1) + (2k+1)\xi\frac{d}{d\xi} + k - \frac{\beta_2^2}{\alpha^2}\xi^2 + \frac{\beta_1^2}{\alpha_2}\xi - \frac{\epsilon_{nl}^2}{\alpha^2}]F_{nl}(\xi) = 0 \quad (2.38)$$

$$[\xi^2\frac{d^2}{d\xi^2} + (2k+1)\xi\frac{d}{d\xi} - \frac{\beta_2^2}{\alpha^2}\xi^2 + \frac{\beta_1^2}{\alpha_2}\xi + K^2 - \frac{\epsilon_{nl}^2}{\alpha^2}]F_{nl}(\xi) = 0 \quad (2.39)$$

we impose this into our expression :

$k = \frac{\epsilon_{nl}}{\alpha}$

we obtain :

$$[\xi\frac{d^2}{d\xi^2}+(2\frac{\epsilon_{nl}}{\alpha}+1)\frac{d}{d\xi}-(\frac{\beta_2^2}{\alpha^2})^2\xi+(\frac{\beta_1^2}{\alpha_2})^2]F_{nl}(\xi)=0$$

(2.40)

By substituting this new variable into the equation above , we obtain this equation , which does not contain the exponential term. This is because the new variable $\xi$ absorbs the effect of this term, making the resulting equation easier to solve analytically.

In other words, the new variable $\xi$ helps to simplify the mathematical expression by absorbing the effect of the exponential term. This is a common technique in mathematical modeling and allows us to solve equations that would otherwise be difficult or impossible to solve. The centrifugal term and the exponential term are both singularities in the equation. A singularity is a point where a mathematical function becomes undefined or where its behavior is not well-defined.

## Further notes :

In the case of the centrifugal term, it becomes infinite when the distance r becomes zero, which is the center of rotation. This means that the centrifugal term dominates the behavior of the equation near the center of rotation, making it very difficult to solve for the behavior of the system in that region.

On the other hand, the exponential term becomes infinite as the distance r goes to infinity, meaning that it dominates the behavior of the system far away from the center of rotation.

When the centrifugal term is combined with the exponential term, the exponential term serves to modulate the effect of the centrifugal term, making it stronger or weaker depending on the value of the distance r. Near the center of rotation, the exponential term can help to reduce the strength of the centrifugal term, making it easier to analyze the behavior of the system. Far away from the center of rotation, the exponential term can enhance the effects of the centrifugal term, allowing it to have a stronger impact on the system.

## Summary :

The pekeris approximation it is powerful mathematical thechnique not just allow us to remove the singularities problems but also allow us to study the general cas (l=0 , non zero l)

## 2.2 Part 2 : Curvilinear Laplace Transform and Conditions on the Wave Function.

The Curvilinear Laplace Transform (CLT) is a mathematical tool used in the analysis of differential equations, particularly in cases involving curvilinear coordinates. Unlike the standard Laplace transform, which is typically applied to problems in Cartesian coordinates, the CLT is designed to handle problems where the geometry or the boundary conditions are more naturally expressed in curvilinear coordinates such as cylindrical or spherical systems. The Curvilinear Laplace Transform is defined for a function f(t) in a given curvilinear coordinate system by the integral [7] :

$$L[f(t)] = F(s) = f(t)e^{-st}dt \tag{2.41}$$

where s is a complex number parameter. This transform converts a function of time t into a function of the complex variable s. Now let us consider the function $F_{nl}(\xi)$ can be expressed in this forme :

$$F_{nl}(\xi) = \oint_c Q(t)e^{\xi t}dt \tag{2.42}$$

such that the function Q(t) is an unknown function to be determined. Here, C denotes the integration contour on the real axis used in order to impose on the true Equation (5) the boundary conditions and independent of the variable $\xi$.the integral (6) is often called the curvilinear laplace transform.

then by applying the $n^{th}$ derivative with respect of $\xi$ , we have this forme :

$$F_{nl}(\xi) = \oint_c Q(t)e^{\xi t}dt \tag{2.43}$$

now we have the n-derivative forme :

$$F_{nl}^{(n)}(\xi) = \oint_c t^n Q(t)e^{\xi t}dt \tag{2.44}$$

we performe derivation by parts we get :

$u = Q(t) \quad du = Q'(t)$
$dv = e^{\xi t} \quad v = \frac{e^{\xi t}}{\xi}$

$$F(\xi) = \frac{1}{\xi}\left[Q(t)e^{\xi t}\right]_c - \frac{1}{\xi}\oint_c \frac{dQ(t)}{dt}e^{\xi t}dt \tag{2.45}$$

$$F_-^{(n)}(\xi) = \frac{1}{\xi}\left[t^n Q(t)e^{\xi t}\right]_c - \frac{1}{\xi}\oint_c \frac{dt^n Q(t)}{dt}e^{\xi t dt} \tag{2.46}$$

we multply by $\xi$ then we get :

$$\varepsilon\mathcal{F}^{(n)}(\xi) = \left[t^n Q(t)e^{\xi t}\right]_c - \oint_c \frac{dt^n Q(t)}{dt}e^{\xi t}dt \tag{2.47}$$

where the symbolism $M(\xi,t)_c$ in equation (2.47) designates the growth of the function $M(\xi,t) = t^n Q_{nl}(t)e^{t\xi}$ when t describes the entire contour C.
we substituting (2.45) , (2.46) , (2.47) into (2.48) :

$$[\xi\frac{d^2}{d\xi^2} + (\frac{2\epsilon_{nl}}{\alpha}+1)\frac{d}{d\xi} - (\frac{\beta_2}{\alpha})^2\xi + (\frac{\beta_1}{\alpha})^2]F(\xi) = 0 \tag{2.48}$$

$$\xi\frac{d^2}{d\xi^2}F(\xi) + (\frac{2\epsilon_{n\ell}}{\alpha}+1)\frac{d}{d\xi}F(\xi) - (\frac{\beta_2}{\alpha})^2\xi F(\xi) + (\frac{\beta_1}{\alpha})^2 F(\xi) = 0 \tag{2.49}$$

$$\begin{aligned}[t^2Q_{nl}(t)e^{\xi t}]_c - \oint_c \frac{d[t^2Q_{nl}(t)]}{dt}e^{\xi t}dt + (\frac{2\epsilon_{nl}}{\alpha}+1)(\oint_c tQ_{nl}(t)e^{\xi t}dt)\\ - (\frac{\beta_2}{\alpha})^2([Q_{nl}(t)e^{\xi t}]_c - \oint_c \frac{dQ_{nl}(t)}{dt}e^{\xi t}dt) + (\frac{\beta_1}{\alpha})^2\oint_c Q_{nl}(t)e^{\xi t}dt = 0\end{aligned} \tag{2.50}$$

$$\begin{aligned}[t^2Q_{nl}(t)e^{\xi t}]_c-\oint_c(2tQ_{nl}+\frac{dQ_{nl}(t)}{dt}t^2)e^{\xi t}dt+(\frac{2\epsilon_{nl}}{\alpha}+1)(\oint_c tQ_{nl}(t)e^{\xi t}dt)&\\ -(\frac{\beta_2}{\alpha})^2([Q_{nl}(t)e^{\xi t}]_c-\oint_c\frac{dQ_{nl}(t)}{dt}e^{\xi t}dt)+(\frac{\beta_1}{\alpha})^2\oint_c Q_{nl}(t)e^{\xi t}dt=0&\end{aligned}\tag{2.51}$$

$$\begin{aligned}\Bigg\{\left(t^2-\left(\frac{\beta_2}{\alpha}\right)^2\right)Q_{n1}(t)e^{\xi t}\Bigg]_c-\oint_c O'_{n1}(t)\left(t^2-\left(\frac{\beta_2}{\alpha}\right)^2\right)e^{\xi t}dt&\\ +\oint_c\left(-2t+\left(\frac{2\epsilon_{n1}}{\alpha}+1\right)t+\left(\frac{\beta_n}{\alpha}\right)^2\right)Q_{n1}(t)e^{\xi t}dt=0&\end{aligned}\tag{2.52}$$

$$\begin{aligned}\Bigg[\left(t^2-\left(\frac{\beta_2}{\alpha}\right)^2\right)Q_{nt}(t)e^{\xi t}\Bigg\}_c-\oint_c O'_n(t)\left(t^2-\left(\frac{\beta_2}{\alpha}\right)^2\right)e^{\xi t}dt&\\ -\oint_c\left(1-\frac{2\epsilon_{n1}}{\alpha}\mid t-\left(\frac{\beta_1}{\alpha}\right)^2\right)Q_{nt}(t)e^{\xi t}dt=0&\end{aligned}\tag{2.53}$$

$$\begin{aligned}\Bigg\{\left(t^2-\left(\frac{\beta_2}{\alpha}\right)^2\right)Q_{nt}(t)e^{\xi t\}_c}&\\ -\oint_c\Bigg\{Q'_{n1}(t)\Bigg(t^2-\left(\frac{\beta_2)^2}{\alpha}\right)^2+\left[\left(1-\frac{2t_{n1}}{\alpha}\right)t-\left(\frac{\beta_n}{\alpha}\right)^2\right]Q_{nt}(t)\Bigg\}e^{\xi t}dt=0&\end{aligned}\tag{2.54}$$

we obtain this :

$$[Q_{nl}(t)(t^2-\frac{\beta_2^2}{\alpha^2})e^{\xi t}]_c-\oint_c[[(\frac{-2\epsilon_{nl}}{\alpha}-1)t-(\frac{\beta_1}{\alpha})^2]Q_{nl}(t)+[t^2-(\frac{\beta_l}{\alpha})^2]Q'_{nl}(t)]e^{\xi t}dt=0 \tag{2.55}$$

where We note in effect that (2.55) is well and truly satisfied if only if the two terms that compose it cancel each other out so The condition involves the behavior of the function under the specific contour integral is important to cancel the terms.
from second term we find :
This eqt is a first order differential eqt. To solve it therefore, we use the integration By application of the Method for solving differential equations with separable variables [6], it comes :

$$Q'_{n1}(t)\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)+\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]Q_{n1}(t)=0 \tag{2.56}$$

$$Q'_{n1}(t)\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)=-\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]Q_{n1}(t) \tag{2.57}$$

$$\frac{dQ_{n1}(t)}{Q_{n1}(t)}=-\frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt \tag{2.58}$$

$$\int\frac{dQ_{n1}(t)}{Q_{n1}(t)}=-\int\frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt \tag{2.59}$$

$$\operatorname{Ln}Q_{n1}(t)+\operatorname{Ln}N=-\int\frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt \tag{2.60}$$

$$\operatorname{Ln}\frac{Q_{n1}(t)}{N}=-\int\frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt \tag{2.61}$$

Let's solve the second member by the Method of integration of a rational fraction it must be decomposed into simple elements like we see here in details :

$$-\int \frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt = -\int \frac{\left[\left(1-\frac{2\epsilon_{nl}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t-\frac{\beta_2}{\alpha}\right)\left(t+\frac{\beta_2}{\alpha}\right)}dt \tag{2.62}$$

$$= \int \frac{B}{\left(t-\frac{\beta_2}{\alpha}\right)}dt + \int \frac{D}{\left(t+\frac{\beta_2}{\alpha}\right)}dt$$

(2.63)

$$= \int \frac{B\left(t+\frac{\beta_2}{4}\right)+D\left(t-\frac{\beta_2}{\alpha}\right)}{\left(t-\frac{\beta_2}{\alpha}\right)\left(t+\frac{\beta_2}{\alpha}\right)}dt \tag{2.64}$$

$$= \int \frac{(B+D)t+\frac{\beta_2}{\alpha}(B-D)}{\left(t-\frac{\beta_2}{\alpha}\right)\left(t+\frac{\beta_2}{\alpha}\right)}dt \tag{2.65}$$

by identification :

$$\begin{cases} B+D = 1-\frac{2\epsilon_{n1}}{\alpha} \Rightarrow B = 1-\frac{2\epsilon_n}{\alpha}-D \\ B-D = -\frac{B_1^2}{\alpha\beta_2} \end{cases}$$

we find :

$$D = \frac{\beta_1^2}{2\alpha\beta_2}-\frac{\epsilon}{\alpha}+\frac{1}{2} \tag{2.66}$$

$$B = \frac{1}{2}-\frac{E}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2} \tag{2.67}$$

The second member is therefore written :

$$-\int \frac{\left[\left(1-\frac{2\epsilon_{n1}}{\alpha}\right)t-\frac{\beta_1^2}{\alpha^2}\right]}{\left(t^2-\frac{\beta_2^2}{\alpha^2}\right)}dt = \left(\frac{1}{2}-\frac{\epsilon}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2}\right)\int \frac{dt}{\left(t-\frac{\beta_2}{\alpha}\right)} + \left(-\frac{1}{2}+\frac{\epsilon}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2}\right)\int \frac{dt}{\left(t+\frac{\beta_2}{\alpha}\right)} \tag{2.68}$$

$$= \left(-\frac{1}{2}+\frac{\epsilon}{\alpha}+\frac{\beta_1^2}{2\alpha\beta_2}\right)\mathrm{Ln}\left(t-\frac{\beta_2}{\alpha}\right) + \left(-\frac{1}{2}+\frac{\epsilon}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2}\right)\mathrm{Ln}\left(t+\frac{\beta_2}{\alpha}\right) \tag{2.69}$$

$$= \mathrm{Ln}\left(t-\frac{\beta_2}{\alpha}\right)^{-\frac{1}{2}+\frac{t}{\alpha}+\frac{\beta_1^2}{2\alpha\beta_2}} + \mathrm{Ln}\left(t+\frac{\beta_2}{\alpha}\right)^{-\frac{1}{2}+\frac{\epsilon}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2}} \tag{2.70}$$

$$= \mathrm{Ln}\left(t-\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}+\frac{\beta_2^2}{2\alpha\beta_2}+\frac{1}{2}-1} + \mathrm{Ln}\left(t+\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}-\frac{\beta_2^2}{2\alpha\beta_2}+\frac{1}{2}-1} \tag{2.71}$$

$$= \mathrm{Ln}\left(t-\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}+\frac{\beta_2^2}{2\alpha\beta_2}+\frac{1}{2}-1} \left(t+\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}-\frac{\beta_2^2}{2\alpha\beta_2}+\frac{1}{2}-1} \tag{2.72}$$

then becomes :

$$L_n\frac{O_{pq}(t)}{N_{pq}} = \mathrm{Ln}\left(t-\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}+\frac{\beta_2^2}{2\alpha\beta_2}+\frac{1}{2}-1} \left(t+\frac{\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}-\frac{\beta_1^2}{2\alpha\beta_2}+\frac{1}{2}-1} \tag{2.73}$$

$$Q_{pq}(t) = N_{pq}\left(t - \frac{\beta_2}{\alpha}\right)^{q-1}\left(t + \frac{\beta_2}{\alpha}\right)^{p-1} \tag{2.74}$$

From the first terme of equation (8) we can write :

$$\begin{cases} t^2 - \frac{\beta_2^2}{\alpha^2} = 0 \\ -t^2 + \frac{\beta_2^2}{\alpha^2} = 0 \Rightarrow \left(\frac{\beta_2}{\alpha^2} - t\right)\left(\frac{\beta_2}{\alpha} + t\right) = 0 \end{cases}$$

So :

$$Q_{pq}(t) = N_{pq}\left(\frac{\beta_2}{\alpha} - t\right)^{q-1}\left(\frac{\beta_2}{\alpha} + t\right)^{p-1} \tag{2.75}$$

where N is normalization constant , and the values of the parameter of p and q :

$$\begin{cases} q = \frac{\epsilon}{\alpha} + \frac{\beta_1^2}{2\alpha\beta_2} + \frac{1}{2} \\ p = \frac{\epsilon}{\alpha} - \frac{\beta_1^2}{2\alpha\beta_2} + \frac{1}{2} \end{cases}$$

$wereplace\mathrm{O}_{pq}(t)$ in (1) and we obtains a new representation :

$$F_{p,q}(\xi) = N\oint_c \left(\frac{\beta_2}{\alpha} - t\right)^{q-1}\left(\frac{\beta_2}{\alpha} + t\right)^{p-1} e^{\xi t}dt \tag{2.76}$$

by performing the change of variable $\frac{\beta_2(2z-1)}{\alpha}$ in the equation we obtain and we will demonstrat that this equation admits two branche point :

$$Q = N\left(\frac{\beta_2}{\alpha} - \frac{\beta_2(2z-1)}{\alpha}\right)^{q-1}\left(\frac{\beta_2}{\alpha} + \frac{\beta_2(2z-1)}{\alpha}\right)^{p-1} \tag{2.77}$$

$$= N\left(\frac{\beta_2 - \beta_2(2z-1)}{\alpha}\right)^{q-1}\left(\frac{\beta_2 + \beta_2(2z-1)}{\alpha}\right)^{p-1} \tag{2.78}$$

$$= N\left(\frac{\beta_2(1 - 2z + 1)}{\alpha}\right)^{q-1}\left(\frac{\beta_2(1 + 2z - 1)}{\alpha}\right)^{p-1} \tag{2.79}$$

$$= N\left(\frac{\beta_2(2 - 2z)}{\alpha}\right)^{q-1}\left(\frac{\beta_2(2z)}{\alpha}\right)^{p-1} \tag{2.80}$$

$$= N \left( \frac{2\beta_2(1-z)}{\alpha} \right)^{q-1} \left( \frac{2\beta_2 z}{\alpha} \right)^{p-1} \tag{2.81}$$

$$= N \left( \frac{2\beta_2}{\alpha} \right)^{q-1} (1-z)^{q-1} \left( \frac{2\beta_2}{\alpha} \right)^{p-1} z^p \tag{2.82}$$

$$= N \left( \frac{2\beta_2}{\alpha} \right)^{q-1} \left( \frac{2\beta_2}{\alpha} \right)^{p-1} \frac{1}{(1-z)} (1-z)^q z^p \tag{2.83}$$

from this we have two branch point :

$$\begin{cases} 1 - z = 0 \Rightarrow z_1 = 1 \\ z_0 = 0 \end{cases}$$

For the parametres p and q not an integer, therefore we found that the have two branch point $z_0 = 0$ and $z_n = 1$, and the product $f(z) = z^p\,(1-z)^q$ in the terme $\left\{ \left(\frac{\beta_2}{\alpha} - t\right)^{p-1} \left(\frac{\beta_2}{\alpha} + t\right)^{q-1} e^{\xi t} \right]_c$ will Cancel at this two point (with $p - 1 > 0$ and $q - 1 > 0$) and This condition allows us to choose a contour that encloses both branch points without encountering any discontinuity and will lead that the integrand is single-valued in this contour otherwise f(z) it would imply that the integrand in equation multivalued function when the point in the z-plane coincide with given phase $\theta$

To ensure the integrand is single-valued and to simplify the integration process [1], it is desirable for the product $z^p(1-z)^q$ to vanish at the branch points z0 and z1. This condition allows us to choose a contour that encloses both branch points without encountering any discontinuity

By taking the line segment joining z0 = 0 and z1 = 1 as a cut line, this will ensures that the integrand remains well-defined and single-valued for the chosen contour

So the segment represent cut line

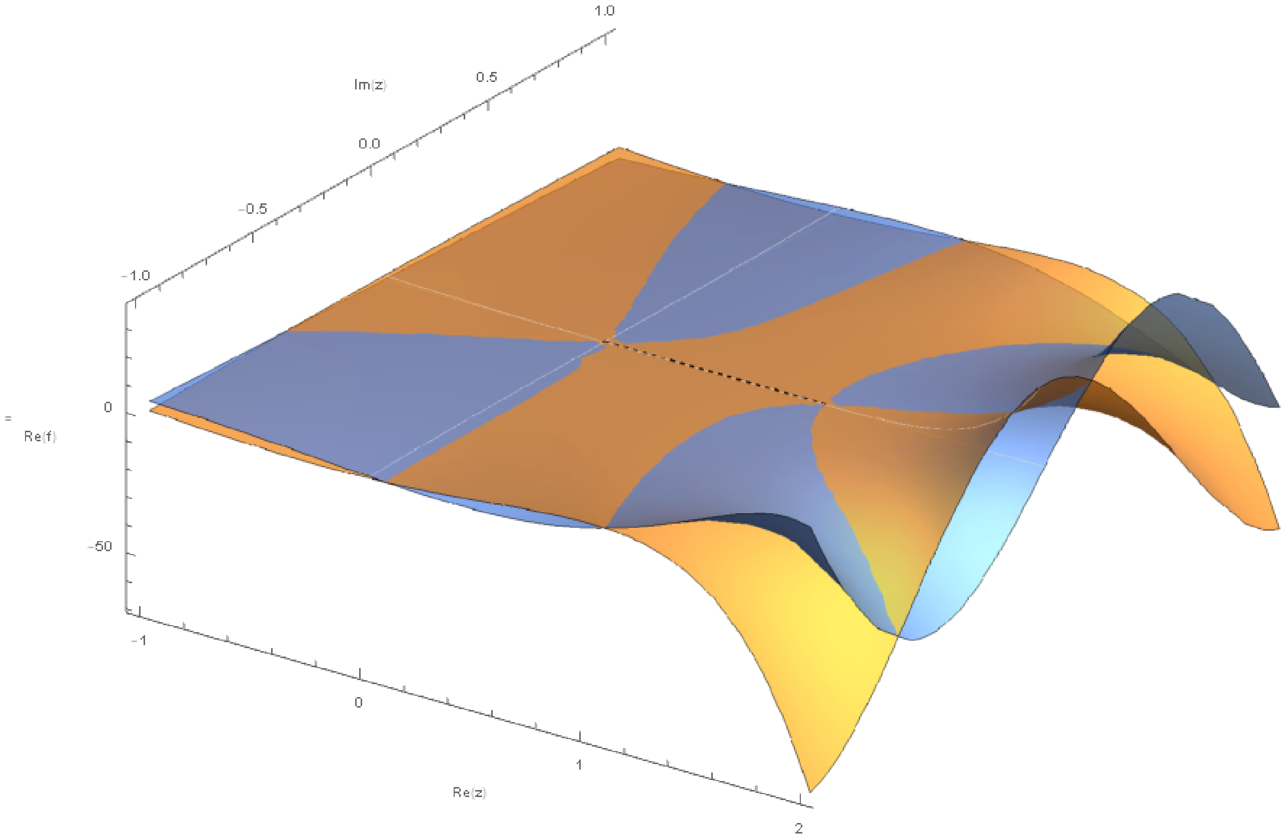

**Figure 2.1:** plot represent the riemann surfaces of the function with the cut line with the black dashed line

The two surfaces represent different branches of the function due to its multivalued nature. As we move along the branch cut,we transition from one sheet to the other. The dashed black line represents the branch cut, and crossing it indicates moving from one sheet to another.

we impose this $t = \beta_2(2z-1)/\alpha$ then the function $F_{p,q}(\xi)$ can be

$$F_{p,q}(\xi) = N \oint_c \left(\frac{2\beta_2(1-z)}{\alpha}\right)^{q-1} \left(\frac{2\beta_2 z}{\alpha}\right)^{p-1} e^{\frac{\xi\beta_2(2z-1)}{\alpha}} \frac{2\beta_2}{\alpha} dz \tag{2.84}$$

$$F_{p,q}(\xi) = N e^{-\frac{\xi\beta_2}{\alpha}} \left(\frac{2\beta_2}{\alpha}\right)^{q-1} \left(\frac{2\beta_2}{\alpha}\right)^{p-1} \frac{2\beta_z}{\alpha} \oint_c (1-z)^{q-1} z^{p-1} e^{\lambda\xi z} dz \tag{2.85}$$

$$F_{p,q}(\xi) = N e^{-\frac{\xi\beta_2}{\alpha}} \left(\frac{z\beta_2}{\alpha}\right)^{q} \left(\frac{2\beta_2}{\alpha}\right)^{p} \frac{\alpha}{2\beta_2} \oint_c (1-z)^{q-1} z^{p-1} e^{\lambda\xi z} dz \tag{2.86}$$

after the imposing of t and $\mathcal{F}_{p,q}(\xi) = \mathrm{e}^{-\frac{\beta_2}{\alpha}\xi} f_{p,q}(\xi)$ then it will become

$$f_{p,q}(\xi) = N \left(\frac{2\beta_2}{\alpha}\right)^{q} \left(\frac{2\beta_2}{\alpha}\right)^{p} \frac{\alpha}{\alpha\beta_2} \oint_c (1-z)^{q-1} z^{p-1} e^{\lambda\xi z} dz \tag{2.87}$$

and yes, the resulting forme shape like a forme we already known about and it is the integral representation of the confluent hyper geometric function, if we set choice of contour $[0,1]$ the integral representation :

the integral representation of the confluent hyper geometric function [9]

$$ {}_1F_1(\alpha,\gamma,x) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1} e^{xt} dt \tag{2.88} $$

$$ \frac{\Gamma(\alpha)\Gamma(\gamma-\alpha)}{\Gamma(\gamma)} {}_1F_1(\alpha,\gamma,x) = \int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1} e^{xt} dt \tag{2.89} $$

our integrale form by integral representation will be :

$$ \int_0^1 z^{p-1}(1-z)^{q-1} e^{\lambda\xi z} dz = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)} {}_1F_1(p,q,\xi) \tag{2.90} $$

therfore :

$$ F_{p,q}(\xi) = N e^{-\xi \frac{\beta_2}{\alpha}} \left(\frac{2\beta_2}{\alpha}\right)^q \left(\frac{2\beta_2}{\alpha}\right)^p \frac{\alpha}{2\beta_2} \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)} {}_1F_1(p,q,\xi) \tag{2.91} $$

with :

$$ B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)} \tag{2.92} $$

7. The value of $\lambda$ :

$$ \lambda = \frac{2\beta_2}{\alpha} \tag{2.93} $$

## 2.3 Part 3 : Integral Transformation of the Inverse Contour Representation

In this third part of the article, we introduce a mathematical technique called the functional integral transformation, which is attributed to Mackie [11]. This approach involves using contour integration to handle differential equations effectively. By employing this method, we aim to obtain the states (wave functions and energy spectrum) corresponding to the radial Morse potential. Contour integration is a powerful tool for evaluating certain types of integrals and allows for the manipulation of complex functions, making it valuable in solving differential equations associated with the rotating Morse potential problem. Through this approach, we seek to gain insights into the behavior of the potential function and better understand the wave functions and energy levels associated with it.
To illustrate the technique, let's consider two complex variable functions, for example, f(z) and g(z), defined as analytic within a closed contour C. Then, the inverse contour representation refers to a pair of functions that satisfy specific transformations :

$$\begin{cases} g(z) = \int_0^1 (1-x)^{n-1} f'(xz)dx \\ \\ f(\xi) = \frac{1}{2\pi i} \oint_e \left(\frac{z}{z-\xi}\right)^n g(z)dz \end{cases} \tag{2.94}$$

In the context of the problem, where n is a positive integer, and $z^n/(z-\xi)^n$ is an analytic function with a branch cut along an axis connecting the point 0 to z, the transformations (2.93) are referred to as the forward and inverse transforms, respectively.

Later on, we will see that precisely the transformations (2.93) will describe the quantum characteristics (wave functions and energy spectrum) of the radial Morse potential. To achieve this, we assume that $f(\xi)$ and $g(\xi)$ have a power series expansion of the form :

$$\begin{cases} g(\xi) = \sum_{k=0}^{+\infty} C_k \xi^k \\ \\ f(\xi) = \sum_{k=0}^{\infty} b_k \xi^k \end{cases} \tag{2.95}$$

where $b_k$ and $c_k$ are coefficients of the two series, and our objective is to establish the relationship connecting them.

we have those two :

$$\begin{cases} g(z) = \int_0^1 (1-x)^{n-1} f'(xz)dx \\ \\ f(\xi) = \sum_{k=0}^{\infty} b_k \xi^k \end{cases} \tag{2.96}$$

So, now we will proceed with the application first thing we insert (11.2) and (12.1) into (11.1) and by interchanging the order of integration of course with respect of the variables x and z and then we performe some manipulation inside this lead us to introduce new formula called the Euler beta function then with identification with the first sommation (12.1) as we can see here in details :

$$f(\xi) = \frac{1}{2\pi i} \oint_e \left( \frac{z}{z-\xi} \right)^n g(z)dz \tag{2.97}$$

$$= \frac{1}{2\pi i} \oint_c \left( \frac{z}{z-\xi} \right)^n \int_0^1 (1-x)^{n-1} \sum_{k=0}^{+\infty} b_k k (zx)^{k-1} dxdz \tag{2.98}$$

$$= \sum_{k=0}^{+\infty} b_k \frac{k}{2\pi i} \int_0^1 (1-x)^{n-1} x^{k-1} dx \oint_c \frac{z^{n+k-1}}{(z-\xi)^n} dz \tag{2.99}$$

$$= \sum_{k=0}^{+\infty} b_k \frac{k}{2\pi i} B(n,k) \oint_c \frac{z^{n+k-1}}{(z-\xi)^n} dz \tag{2.100}$$

then we obtain :

$$\xi^k = \frac{k}{2\pi i} B(n,k) \oint_c \frac{z^{n+k-1}}{(z-\xi)^n} dz \tag{2.101}$$

where B(n, k) = (n)(k)/(n + k) is Euler's beta function, On the other hand, by inserting (12.2) into (11.1) and do some manipulation as we can see here we have those :

$$\begin{cases} g(\xi) = \sum_{k=0}^{+\infty} C_k \xi^k \\ f(\xi) = \frac{1}{2\pi i} \oint_c \frac{z^n}{(z-\xi)^n} g(z)dz \end{cases} \tag{2.102}$$

$$f(\xi)=\frac{1}{2\pi i}\oint_c \frac{z^n}{(z-\xi)^n}\sum_{k=0}^{+\infty} c_k\xi^k dz \tag{2.103}$$

we obtain :

$$f(\xi)=\sum_{k=0}^{+\infty}\frac{c_k}{2\pi i}\oint_c \frac{z^{n+k}}{(z-\xi)^n}dz \tag{2.104}$$

Now, to calculate this integral we have to apply the residues theorem but before that we apply change of variable to last formula that we get , $z = 1/u$ by applying it and do some manipulation we transform this inegrale to as we can see here the steps :

$$f(\xi)=\sum_{k=0}^{+\infty} c_k\left(-\frac{1}{2\pi i}\oint_c \frac{\left(\frac{1}{u}\right)^{n+k}}{\left(\left(\frac{1}{u}\right)-\xi\right)^n}\left(\frac{1}{u^2}\right)du\right) \tag{2.105}$$

$$=\sum_{k=0}^{+\infty} c_k\left(-\frac{1}{2\pi i}\oint_c \frac{\left(\frac{1}{u}\right)^{n}\left(\frac{1}{u}\right)^{k}}{\left(\frac{1}{u}\right)^n(1-\xi u)^n}\frac{1}{u^2}du\right) \tag{2.106}$$

$$=\sum_{k=0}^{+\infty} c_k\left(-\frac{1}{2\pi i}\oint_c \frac{(1-\xi u)^{-n}}{u^{k+2}}du\right) \tag{2.107}$$

which have a pole at u = 0 of order k+2

Know will integrate this new formula by applying residues theorem, first we introduce this theorem formula , so if we have $u_0$ pole of an order of $m$ then we introduce this formula :

$$\operatorname{Res}[u_0]=\frac{1}{(m-1)!}\lim_{u\to u_0}\frac{d^{m-1}}{du^{m-1}}\left[(u-u_0)^m f(u)\right] \tag{2.108}$$

So, by apply this theorem directly we calculate the residue with performing the $(k+1)^th$ derivative and then apply the limite as we can see here :

$$\text{Res}\left[\frac{(1-\xi u)^{-n}}{u^{k+2}},0\right]=\frac{1}{(k+1)!}\lim_{u\to 0}\frac{d^{k+1}}{du^{k+1}}\left[(u-0)^{k+2}\frac{(1-\xi u)^{-n}}{u^{k+2}}\right] \tag{2.109}$$

$$=\frac{1}{(k+1)!}\lim_{u\to 0}\frac{d^{k+1}}{du^{k+1}}\left[(1-\xi u)^{-k}\right] \tag{2.110}$$

$$=\frac{1}{(k+1)!}\lim_{u\to 0}\xi^{k+1}n(n+1)\dots(n+k)(1-\xi u)^{-(n+k+1)} \tag{2.111}$$

$$=\frac{1}{\Gamma(k+2)}\xi^{k+1}(n)_{k+1} \tag{2.112}$$

and then we obtain :

$$f(\xi)=\sum_{k=0}^{+\infty}C_k\frac{(n)_{k+1}}{\Gamma(k+2)}\xi^{k+1} \tag{2.113}$$

where $(n)_k+1=\frac{\Gamma(n+k+1)}{\Gamma(n)}$ is the Pochhammer symbol defined by $(a)_k=a(a+)(a+2)....(a+k+1)$

We can see that (11.1) by deduction can be rewright as the cauchy residues theorem we apply it directly to this integrale with applying the limit of this theorem as we can see here :

$$f(\xi)=\frac{1}{2\pi i}\oint_c\left(\frac{z}{z-\varepsilon}\right)^n g(z)dz \tag{2.114}$$

$$=\frac{1}{(n-1)!}\lim_{z\to\xi\infty}\frac{d^{n-1}}{dz^{n-1}}\left[(z-\xi)^n\frac{z^n}{(z-\xi)^n}g(z)\right] \tag{2.115}$$

$$=\frac{1}{(n-1)!}\frac{d^{n-1}}{d\xi^{n-1}}\xi^n g(\xi) \tag{2.116}$$

$$=\frac{1}{\Gamma(n)}\frac{d^{n-1}}{d^{n-1}}\xi^n g(\xi) \tag{2.117}$$

and then we do further calculation leads to (12.1) so firstly we can see with some identification with formula (14) , and inserting (12.2) into what we deducted in (15) so as we see that :

$$f(\xi) = \sum_{k=0}^{+\infty} c_k \frac{1}{\Gamma(n)} \frac{d^{n-1}}{d\xi^{n-1}} \xi^n \xi^k = \sum_{k=0}^{+\infty} c_k \frac{(n)_{k+1}}{\Gamma(k+2)} \xi^{k+1} \tag{2.118}$$

$$= \sum_{k=0}^{+\infty} c_k \frac{\Gamma(n+k+1)}{\Gamma(n)\Gamma(k+2)} \xi^{k+1} \tag{2.119}$$

we find the expression that connect the coefficient $b_{k+1}$ and $c_k$ :

$$b_{k+1} = \frac{\Gamma(n+k+1)}{\Gamma(n)\Gamma(k+2)} C_k \tag{2.120}$$

as we can do the same thing, will lead to refind the sommation (12.2) by inserting (12.1) into (11.2) but not directly we have those here :

$$\left\{ \; g(z) = \textstyle\int_0^1 (1-x)^{n-1} f'(xz) dx (2.121) \;\; f(\xi) = \sum b_k \xi^k \right. \tag{2.121}$$

we have to change the variable and applying the first derivative to (12.1) as we can see here :

$$\left\{ \; f(xz) = \textstyle\sum b_k (xz)^k (2.122) \;\; f'(xz) = \sum b_k k (xz)^{k-1} \right. \tag{2.122}$$

we insert it and interchanging the order between the sommation and the integral and defined this integral as beta euler function , then change the order from k to k+1 and of course taking into account the reccurence relation (16) as we can see here :

$$g(z) = \int_0^n (1-x)^{n-1} \sum b_k k (xz)^{k-1} dx \tag{2.123}$$

$$= \sum b_k k z^{k-1} \int_0^1 (1-x)^{n-1} x^{k-1} dx \tag{2.124}$$

$$= \sum b_k k z^{k-1} B(n,k) \tag{2.125}$$

$$= \sum b_k k z^{k-1} \frac{\Gamma(n)\Gamma(k)}{\Gamma(n+k)} \tag{2.126}$$

$$= \sum b_k k \xi^{k-1} \frac{\Gamma(n)\Gamma(k)}{\Gamma(n+k)} \tag{2.127}$$

$$= \sum b_{k+1}(k+1)\xi^k \frac{\Gamma(n)\Gamma(k+1)}{\Gamma(n+k+1)} \tag{2.128}$$

$$= \sum (k+1)\xi^k c_k \frac{\Gamma(n+k+1)}{\Gamma(n)\Gamma(k+2)} \frac{\Gamma(n)\Gamma(k+1)}{\Gamma(n+k+1)} \tag{2.129}$$

$$= \sum c_k (k+1) \frac{\Gamma(k+1)}{\Gamma(k+2)} \xi^k \tag{2.130}$$

we obtain :

$$= \sum c_k \xi^k (k+1) \frac{\Gamma(k+1)}{\Gamma(k+2)} \tag{2.131}$$

### 2.3.1 Part 4 : Deduction of the wave function and energy spectrum

In this section, we aim to establish the wave functions and energy spectrum for the radial Morse potential, considering the mathematical results derived in the previous part. By doing so, we observe that the wave function f(e) obtained in equation (10) can be associated with equation (11.1). From this correspondence, the role played by the coefficient b(k+1) in determining the normalization constant becomes apparent.

To achieve this, we utilize the inverse contour representation method, which involves contour integration techniques and mathematical manipulations. We start by analyzing the results obtained in the previous section, particularly equation (10) and equation (11.1). By establishing a connection between these expressions, we can deduce the significance of the coefficient b(k+1) in determining the normalization constant for the wave function. This understanding helps us derive the wave functions and energy spectrum associated with the radial Morse potential. The integration and manipulation techniques used are based on well-known mathematical tools and principles, ensuring accurate results

Now, for the calculation firstly we began with equation (10) by expanding the exponential terme in taylor series and by inserting of course $\lambda$ value , also interchanging the order between the sommation and integral then introducing the beta function, inside we expresse wave function in new forme , like we see here in the folowing steps :

$$f(\xi) = N\left(\frac{2\beta_2}{\alpha}\right)^q \left(\frac{2\beta_2}{\alpha}\right)^p \frac{\alpha}{2\beta_2} \oint_c (1-z)^{q-1} z^{p-1} e^{\lambda\xi z} dz \tag{2.132}$$

$$= N\lambda^{q+p-1} \oint_c (1-z)^{q-1} z^{p-1} \sum \frac{(\lambda\xi z)^n}{n!} dz \tag{2.133}$$

$$= N\sum \frac{(\lambda\xi)^n}{n!} \lambda^{q+p-1} \oint_c (1-2)^{q-1} z^{p+n-1} dz \tag{2.134}$$

$$= N\sum \frac{(\lambda\xi)^n}{n!} \lambda^{q+p-1} B(p+n,q) \tag{2.135}$$

$$= N\sum \frac{(\lambda\xi)^{k+1}}{\Gamma(k+2)}\lambda^{q+p-1}B(p+k+1,q) \tag{2.136}$$

From this new expression we can deduce the coefficient $b_{k+1}$ like we see here :

$$f(\xi) = N\lambda^{q+p+k}\sum \frac{\xi^{k+1}}{\Gamma(k+2)}B(p+k+1,q) = N\lambda^{q+p+k}\sum \frac{\xi^{k+1}}{\Gamma(k+2)}\frac{\Gamma(p+k+1)\Gamma(q)}{\Gamma(p+k+q+1)} \tag{2.137}$$

then the coefficient becomes :

$$b_{k+1} = N\lambda^{q+p+k}\frac{\Gamma(p+k+1)\Gamma(q)}{\Gamma(k+2)\Gamma(p+q+k+1)} \tag{2.138}$$

We can also by taking into account the previous result , we can expresse the wave function $f(\xi)$ by doing further calculation and inserting the pochhammer symbol we get new forme as we can see here :

$$f(\xi) = N\lambda^{p+q-1}\oint_c z^{p-1}(1-z)^{q-1}\sum \frac{(\lambda\xi z)^n}{n!}dz \tag{2.139}$$

$$= N\lambda^{p+q-1}\sum \frac{(\lambda\xi)^k}{k!}\oint_c z^{p+k-1}(1-z)^{q-1}dz \tag{2.140}$$

$$= N\lambda^{p+q-1}\sum \frac{(\lambda\xi)^k}{k!}\frac{\Gamma(p+k)\Gamma(q)}{\Gamma(p+q+k)} \tag{2.141}$$

$$= N\lambda^{p+q-1}\sum \frac{(\lambda\xi)^k}{k!}\frac{(p)_k\Gamma(p)\Gamma(q)}{(p+q)_k\Gamma(p+q)} \tag{2.142}$$

$$= N\lambda^{p+q-1}\sum \frac{(p)_k}{(p+q)_k}\frac{(\lambda\xi)^k}{k!}B(p,q) \tag{2.143}$$

$$= N\lambda^{p+q-1} B(p,q)_1 F_1(p, p+q, \lambda\xi) \tag{2.144}$$

where ${}_1F_1$ here is The Gaussian hypergeometric function is given by :

$${}_1F_1(p, p+q, \lambda\xi) = \sum \frac{(p)_k}{(p+q)_k} \frac{(\lambda\xi)^k}{k!} \tag{2.145}$$

and from the relations we deducted in part two :

$$\begin{cases} q = \frac{\epsilon}{\alpha} + \frac{\beta_1^2}{2\alpha\beta_2} + \frac{1}{2} \\ p = \frac{\epsilon}{\alpha} - \frac{\beta_1^2}{2\alpha\beta_2} + \frac{1}{2} \end{cases} \tag{2.146}$$

we note that $k = \frac{\epsilon}{\alpha}$ then we can express them like this :

$$\begin{cases} p + q = \frac{2\epsilon}{\alpha} + 1 = 2k + 1 \\ p + q - 1 = \frac{2\epsilon}{\alpha} = 2k \end{cases} \tag{2.147}$$

In the context of special functions in mathematical physics, it is widely recognized that when we substitute p = -n in equation (19), a condition known as the quantization condition, the hypergeometric function F transforms into a degenerate form. As a consequence, it no longer behaves as a standard function but becomes a finite expression represented by an associated Laguerre polynomial. Before the quantization condition, the hypergeometric function F behaves like a standard function, meaning it can be represented by a well-defined formula involving a series of terms with infinite possibilities, depending on the values of the parameters.

After imposing the quantization condition, the hypergeometric function F transforms into a degenerate form, and it no longer behaves like a standard function. Instead, it takes on a finite expression represented by an associated Laguerre polynomial. In this case, the function becomes limited to a specific set of terms, making it finite and well-behaved. This condition is used to restrict the values of "p" and results in the confluent hypergeometric function becoming a polynomial, specifically an associated Laguerre polynomial.

By applying this quantization condition, we ensures that the expression for the confluent hypergeometric function simplifies to a finite polynomial form. This is advantageous for the study of the rotating Morse potential and allows for the determination of energy eigenvalues and wave functions associated with the problem.such that :

$$ {}_1F_1(-n;2k+1;\lambda\xi)=\frac{\Gamma(n+1)\Gamma(2k+1)}{\Gamma(n+2k+1)}L_n^{(2k)}(\lambda\xi) \tag{2.148}$$

and now taking into account the previous result of part 1 and 2 we have this two :

$$\begin{cases} F(\xi)=e^{-\frac{\beta_2}{\alpha}\xi}f(\xi) \\ R_{nl}(\xi)=\xi^k F(\xi) \end{cases} \tag{2.149}$$

and of course the last form of $f(\xi)$ we find :

$$f(\xi)=N\lambda^{p+q-1}B(p,q),F_1(p,p+q,\lambda\xi) \tag{2.150}$$

then by substitues this last expressions we get :

$$R_{nl}(\xi)=\xi^k e^{-\frac{\beta_2}{q}\xi}N\lambda^{p+q-1}B(p,q)_nF_1(p,p+q,d\xi) \tag{2.151}$$

then we insert the condition $p=-n$ and substitue the transformed forme associated Laguerre polynomial into the radial fonction we get :

$$R_{nl}(\xi)=C\xi^k e^{-\frac{\lambda}{2}\xi}L_n^{(2k)}(\lambda\xi) \tag{2.152}$$

where :

$$C=N_{pq}B(p,q)\frac{\Gamma(n+1)\Gamma(kk+1)}{\Gamma(n+2k+1)}\lambda^{p+q-1}$$

is the new constant of normalization we find in terms of $N_{pq}$(2.153)

In order to determine the analytical expression of the energy spectrum $E_{nl}$, we will use the quantization condition p = -n, where p has already been deduced in Part 2 and n is energy level . We will demonstrate that by substituting the values of $\epsilon_{nl}^2$, $\beta_1^2$, $\beta_2^2$ and $\gamma$ into this equation :

$$p=n=\frac{E}{\alpha}+\frac{1}{2}-\frac{\beta_1^2}{2\alpha\beta_2} \tag{2.154}$$

after the substitue and some manipulation we find the expression of the energy spectrum as we here in details :

$$n = -\frac{E}{\alpha} - \frac{1}{2} + \frac{\beta_1^2}{2\alpha\beta_2} \tag{2.155}$$

$$n = -\Lambda_0 \sqrt{(\gamma_{a_0} - E)}\frac{1}{\alpha} - \frac{1}{2} + \frac{\beta_1^2}{2\alpha\beta_2} \tag{2.156}$$

$$\Lambda_0 \sqrt{(\gamma a_0 - E)}\frac{1}{\alpha} = -n - \frac{1}{2} + \frac{\beta_1^2}{2\alpha\beta_2} \tag{2.157}$$

$$\sqrt{(\gamma_{a_0} - E)} = -n\frac{\alpha}{\Lambda_0} - \frac{1}{2}\frac{\alpha}{\Lambda_0} + \frac{\beta_1^2}{2\alpha\beta_2}\frac{\alpha}{\Lambda_0} \tag{2.158}$$

$$= -\frac{\alpha}{\Lambda_0}\left(n + \frac{1}{2}\right) + \frac{\beta_1^2}{2\alpha\beta_2}\frac{\alpha}{\Lambda_0} \tag{2.159}$$

$$= \frac{1}{2}\frac{\alpha}{\Lambda_0}\frac{1}{\alpha}\left[-(2n+1)\alpha + \frac{\beta_1^2}{\beta_2}\right] \tag{2.160}$$

$$\gamma a_0 - E = \frac{\hbar^2}{8r_e^2\mu}\left[-(2n+1)\alpha + \frac{\beta_1^2}{\beta_2}\right] \tag{2.161}$$

$$E = -\frac{\hbar^2}{8r_e^2\mu}\left[-(2n+1)\alpha + \frac{\beta_1^2}{\beta_2}\right] + \gamma a_0 \tag{2.162}$$

and this is the expression energy eigenvalues :

$$E_{nl} = \frac{\hbar^2 l(l+1)}{2\mu r_e^2} - \frac{\hbar^2}{8\mu r_e^2}\left[\frac{\Lambda_0\left(2V_0 - \gamma a_1\right)}{\sqrt{(V_0 + \gamma a_2)}} - (2n+1)\alpha\right] \tag{2.163}$$

Let's now focus on the radial wave function (21). More specifically, we aim to determine the normalization constant C, or N. To evaluate C, we will need some mathematical identities.for exempl :

$$L_n^{(2k)}(\varphi)=\sum_{k=0}^{n}(-1)^k\frac{\Gamma(2k+n+1)}{\Gamma(n-k+1)\Gamma(2k-k+1)}\frac{\varphi^k}{k!} \tag{2.164}$$

$$\int_0^{+\infty}\varphi^{\tau-1}e^{-\varphi}L_n^{(\nu)}(\varphi)d\varphi=\frac{\Gamma(\tau)\Gamma(n+\nu+1-\tau)}{\Gamma(n+1)\Gamma(\nu+1-\tau)},\qquad [R(\tau)>0] \tag{2.165}$$

Subsequently, we make the change of variable $\varphi=\lambda\xi$.

Now ; we will find the constant of normalization $C_pq$ , firstly will introduce the rule of normalization to find certin integral of the type like follow in this :

the rule of normalization :

$$\int_{\mathbb{R}}R_{nl}^*(x)R_{nl}(x)dx=1 \tag{2.166}$$

now we will make change of variable $\xi=e^{-\alpha x}$ :

$$\begin{cases}\xi=e^{-\alpha x}\\ \\ dx=-\frac{1}{\alpha\xi}\end{cases}\Rightarrow\begin{cases}x=-\infty\rightarrow\xi=+\infty\\ \\ x=+\infty\rightarrow\xi=0\end{cases}$$

we find that :

$$-\int_{+\infty}^{0}\left|R_{nl}(\xi)^2\right|\frac{d\xi}{\alpha\xi}=1 \tag{2.167}$$

$$\int_0^{+\infty}\left|R_{nl}(\xi)^2\right|\frac{d\xi}{\alpha\xi}=1 \tag{2.168}$$

we apply directly the rule then we find :

$$\int_0^{+\infty}C_{pq}^2\xi^{2k}e^{-\lambda\xi}\left[L_n^{(2k)}(\lambda\xi)\right]^2\frac{d\xi}{\alpha\xi}=1 \tag{2.169}$$

then we do change of varialbe we impose first $\varphi = \lambda\xi$ :

$$\begin{cases} \varphi = \lambda\xi \\ \frac{d\varphi}{\lambda} = d\xi \end{cases} \tag{2.170}$$

we insert this last into our integral we get as we see here in steps :

$$C_{pq}^2 \int_0^{+\infty} \left(\frac{\varphi}{\lambda}\right)^{2k} e^{-\varphi} \left[L_n^{(2k)}(\varphi)\right]^2 d\varphi = \alpha\xi\lambda \tag{2.171}$$

$$C_{pq}^2 \int_0^{+\infty} \varphi^{2k-1} e^{-\varphi} \left[L_n^{(2k)}(\varphi)\right]^2 d\varphi = \alpha\lambda^{2k} \tag{2.172}$$

Now, we will calculate this integral by inserting only a single Laguerre polynomial from equation (23) into equation (25) and integrating with respect to $\varphi$ using equation (24), the integral in equation (25) is given by as we can see here in details :

$$\int_0^{+\infty} \varphi^{2k-1} e^{-\varphi} L_n^{(2k)}(\varphi) L_n^{(2k)}(\varphi) d\varphi = \sum (-1)^k \frac{\Gamma(2k+n+1)}{\Gamma(k+1)\Gamma(n-k+1)((2k-k+1)} \int_0^{+\infty} \varphi^{2k+k-1-e} e^{-\varphi} L_n^{(2k)}( \tag{2.173}$$

$$= \frac{\Gamma(2k+n+1)}{\Gamma(n+1)} \sum_{k=0}^{n} (-1)^n \frac{\Gamma(2k+k)\Gamma(n+1-k)}{\Gamma(k+1)\Gamma(n-k+1)\Gamma(2k-k+1)\Gamma(1-k)} \tag{2.174}$$

$$= \frac{\Gamma(2k+n+1)}{\Gamma(n+1)} \sum (-1)^n \frac{\Gamma(2k+k)}{\Gamma(k+1)\Gamma(2k-k+1)\Gamma(1-k)} \tag{2.175}$$

then we can find the constant of normalization $C_{pq}$ by inserting this new form of the integral we find into equation (25) and then we take the first terme of the sommation for k=0 then C will be given as shown here by :

$$\alpha\lambda^{2k} = C_{pq}^2 \int_0^{+\infty} \varphi^{2k-1} e^{-\varphi} \left[L_n^{(kk)}(\varphi)\right]^2 d\varphi \tag{2.176}$$

$$= C^2 \frac{\Gamma(2k+n+1)}{\Gamma(n+1)} \sum (-1)^n \frac{\Gamma(2k+k)}{\Gamma(k+1)\Gamma(2k-k+1)\Gamma(1-k)} \tag{2.177}$$

$$= C^2 \frac{\Gamma(2k+n+1)}{\Gamma(n+1)} \sum_{k=0}^{+\infty} (-1)^n \frac{\Gamma\left(2k+\frac{\epsilon}{\alpha}\right)}{\Gamma\left(\frac{\epsilon}{\alpha}+1\right)\Gamma(2k-k+1)\Gamma(1-k)} \tag{2.178}$$

for k=0 :

$$\alpha\lambda^{2k} = C^2 \frac{\Gamma(2k+n+1)}{\Gamma(n+1)} \frac{\alpha}{\epsilon} \tag{2.179}$$

$$C = \left(\frac{2\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}} \sqrt{\frac{\epsilon\Gamma(n+1)}{\Gamma\left(2\frac{\epsilon}{\alpha}+n+1\right)}} \tag{2.180}$$

we can also express the radial wave function $R_{nl}(\xi)$ as :

$$R_{nl}(\xi) = \left(\frac{2\beta_2}{\alpha}\right)^{\frac{\epsilon}{\alpha}} \sqrt{\frac{\epsilon\Gamma(n+1)}{\Gamma\left(n+\frac{2\epsilon}{\alpha}+1\right)}} \xi^k e^{-\frac{\lambda}{2}\xi} L_n^{(2k)}(\lambda\xi) \tag{2.181}$$

### 2.3.2 Part 5 : NUMERICAL APPLICATION

In this fifth and final part, we focus entirely on applying all our results, which, of course, depend on the Pekeris approximation used, to four (4) diatomic molecules : H2, HCl, CO, and LiH. We will compare our numerical results with those obtained using other methods such as

EQR, SUSY, variational, MSE, NU, AIM, and so on [9], [4] . after calculation using mathematica the energy spectrum according to diffrent quantum numbers n and l at diffrent molecule we find that the result we obtaind appriximatly matched the result obtained when the deffrent methodes has been used

#### 2.3.2.1 We will then numerically calculate, using Mathematica, the energy spectrum (22) according to the different quantum numbers nn and ll for the various molecules mentioned above. We will also graphically illustrate the radial Morse potential with the Pekeris approximation as the centrifugal term..

This section presents the numerical results of the energy spectra for four diatomic molecules : H2_22, HCl, CO, and LiH. Using the Pekeris approximation, the bound-state energy eigenvalues are calculated for various vibrational (nnn) and rotational (lll) quantum numbers. These results are compared with those obtained from other established methods, such as EQR, SUSY, and variational approaches, to validate the accuracy of the approximation. The tables provide a detailed comparison, highlighting the consistency of the Pekeris approximation with experimental and theoretical benchmarks.

**Tableau 2.1:** Bound-state energy eigenvalues ($-E$) for the $H_2$ molecule (in eV ) for different values of the rotational $\ell$ and vibrational $n$ quantum numbers

| $n$ | $\ell$ | Our work | TJMR | SUSY | AIM | Variational |
|---|---|---|---|---|---|---|
| 0 | 0 | 4.47601 | 4.4760131 | 4.476 01 | 4.476 01 | 4.4758 |
| | 5 | 4.29987 | 4.2590180 | 4.258 80 | 4.258 80 | 4.2563 |
| | 10 | 3.87255 | 3.7247471 | 3.721 93 | 3.721 93 | 3.7187 |

**Tableau 2.2:** Bound-state energy eigenvalues ($-E$) for the Hcl molecule (in eV ) for different values of the rotational $\ell$ and vibrational $n$ quantum numbers

| $n$ | $\ell$ | Our work | TJMR | EQR | SUSY | AIM | Variational |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 4.36398 | 4.435 5522 | 4.435 56 | 4.435 56 | 4.4356 | 4.4360 |
| | 5 | 4.29948 | 4.396 8066 | 4.396 81 | 4.396 81 | 4.3968 | 4.3971 |
| | 10 | 4.12965 | 4.294 0628 | 4.284 07 | 4.284 08 | 4.2841 | 4.2840 |

**Tableau 2.3:** Bound-state energy eigenvalues $(-E)$ for the CO molecule (in eV ) for different values of the rotational $\ell$ and vibrational $n$ quantum numbers

| $n$ | $\ell$ | Our work | TJMR | EQR | SUSY | NU | Variational |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 10.7345 | 11.091 5353 | 11.0915 | 11.0915 | 11.091 | 11.093 |
|  | 5 | 10.6525 | 11.084 3875 | 11.0844 | 11.0844 | 11.084 | 11.084 |
|  | 10 | 10.4353 | 11.065 3334 | 11.0653 | 11.0653 | 11.065 | 11.0653 |

**Tableau 2.4:** Bound-state energy eigenvalues $(-E)$ for the LiH molecule (in eV ) for different values of the rotational $\ell$ and vibrational $n$ quantum numbers

| $n$ | $\ell$ | Our work | TJMR | EQR | SUSY | NU | Variational |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 2.40129 | 2.4288627 | 2.42886 | 2.42886 | 2.4287 | 2.4291 |
|  | 5 | 2.35986 | 2.4013352 | 2.40133 | 2.40133 | 2.4012 | 2.4014 |
|  | 10 | 2.25214 | 2.3288530 | 2.32883 | 2.32883 | 2.3287 | 2.3287 |

## 2.4 Graph of the radial Morse effective potential with the Pekeris approximation as the centrifugal term

This section explores the graphical representation of the radial Morse effective potential and its modification using the Pekeris approximation to account for the centrifugal term. The original Morse potential effectively describes the vibrational energy of diatomic molecules, while the Pekeris approximation incorporates rotational dynamics, enabling an approximate analytical solution to the Schrödinger equation. By comparing the two potentials, the graphs illustrate the impact of the centrifugal term and the accuracy of the approximation in describing molecular interactions.

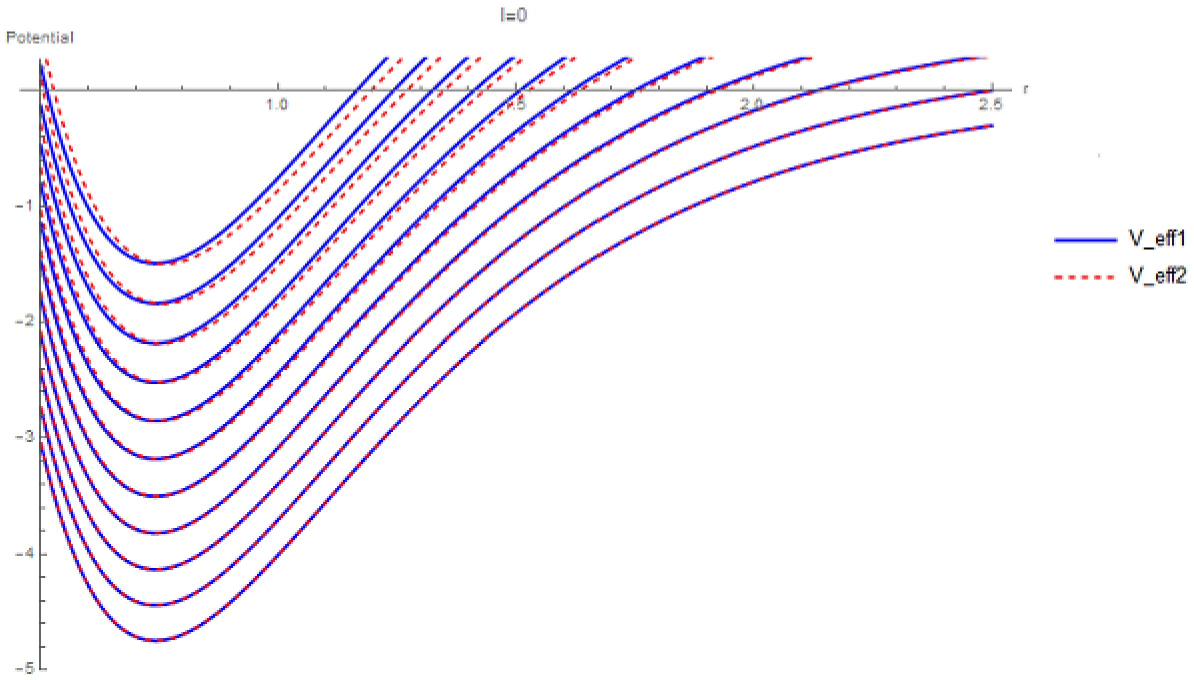

**Figure 2.2:** The morse potential $V_eff1$ (bleu line) and the approximate new morse potential $V_eff2$ (dached red line) of the molecule $H_2$

The blue line represents the original Morse potential, which models the interaction energy of diatomic molecules as a function of the interatomic distance . This potential exhibits a distinct minimum at the equilibrium bond length, corresponding to the molecule's most stable bound state. As the atoms approach each other, the potential rises sharply, reflecting strong repulsive forces. Conversely, as the distance increases , the potential asymptotically approaches zero, representing the dissociation of the molecular bond. This graph highlights the Morse potential's ability to accurately capture anharmonicity in molecular vibrations, providing a more realistic depiction of molecular interactions than the harmonic oscillator approximation.

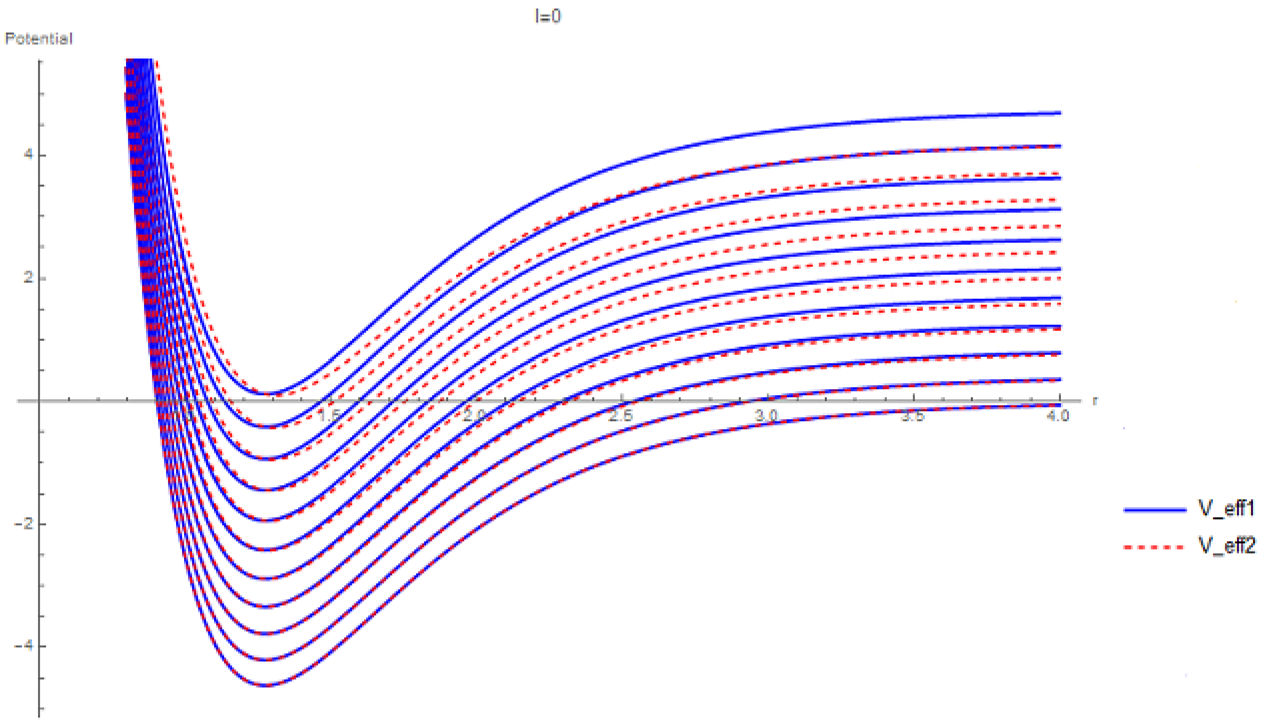

**Figure 2.3:** The morse potential $V_eff1$ (bleu line) and the approximate new morse potential $V_eff2$ (dached red line) of the molecule HcL

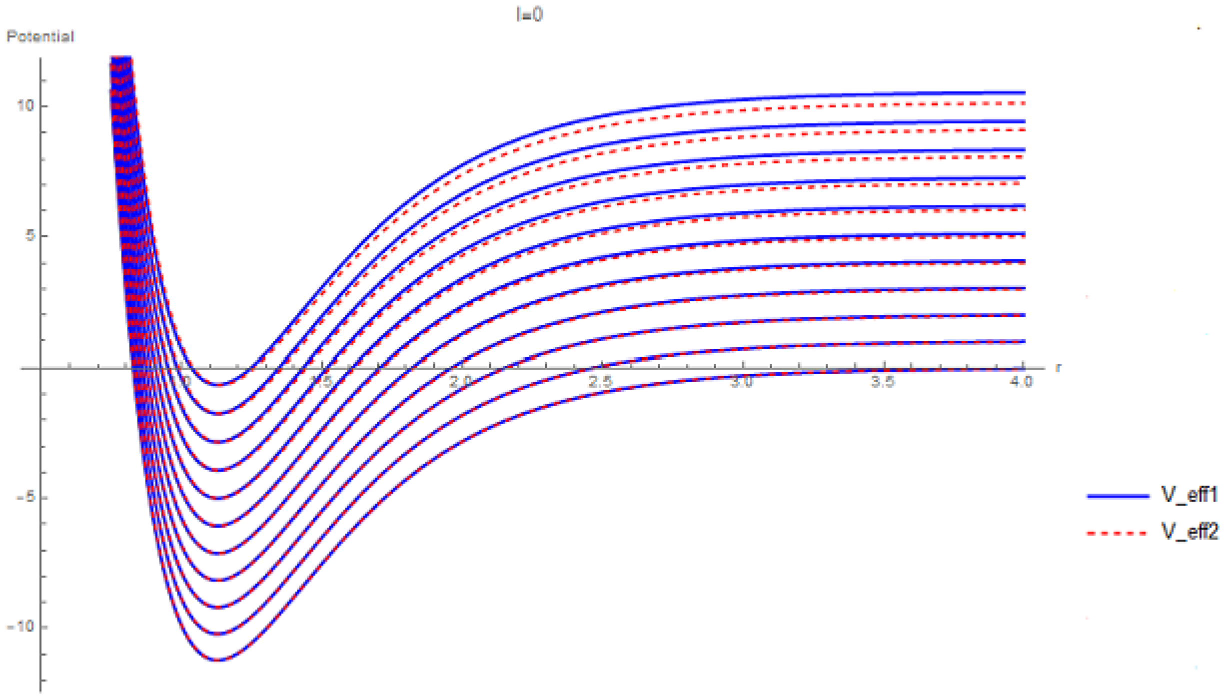

**Figure 2.4:** The morse potential $V_eff1$ (bleu line) and the approximate new morse potential $V_eff2$ (dached red line) of the molecule CO

The dashed red line illustrates the modified Morse potential incorporating the Pekeris approximation, which accounts for the centrifugal term's contribution. The modified potential retains the overall shape of the original Morse potential but features a slightly elevated energy curve at smaller interatomic distances. This adjustment reflects the additional rotational energy introduced by the centrifugal term. Despite this modification, the Pekeris approximation preserves the essential characteristics of the Morse potential, ensuring both analytical solvability and physical relevance in the description of molecular dynamics.

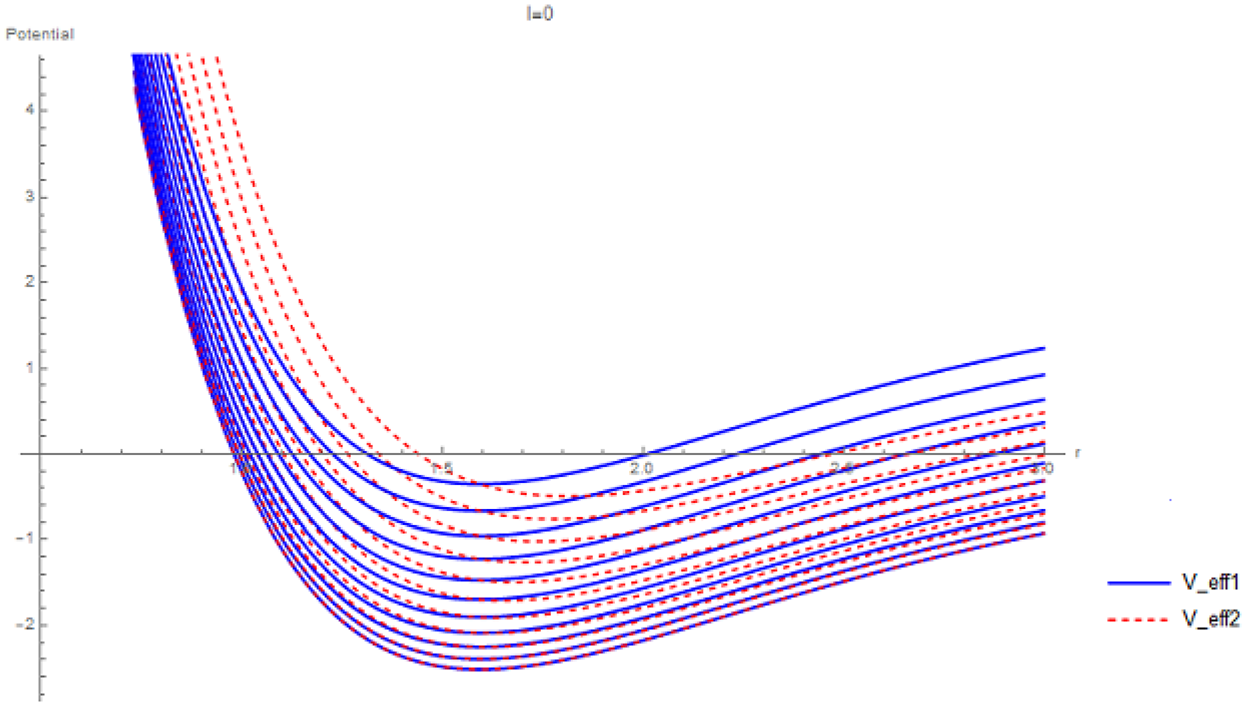

**Figure 2.5:** The morse potential $V_eff1$ (bleu line) and the approximate new morse potential $V_eff2$ (dached red line) of the molecule LiH

The combined graph overlays the original Morse potential (Veff1V_\text{eff1}Veff1) and the modified potential (Veff2V_\text{eff2}Veff2) for direct comparison. The two curves align closely, particularly near the equilibrium bond length , where the molecule is most stable. However, noticeable deviations occur at smaller interatomic distances, where the centrifugal term's effects are more pronounced. This comparison underscores the practicality and accuracy of the Pekeris approximation. The minimal deviations between the two potentials demonstrate that the approximation provides a reliable modification for incorporating rotational dynamics into the Morse potential while maintaining its core descriptive capabilities.

# Conclusion

this thesis aimed to find the bound-state solutions (energy levels) of the rotating Morse potential, which is a mathematical model used in physics to describe the behavior of molecules. Specifically, the goal was to solve the Schrödinger equation (which describes quantum systems) for this potential in a new and more straightforward way using a technique called Inverse Contour Representation (ICR). The solution of the radial Schrödinger equation with the Morse potential becomes challenging for non-zero angular momentum states (l  0) so we used approximations of Pekeris to handle the centrifugal term that complicates the exact solution. so by expressing the Solution in Terms of Contour Integrals the differential equation (Schrödinger equation) is transformed into an integral over a contour C in the complex plane and the integrals are chosen such that they satisfy the boundary conditions, leading to a form for Q(t),

But Using integral transformations to solve differential equations, like the Schrödinger equation, is challenging because The integral representations are often unwieldy unless the integrand can be expressed in terms of known special functions (Euler's Beta function and Laguerre polynomials) and The specific choice of the contour of integration C is non-trivial. For complex integrals, many contours are possible, and selecting the correct one to simplify the solution is critical , so the ICR method simplifies the process by connecting the solution to the Euler Beta function so the Beta function can be employed to compute the inverse contour representation, enabling a direct connection to residue calculus : The poles of the integrand represent the quantized energy levels of the system. By applying the calculus of residues, the integral is evaluated , and with ICR we don't have to search for the right contour so Instead of requiring one exact contour, the method provides a general framework where the choice of C is no longer restrictive, as long as fundamental conditions (encircling poles z=0 and z=1) are met.

The final solution for the radial wavefunction is expressed in terms of a confluent hypergeometric function, which can be rewritten as a sum involving Laguerre polynomials when the quantum number p is a negative integer and the wave function must be normalized, which is done by integrating over the domain and determining the appropriate normalization constant. The constant depends on the energy eigenvalues and the form of the Laguerre polynomials so the final form of the radial wave function is obtained, which includes a normalization constant and a Laguerre polynomial that represents the vibrational states of the molecule.

The numerical results align well with other established methods, validating the approximation's reliability. The graphical representation underscores the accuracy of the modified potential, making the method highly applicable for studying vibrational and rotational dynamics in diatomic molecules.

It is worthwhile to generalize the ICR method and approach it with all potential related to hypergeometric functions.for those higher rovibrational states the method loses its accuracy We notice that for low energies the effective potential is quite similar to the real Morse potential and this is why our results are in such a good agreement with the other results.ICR offers flexibility that may outperform other methods by providing an easy-to-apply contour integration approach that can generalize to different and ICR direct use of contour integrals makes it simpler compared to the more complex recursive or iterative approaches and ICR may be adaptable to a variety of potentials, including those governed by hypergeometric functions, which could be advantageous when moving beyond the specific cases studied in some of the methods.

# Bibliographie

[1] George B Arfken and Hans J Weber. *Mathematical methods for physicists ; 4th ed.* Academic Press, San Diego, CA, 1995.

[2] M Bag, MM Panja, R Dutt, and YP Varshni. Modified shifted large-n approach to the morse oscillator. *Physical Review A*, 46(9) :6059, 1992.

[3] ORHAN Bayrak and I Boztosun. Arbitrary -state solutions of the rotating morse potential by the asymptotic iteration method. *Journal of Physics A : Mathematical and General*, 39(22) :6955, 2006.

[4] Cüneyt Berkdemir and Jiaguang Han. Any l-state solutions of the morse potential through the pekeris approximation and nikiforov–uvarov method. *Chemical physics letters*, 409(4-6) :203–207, 2005.

[5] Yurii Aleksandrovich Brychkov. Practical quantum mechanics : S. flugge. 331+ 287+ xvi p. springer, new york–heidelberg–berlin, 1974. book review. *Zhurnal Vychislitel'noi Matematiki i Matematicheskoi Fiziki*, 16(5) :1366–1367, 1976.

[6] Gang Chen. The exact solutions of the schrödinger equation with the morse potential via laplace transforms. *Physics Letters A*, 326(1) :55–57, 2004.

[7] D. Doetsch. *Guide to the Applications of Laplace Transforms, Princeton Univ.Press, Princeton,1961.* Van Nostrand, 1961.

[8] Elso Drigo Filho and Regina Maria Ricotta. Morse potential energy spectra through the variational method and supersymmetry. *Physics Letters A*, 269(5-6) :269–276, 2000.

[9] I. S. Gradshteyn and I. M. Ryzhik. *Table of integrals, series, and products.* Elsevier/Academic Press, Amsterdam, seventh edition, 2007. Translated from the Russian, Translation edited and with a preface by Alan Jeffrey and Daniel Zwillinger, With one CD-ROM (Windows, Macintosh and UNIX).

[10] Tom D Imbo and Uday P Sukhatme. Supersymmetric quantum mechanics and large-n expansions. *Physical review letters*, 54(20) :2184, 1985.

[11] A. G. MACKIE. Contour integral solutions of a class of differential equations. *Journal of Rational Mechanics and Analysis*, 4 :733–750, 1955.

[12] Daniel A Morales. Supersymmetric improvement of the pekeris approximation for the rotating morse potential. *Chemical physics letters*, 394(1-3) :68–75, 2004.

[13] Philip M. Morse. Diatomic molecules according to the wave mechanics. ii. vibrational levels. *Phys. Rev.*, 34 :57–64, Jul 1929.

[14] GA Natanzon. Vestnik leningrad univ. 10, 22 (1971). *Teor. Mat. Fiz*, 38 :146, 1979.

[15] CL Pekeris. The rotation-vibration coupling in diatomic molecules. *Physical Review*, 45(2) :98, 1934.

[16] Wen-Chao Qiang and Shi-Hai Dong. Arbitrary l-state solutions of the rotating morse potential through the exact quantization rule method. *Physics Letters A*, 363(3) :169–176, 2007.

# Annexe A

# Exemple of the codes that we did in mathematica

## A.1 the code of the graphe

**Algorithme A.1 :** the code of the graphe of the molecule $H_2$ in mathematica

```
$V0 = 4.7446$
$\sigma = 1.9425$
$re = 0.7416$
$\alpha = 1.440558$
$A1 = -0.114575538605$
$A2 = 0.7514632207596$
$A0 = 0.3631123178455$
$\gamma = (l * (l + 1)/241.09) * re^2;$
$Veff1[l_,r_] := V0 * (Exp[-2 * \alpha * ((r - re)/re)] - 2 * Exp[-\alpha * ((r - re)/re)]) + \gamma;$
$Veff2[l_,r_] := V0 * (Exp[-2 * \alpha * ((r - re)/re)] - 2 * Exp[-\alpha * ((r - re)/re)]) + \gamma *$
  $(A0 + A1 * Exp[-\alpha * ((r - re)/re)] + A2 * Exp[-2 * \alpha * ((r - re)/re)]);$
$n = 10;$
$Show[Table[\ Plot[Veff1[l, r], Veff2[l, r], r, 0.5, 2.5,$
  $PlotStyle- > Directive[Blue, Thick], Directive[Red, Dashed],$
  $PlotLegends- > "V_eff1", "V_eff2",\ AxesLabel- > "r", "Potential",$
  $PlotLabel- > StringForm["l = `1`", l]], l, 0, n]]$
```

## A.2 the code of the bound state energy eigenvalues

**Algorithme A.2 :** the code of calculating the Bound-state energy eigenvalues (E) for the molecule LiH in mathematica

```
(*Function to calculate the energy eigenvalue*)
energyEigenvalue[n_,l_,r_,V0_,Z_,a_] :=Module[{A0,A1,A2,term},A0=0.2592760585180616 ;
A1=0.3702360219773695 ;
A2=0.3704879195045688 ;
term = (l ∗ (l + 1) ∗ A0)/(2 ∗ 241.09 ∗ (1.5956)^2)−
(1/(4 ∗ 241.09 ∗ (1.5956)^2))
((Z ∗ ((2 ∗ V0) − (l ∗ (l + 1) ∗ A1/(241.09 ∗ 1.5956^2)))/
Sqrt[V0 + ((l ∗ (l + 1) ∗ A2)/(241.09 ∗ 1.5956^2))]) − (2 ∗ n + 1) ∗ a)^2;
term];

(*Constants and parameters for the calculation*)
nValues = Range[0, 3]; (*Principalquantumnumber(n)rangingfrom0to10*)
lValues = Range[0, 3]; (*Azimuthalquantumnumber(l)rangingfrom0ton − 1foreachn*)
r = 1.5956; (*restassocieéàladistanceinternucléaireàl′équilibreentremolécules*)
V0 = 2.51518226; (*V0estl′énergiedeséparationdelamolécule*)
Z = 24.77499788703119;
a = 1.7998368;
(*Calculate the energy eigenvalues for different n and l*)
energyValues =
Flatten[Table[{n, l, energyEigenvalue[n, l, r, V0, Z, a]}, {n, nValues}, {l, lValues}], 1];

(*Display the result as a table*)
TableForm[energyValues, TableHeadings → {None, {n, l, "Energy (eV)"}}]
```

# Annexe B

# Parameters of the Molecules.

## B.1 Here, some data characterizing the different molecules will be provided.

**Tableau B.1:** Parameters of the Molecules

| | Quantités | $V_0$ | $\sigma = \alpha/r_F$ | $r_e$ | $\mu$ |
|---|---|---|---|---|---|
| | Unités | (eVoucm | $(\mathbb{A}^{-1})$ | $(A)$ | (uma) |
| Molécules | $H_2$ | 4.7446eV | 1.9425 | 0.7416 | 0.50391 |
| | HCl | 37255 $\mathrm{cm}^{-1}$ | 1.8677 | 1.2746 | 0.9801045 |
| | CO | 90540 $\mathrm{cm}^{-1}$ | 2.2994 | 1.1283 | 6.8606719 |
| | LiH | 20287 $\mathrm{cm}^{-1}$ | 1.1280 | 1.5956 | 0.8801221 |

Atomic units : $\hbar c \approx 1973.29\mathrm{eVA}$, $\mu c^2 \approx \mu \times 931.481 \times 10^5\mathrm{eV}$, $1\ \mathrm{cm}^{-1} \approx 1.2398 \times 10^{-4}\mathrm{eV}$.