

# Bachelor's Thesis

## Theoretical Investigation of the Kratzer and Morse Potentials in Higher-Dimensional Quantum Mechanics

*Theoretische Untersuchung des Kratzer- und des Morse Potentials in der Höher  
Dimensionalen Quantenmechanik*

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# 1 Introduction

In the last century there were formed two new fundamental concepts: theory of relativity and quantum mechanics.

Predictions of these two models seem to be accurate each within its boundaries. One of the most important predictions which could be proved was the discovery of the Higgs boson in 2012 [Greene].

However these two theories can't be unified. The most promising attempt is the string theory. Our three dimensional space is embedded in a higher dimensional space. It was amazing that the force which influences until infinity range is so small compared to the electromagnetic force for example. Maybe we experience only a small part of it in our three dimensions and the major part is distributed to other dimensions we can't perceive [Randall].

So it is useful to deal with quantum mechanics in higher dimensions [Dong].

Two-atomic molecules have more degrees of freedom than one-atomic ones. The Morse potential describes the vibrations [Flügge182] and the Kratzer potential specifies "the rotation-vibration spectrum" [Flügge178].

So this bachelor's thesis applies the higher dimensional formalism to these two potentials. To investigate wave equations in higher dimensions there has to be introduced a formalism to handle with. It has to be defined hyperspherical coordinates  $r$  and  $\theta_b$ , such as the Laplacian, the volume element and the angular momentum operator in polar coordinates. For the investigation of the Kratzer potential the wave equation has to be developed in  $D$ -dimensions. The radial wave function is determined by analysing the behaviour at infinity and at zero. This result is applied to three dimensions. After normalisation there is derived an expression for the energy levels. The levels are investigated according to the dimension and the quantum numbers referred to the shell and the angular momentum. For the investigation of the Morse potential the same formalism is applied to the Morse potential to get the wave function.

## 2 Basics

The consideration of potentials in higher dimensions requires a suitable formalism. Here it is followed the nomenclature and the explanation by [Dong]. The two potentials are rotation-symmetric, so a description of hyperspherical coordinates is needed. To check that the formalism works it will be applied to two and three dimensions.

### 2.1 Hyperspherical Coordinates

First of all the transformation between the Cartesian coordinates  $x_i$  and the hyperspherical coordinates  $r$  and  $\theta_b$  in a  $D$ -dimensional space is defined by

$$\begin{aligned} x_1 &= r \cdot \cos \theta_1 \cdot \prod_{b=2}^{D-1} \sin \theta_b, \\ x_2 &= r \cdot \prod_{b=1}^{D-1} \sin \theta_b, \\ x_n &= r \cos \theta_{n-1} \cdot \prod_{b=n}^{D-1} \sin \theta_b, \\ x_D &= r \cos \theta_{D-1}, \end{aligned} \tag{1}$$

where  $r \in [0, \infty)$ ,  $\theta_1 \in [-\pi, \pi]$ ,  $\theta_2, \theta_n \in [0, \pi]$  and  $n \in [3, D - 1]$ . In two dimensions there will be yielded

$$\begin{aligned} x_1 &= r \cdot \cos \theta_1, \\ x_2 &= r \cdot \sin \theta_1, \end{aligned} \tag{2}$$

and in three

$$\begin{aligned} x_1 &= r \cdot \cos \theta_1 \cdot \sin \theta_2, \\ x_2 &= r \cdot \sin \theta_1 \cdot \sin \theta_2, \\ x_3 &= r \cdot \cos \theta_2. \end{aligned} \tag{3}$$

This two sets of hyperspherical coordinates corresponds to the well known sets as used in e. g. [Demtröder], identifying  $\theta_1$  with  $\varphi$  and  $\theta_2$  with  $\vartheta$ .

$r = \sqrt{\sum_{b=1}^D x_b^2}$  is the radius of a  $D$ -dimensional sphere.

### 2.2 The Laplacian in Higher Dimensions

In order to define the Laplacian in polar coordinates a scaling factor  $h$  is needed.

$$h = \prod_{n=1}^{D-1} h_n \tag{4}$$

where  $h_n = \sqrt{\sum_{b=1}^D \left(\frac{\partial x_b}{\partial \theta_b}\right)^2}$  and  $\theta_0 = r$ .  
 $h_n$  can directly be calculated

$$\begin{aligned} h_0 &= 1, \\ h_1 &= r \cdot \prod_{b=2}^{D-1} \sin \theta_b, \\ h_2 &= r \cdot \prod_{b=3}^{D-1} \sin \theta_b, \\ h_n &= r \cdot \prod_{b=n+1}^{D-1} \sin \theta_b, \\ h_{D-1} &= r. \end{aligned} \tag{5}$$

The Laplacian is defined by:

$$\nabla_D^2 = \frac{1}{h} \sum_{b=1}^{D-1} \frac{\partial}{\partial \theta_b} \left( \frac{h}{h_b^2} \frac{\partial}{\partial \theta_b} \right) \tag{6}$$

Now the Laplacian in polar coordinates can be written as

$$\begin{aligned} \nabla_D^2 &= \frac{1}{r^{D-1}} \frac{\partial}{\partial r} \left( r^{D-1} \frac{\partial}{\partial r} \right) \\ &+ \frac{1}{r^2} \sum_{b=1}^{D-2} \left[ \prod_{a=b+1}^{D-1} \frac{1}{\sin^2 \theta_a} \cdot \left( \frac{1}{\sin^{b-1} \theta_b} \left( \frac{\partial}{\partial \theta_b} \sin^{b-1} \theta_b \frac{\partial}{\partial \theta_b} \right) \right) \right] \\ &+ \frac{1}{r^2} \left( \frac{1}{\sin^{D-2} \theta_{D-1}} \left( \frac{\partial}{\partial \theta_{D-1}} \sin^{D-2} \theta_{D-1} \frac{\partial}{\partial \theta_{D-1}} \right) \right). \end{aligned} \tag{7}$$

In two dimensions this leads to

$$\nabla_2^2 = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \cdot \frac{\partial^2}{\partial \theta_{D-1}^2} \tag{8}$$

and in three dimensions to

$$\nabla_3^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{1}{\sin^2 \theta_2} \frac{\partial^2}{\partial \theta_1^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta_2^2}. \tag{9}$$

In the configuration space the differential of the solid angle is given by

$$d\Omega = \prod_{n=1}^{D-1} (\sin \theta_n)^{n-1} d\theta_n. \tag{10}$$

In two dimensions it can be identified by

$$d\Omega = d\theta_1 = d\varphi \quad (11)$$

and in three dimensions by

$$\begin{aligned} d\Omega &= \sin \theta_2 d\theta_2 d\theta_1 = \\ &= \sin \vartheta d\vartheta d\varphi. \end{aligned} \quad (12)$$

Therefore the volume element is given by

$$\prod_{b=1}^D dx_b = r^{D-1} dr d\Omega, \quad (13)$$

where  $r \in [0, \infty)$ ,  $\theta_1 \in [-\pi, \pi]$ ,  $\theta_2, \theta_n \in [0, \pi]$  and  $n \in [2, D-1]$ . This corresponds to the results in two dimensions

$$dA = r dr d\varphi \quad (14)$$

as well as to the results in three dimensions

$$dV = r dr \sin \vartheta d\vartheta d\varphi. \quad (15)$$

## 2.3 The Angular Momentum Operator in Arbitrary Dimensions

In Cartesian coordinates the angular momentum operator  $L_{kl}$  is defined as

$$L_{kl} = x_k p_l - x_l p_k \quad (16)$$

where  $k, l = 1, 2, \dots, D$  and  $\hbar = 1$ <sup>1</sup>.

The Casimir operator  $L^2$ , which commutes with all  $L_{kl}$ , is defined as follows

$$L^2 = \frac{1}{2} \sum_{k,l} (L_{kl})^2. \quad (17)$$

In spheric coordinates is yielded

$$L^2 = L_{D-1}^2 = - \left( \frac{1}{\sin^{D-2} \theta_{D-1}} \frac{\partial}{\partial \theta_{D-1}} \left( \sin^{D-2} \theta_{D-1} \frac{\partial}{\partial \theta_{D-1}} \right) - \frac{L_{D-2}^2}{\sin^2 \theta_{D-1}} \right). \quad (18)$$

$L_{D-2}^2$  can be calculated by the recursive formula

$$L_j^2 = - \left( \frac{1}{\sin^{j-1} \theta_j} \frac{\partial}{\partial \theta_j} \left( \sin^{j-1} \theta_j \frac{\partial}{\partial \theta_j} \right) - \frac{L_{j-1}^2}{\sin^2 \theta_j} \right), \quad (19)$$

$$\begin{aligned} L_2^2 &= - \left( \frac{1}{\sin \theta_2} \frac{\partial}{\partial \theta_2} \left( \sin \theta_2 \frac{\partial}{\partial \theta_2} \right) - \frac{L_1^2}{\sin^2 \theta_2} \right) = \\ &= - \left( \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2} \right), \end{aligned} \quad (20)$$

$$L_1^2 = - \frac{\partial^2}{\partial \theta_1^2}. \quad (21)$$

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<sup>1</sup>In this thesis is followed the convention  $\hbar = 1$ .

It can be seen that equ. (20) corresponds to the Casimir operator in three dimensions and equ. (21) to the Casimir operator in two dimensions Inserted in the Laplacian yields

$$\nabla_D^2 = \frac{1}{r^{D-1}} \frac{\partial}{\partial r} \left( r^{D-1} \frac{\partial}{\partial r} \right) - \frac{L_{D-1}^2}{r^2}. \quad (22)$$

The eigenfunctions of these operators are the spherical harmonics  $Y_{l_{D-2} \dots l_1}^l$ . They achieve the eigenvalue equation

$$L^2 Y_{l_{D-2} \dots l_1}^l = l(l + D - 2) Y_{l_{D-2} \dots l_1}^l. \quad (23)$$

## 2.4 The Radial Momentum Operator

The radial momentum operator  $p_r$  is defined as

$$p_r = -\frac{i}{2} (\nabla \cdot (\hat{\mathbf{r}} \dots) + \hat{\mathbf{r}} \cdot \nabla), \quad (24)$$

where

$$\hat{\mathbf{r}} = \frac{\mathbf{r}}{r}. \quad (25)$$

Writing  $\nabla \cdot (\hat{\mathbf{r}} \dots)$  it has to be kept in mind that the operator  $p_r$  is applied to a wave function. So it has to be calculated

$$\nabla(\hat{\mathbf{r}}\Psi) = \hat{\mathbf{r}} \cdot \nabla\Psi + \Psi\nabla \cdot \hat{\mathbf{r}}. \quad (26)$$

That yields for  $p_r$

$$p_r = -\frac{i}{2} (\nabla \cdot \hat{\mathbf{r}} + 2\hat{\mathbf{r}} \cdot \nabla). \quad (27)$$

It can be shown that

$$\nabla \cdot \hat{\mathbf{r}} = \frac{D-1}{r} \quad (28)$$

and

$$\hat{\mathbf{r}} \cdot \nabla = \frac{\partial}{\partial r}. \quad (29)$$

The result is

$$p_r = -i \left( \frac{\partial}{\partial r} + \frac{D-1}{2r} \right). \quad (30)$$

In two dimensions

$$p_r = -i \left( \frac{\partial}{\partial r} + \frac{1}{2r} \right). \quad (31)$$

and in three dimensions<sup>2</sup>

$$p_r = -i \left( \frac{\partial}{\partial r} + \frac{1}{r} \right). \quad (32)$$

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<sup>2</sup>It can be compared to [Gorgas]

is yielded.

In the Schrödinger equation the radial momentum operator appears squared. So

$$\begin{aligned} p_r^2 &= - \left( \frac{\partial}{\partial r} + \frac{D-1}{2r} \right) \left( \frac{\partial}{\partial r} + \frac{D-1}{2r} \right) = \\ &= - \left( \frac{\partial^2}{\partial r^2} + \frac{D-1}{r} \frac{\partial}{\partial r} + \frac{(D-1)(D-3)}{4r^2} \right). \end{aligned} \quad (33)$$

### 3 Kratzer potential

#### 3.1 Expansion of the Wave Function

Now there are all tools to expand an expression for wave function in the D-dimensional Schrödinger equation

$$-\frac{1}{2} \nabla^2 \Psi(\mathbf{x}) = (E - V(r)) \Psi(\mathbf{x}). \quad (34)$$

The wave function can be separated in a radial part  $R_l(r)$  and an angular part  $Y_{lD-2\dots l_1}^l$ . Furthermore expression (22) for Nabla is used. That yields

$$\frac{1}{r^{D-1}} \frac{d}{dr} \left( r^{D-1} \frac{d}{dr} \right) R_l(r) + \left( 2E - 2V(r) - \frac{l(l+D-2)}{r^2} \right) R_l(r) = 0. \quad (35)$$

Derivation results in a differential equation

$$\frac{d^2}{dr^2} R_l(r) + \frac{D-1}{r} \frac{d}{dr} R_l(r) + \left( 2E - 2V(r) - \frac{l(l+D-2)}{r^2} \right) R_l(r) = 0. \quad (36)$$

To prove if this equation fits to known results in lower dimensions the three dimensional case is looked at. In three dimensions it is <sup>3</sup>

$$\frac{d^2}{dr^2} R_l(r) + \frac{2}{r} \frac{d}{dr} R_l(r) + \left( 2E - 2V(r) - \frac{l(l+1)}{r^2} \right) R_l(r) = 0 \quad (37)$$

As potential there is taken the Kratzer type potential in arbitrary dimensions

$$V(r) = \frac{A}{r^2} - \frac{B}{r}. \quad (38)$$

With

$$\varrho = r\sqrt{-8E} \quad (39)$$

and

$$\tau \equiv B\sqrt{\frac{1}{-2E}} \quad (40)$$

there is yielded

$$\frac{d^2 R_l(\varrho)}{d\varrho^2} + \frac{D-1}{\varrho} \frac{dR_l(\varrho)}{d\varrho} + \left( -\frac{1}{4} + \frac{\tau}{\varrho} - \frac{2A + l(l+D-2)}{\varrho^2} \right) R_l(\varrho) = 0. \quad (41)$$

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<sup>3</sup>This formula for the radial wave function in three dimensions can be found in [Haken168].



To determine  $R_l(\varrho)$  first the behaviour of the function at infinity is analysed. The terms with  $\frac{1}{\varrho}$  or  $\frac{1}{\varrho^2}$  are negligible. So the result is

$$\frac{d^2 R_l(\varrho)}{d\varrho^2} - \frac{1}{4} R_l(\varrho) = 0. \quad (42)$$

A solution for a differential equation of this type is solved by an ansatz of the form

$$R_l(\varrho) = K \cdot e^{-\varrho/2} \quad (43)$$

where  $K$  is an arbitrary magnitude. If  $K$  is chosen as  $\varrho^\lambda \cdot F(\varrho)$

$$R_l(\varrho) = \varrho^\lambda \cdot e^{-\varrho/2} \cdot F(\varrho) \quad (44)$$

can be inserted in equ. (41) results in

$$\begin{aligned} & \varrho^\lambda \left( \frac{d^2 F(\varrho)}{d\varrho^2} - \frac{dF(\varrho)}{d\varrho} \right) \\ + & \varrho^{\lambda-1} \left( (2\lambda + D - 1) \frac{dF(\varrho)}{d\varrho} + \left( \tau - \frac{1}{2}(D - 1) - \lambda \right) F(\varrho) \right) \\ + & \varrho^{\lambda-2} (\lambda(\lambda - 1) + (D - 1)\lambda - (2A + l(l + D - 2))) F(\varrho) = 0. \end{aligned} \quad (45)$$

To determine  $\lambda$  it has to be considered the behaviour of the function near 0. The terms with  $\varrho^\lambda$  or  $\varrho^{\lambda-1}$  are negligible. So the result is

$$\varrho^{\lambda-2} (\lambda(\lambda - 1) + (D - 1)\lambda - (2A + l(l + D - 2))) F(\varrho) = 0. \quad (46)$$

This leads to

$$\lambda = \frac{2 - D + \sqrt{8A + \kappa^2}}{2}, \quad \kappa \equiv 2l + D - 2. \quad (47)$$

Rearranging equ. (45) leads to a form which can be solved by Laguerre polynomials

$$\varrho \frac{d^2 F(\varrho)}{d\varrho^2} + (2\lambda + D - 1 - \varrho) \frac{dF(\varrho)}{d\varrho} + \left( \tau - \frac{D - 1}{2} - \lambda \right) F(\varrho) = 0. \quad (48)$$

The solution of equ. (48) is  $F(\varrho) = L_{\tau - \frac{D-1}{2} - \lambda}^{2\lambda + D - 2}(\varrho)$  [Motschmann].  $L_b^a(t)$  is given by

$$L_n^a(t) = \sum_{j=1}^n \binom{n+a}{n-j} \frac{(-t)^j}{j!}. \quad (49)$$

This leads to the solution of equ. (44)

$$R(\varrho) = \mathcal{N} \varrho^\lambda e^{-\varrho/2} L_{\tau - \frac{D-1}{2} - \lambda}^{2\lambda + D - 2}(\varrho). \quad (50)$$

$\mathcal{N}$  is a factor to normalize  $R(\varrho)$ .

Developing  $F(\varrho) = \sum_{\nu=0}^{\infty} c_{\nu} \varrho^{\nu}$  in equ. (48) leads to

$$\begin{aligned} & \sum_{\nu=0}^{\infty} \nu(\nu-1)c_{\nu}\varrho^{\nu-1} + (2\lambda + D - 1) \sum_{\nu=0}^{\infty} \nu c_{\nu}\varrho^{\nu-1} \\ & - \sum_{\nu=0}^{\infty} \nu c_{\nu}\varrho^{\nu} - \left( \lambda - \tau + \frac{D-1}{2} \right) \sum_{\nu=0}^{\infty} c_{\nu}\varrho^{\nu} = 0. \\ & \sum_{\nu=0}^{\infty} \nu c_{\nu}\varrho^{\nu-1} ((\nu-1) + 2\lambda + D - 1) - \sum_{\nu=0}^{\infty} c_{\nu}\varrho^{\nu} \left( \nu + \lambda - \tau + \frac{D-1}{2} \right) = 0 \\ & \sum_{\nu=0}^{\infty} c_{\nu+1}\varrho^{\nu} (\nu+1) (\nu + 2\lambda + D - 1) - \sum_{\nu=0}^{\infty} c_{\nu}\varrho^{\nu} \left( \nu + \lambda - \tau + \frac{D-1}{2} \right) = 0 \\ & \sum_{\nu=0}^{\infty} \varrho^{\nu} \left( c_{\nu+1}(\nu+1) (\nu + 2\lambda + D - 1) - c_{\nu} \left( \nu + \lambda - \tau + \frac{D-1}{2} \right) \right) = 0. \end{aligned}$$

That this equation can only be fulfilled when the factors are zero leads to a recursion relation

$$c_{\nu+1} = c_{\nu} \frac{\nu + \lambda - \tau + \frac{D-1}{2}}{(\nu+1) (\nu + 2\lambda + D - 1)} \quad (51)$$

For  $\nu^* = (\lambda - \tau + \frac{D-1}{2})$  the coefficient  $c_{\nu^*+1}$  is 0, as well as the coefficients  $c_{\nu^*+c}$  ( $c < 1$ ). So

$$\lambda - \tau + \frac{D-1}{2} = N = 0, 1, 2, \dots \quad (52)$$

where  $N$  is the radial quantum number. The associated principal quantum number is

$$n = N + l + 1 = N + \kappa/2 - D/2. \quad (53)$$

This leads to the condition, that

$$l < n \quad (54)$$

and equ. (50) can be written as

$$R(\varrho) = \mathcal{N} \varrho^{\lambda} e^{-\varrho/2} L_{n-l-1}^{2\lambda+D-2}(\varrho). \quad (55)$$

The corresponding energy levels can be obtained by equ. (40).

$$B \sqrt{\frac{1}{-2E}} = \tau = n - l - 1 + \lambda + \frac{D-1}{2}. \quad (56)$$

Relocated to  $E$  yields

$$E = - \frac{B^2}{2 \left( n - l - 1 + \lambda + \frac{D-1}{2} \right)^2}. \quad (57)$$

With equ. (47) it is obtained

$$E = - \frac{2B^2}{(2n - 2l - 1 + \sqrt{8A + \kappa^2})^2}. \quad (58)$$

There can be considered an approximation for large  $D$

$$E \simeq -2B^2 \left( D^{-2} - 2(2n-3)D^{-3} + (3(2n-3)^2 - 8A - (2l-2)^2)D^{-4} - \dots \right). \quad (59)$$

In this case  $\kappa$  is approximately equal to  $D$ . So  $l$  in equ. (53) can be determined as 1, if the power of  $D$  is small. So the dependence of  $l$  is negligible.

To determine  $\mathcal{N}$  in equ. (50) the normalisation condition

$$\int_0^\infty R(\varrho)^2 r^{D-1} dr = 1 \quad (60)$$

has to be used. With equ. (56) it leads to

$$\int_0^\infty (\mathcal{N} \varrho^\lambda e^{-\varrho/2} L_{n-l-1}^{2\lambda+D-2}(\varrho))^2 r^{D-1} dr = 1. \quad (61)$$

This can be solved by the formula [Nieto]

$$\begin{aligned} J_{m,\alpha}^{(\beta)} &= \int_0^\infty e^{-t} t^{\alpha+\beta} [L_m^\alpha(t)]^2 dt \\ &= \frac{\Gamma(\alpha+m+1)}{\Gamma(m+1)} \sum_{k=0}^m (-1)^k \frac{\Gamma(m-k-\beta)}{\Gamma(-k-\beta)} \frac{\Gamma(\alpha+k+1+\beta)}{\Gamma(\alpha+k+1)} \frac{1}{\Gamma(k+1)\Gamma(m-k+1)}, \\ &\text{with } \operatorname{Re}(\alpha+\beta+1) > 0. \end{aligned} \quad (62)$$

From equ. (60) follows  $\beta = 1$ . Using  $\Gamma(m+1) = m!$  equ. (62) becomes [Dong83]

$$J_{m,\alpha}^{(1)} = \frac{(2m+\alpha+1)\Gamma(\alpha+m+1)}{m!}. \quad (63)$$

Comparing equ. (50) with equ. (62) yields

$$\begin{aligned} m &= n-l-1, \\ \alpha &= 2\lambda+D-2. \end{aligned}$$

So

$$J_{n-l-1, 2\lambda+D-2}^{(1)} = \frac{(2n-2l+2\lambda+D-3)\Gamma(2\lambda+D-2+n-l)}{(n-l-1)!}. \quad (64)$$

So equ. (61) becomes with equ. (64)

$$\frac{\mathcal{N}^2}{2^D \sqrt{-2E}^D} \cdot \frac{(2n-2l+2\lambda+D-3)\Gamma(2\lambda+D-2+n-l)}{(n-l-1)!} = 1. \quad (65)$$

At least  $\mathcal{N}$  becomes

$$\mathcal{N} = \left( \frac{4B}{2n-2l+2\lambda+D-3} \right)^{\frac{D}{2}} \quad (66)$$

$$\cdot \sqrt{\frac{(n-l-1)!}{(2n-2l+2\lambda+D-3)\Gamma(2\lambda+D-2+n-l)}}. \quad (67)$$

The entire wave function is made out to

$$\Psi(\mathbf{x}) = \mathcal{N} \varrho^\lambda e^{-\varrho/2} L_{n-l-1}^{2\lambda+D-2}(\varrho) Y_{l_{D-2}\dots l_1}^l(\theta_1 \dots \theta_{D-1}). \quad (68)$$

### 3.2 Dependence of the Energy by $D$ , $l$ and $n$

Equ. (58) showed the dependence of the energy of the dimension and the quantum numbers  $n$  and  $l$ . First it will be investigated, if there is a special dimension, that the energy is extremal. So the roots of

$$\begin{aligned} \frac{\partial E(n, l, D)}{\partial D} &= \frac{\partial E(n, l, D)}{\partial \kappa} \cdot \underbrace{\frac{\partial \kappa}{\partial D}}_{=1} = \\ &= \frac{4B^2\kappa}{(2n - 2l - 1 + \sqrt{8A + \kappa^2})^3 \sqrt{8A + \kappa^2}} \end{aligned} \quad (69)$$

has to be found, e. g.

$$D = 2(1 - l). \quad (70)$$

Thus  $l$  has to be an integer and less than  $D$ , there is only one solution for this equation

$$l = 0, \quad D = 2.$$

To see, if there is a maximum or a minimum, equ. (69) has to be derived to  $D$ .

$$\begin{aligned} \frac{\partial^2 E(n, l, D)}{\partial D^2} &= \\ &= \frac{4B^2((2n - 2l - 1 + \sqrt{8A + \kappa^2})(\sqrt{8A + \kappa^2} + 2\kappa) + 3\kappa^2\sqrt{8A + \kappa^2})}{(2n - 2l - 1 + \sqrt{8A + \kappa^2})^4(8A + \kappa^2)} \end{aligned} \quad (71)$$

The denominator is greater than 0. The numerator is positive too, since  $4B^2$  is greater than 0,  $n$  is greater than  $l$ , so  $2n - 2l - 1$  is at least 0.  $\sqrt{8A + \kappa^2} > 0$ , so the rest of the numerator is positive. Finally the second derivation of the energy to  $D$  is positive, so it has to be a minimum at  $l = 0$ ,  $D = 2$ . This circumstance is shown in figure 1 and figure 2.

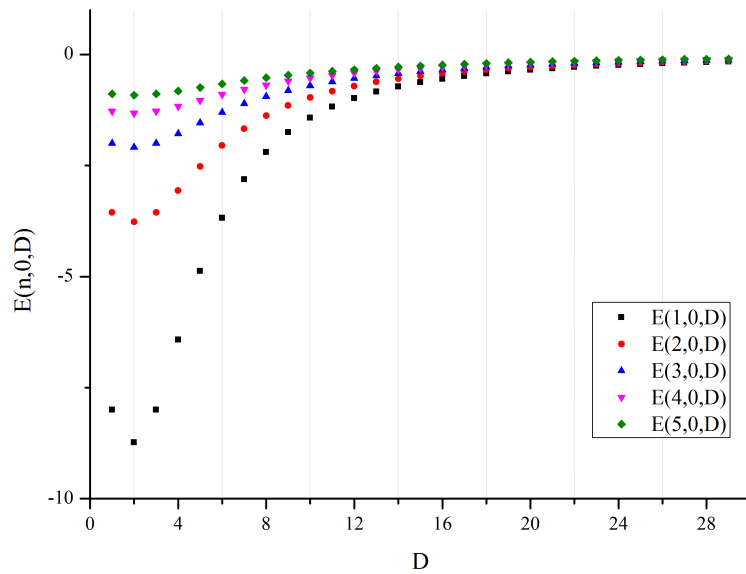


Figure 1: Variation of the energy when the quantum number  $l$  is fixed. ( $A = 1$  and  $B = 8$ .) In this case a minimum can be found at  $D = 2$  for the energy in every state. It can be seen that the curves become smoother when  $n$  is growing up.

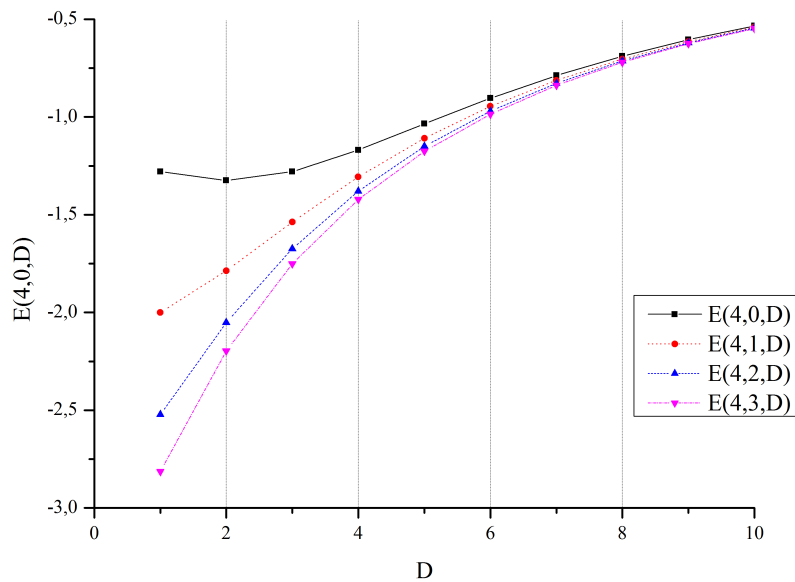


Figure 2: Variation of the energy when the quantum number  $n = 4$  is taken. ( $A = 1$  and  $B = 8$ .) The only case with a local minimum is when  $l = 0$ . The minimum is at  $D = 2$  as expected.

Second it will be considered the dependence of the energy of the quantum number  $l$ .

$$\frac{\partial E(n, l, D)}{\partial l} = \frac{8B^2(\kappa - \sqrt{8A + \kappa^2})}{\sqrt{8A + \kappa^2}((2n - 2l - 1 + \sqrt{8A + \kappa^2})^3)}. \quad (72)$$

As in equ. (71) the denominator is positive.  $\kappa$  is less than  $\sqrt{8A + \kappa^2}$ , so the numerator is negative for all  $D$  or  $l$ . If  $A$  equals 0, the Kratzer potential becomes a Coulomb potential and  $\frac{\partial E(n, l, D)}{\partial l}$  equals 0, so the energy is independent of  $l$  at all. In the one-dimensional case  $D = 1$  the eigenvalues reduce to

$$E_n = -\frac{B^2}{2n^2}. \quad (73)$$

Figure 3 shows the Coulomb potentials for the two-, three-, four- and five-dimensional case. The one-dimensional case follows equ. (73) and has therefore the same shape as  $E(n, 3)$ .

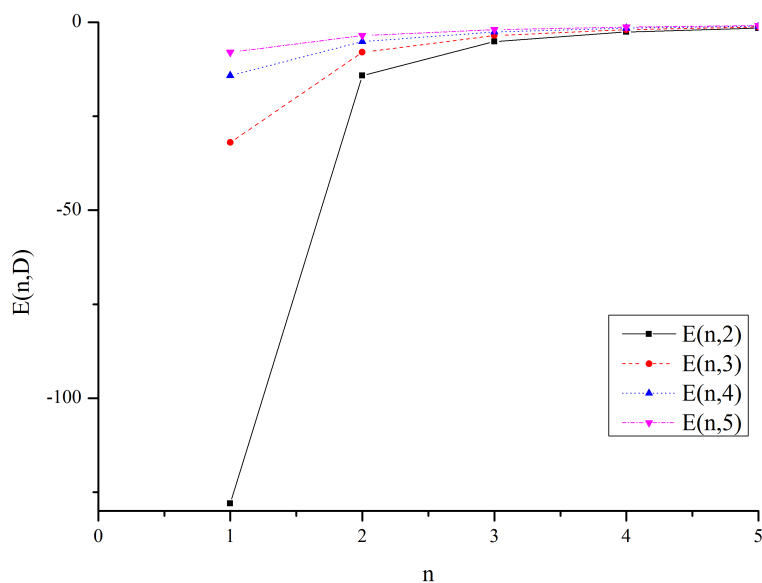


Figure 3: Variation of the energy when  $A = 0$  and  $B = 8$ . This shows the Coulomb potential. Energy is increasing with the dimension in each state.

Third it will be considered the dependence of the energy of the quantum number  $n$ .

$$\frac{\partial E(n, l, D)}{\partial n} = \frac{8B^2}{((2n - 2l - 1 + \sqrt{8A + \kappa^2})^3)}. \quad (74)$$

Since  $2n - 2l$  is greater than or equal 2 the denominator is positive. So the whole expression is positive. This means that there will be no local extremum. The energy increases with increasing quantum number  $n$ . For great  $D$  this expression tends to zero.

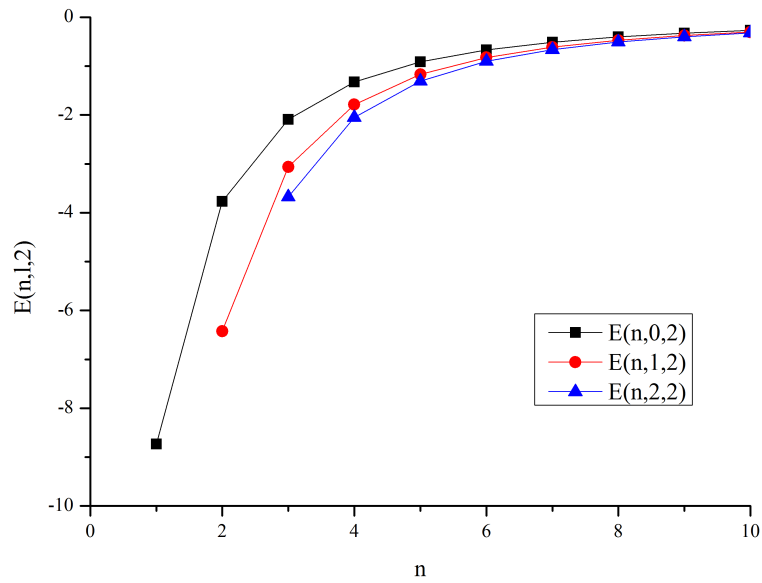


Figure 4: Variation of the energy when  $A = 1$ ,  $B = 8$  and  $D = 2$ . When  $n$  increases the energy increases as well. When  $l$  is increasing the energy decreases in each state.

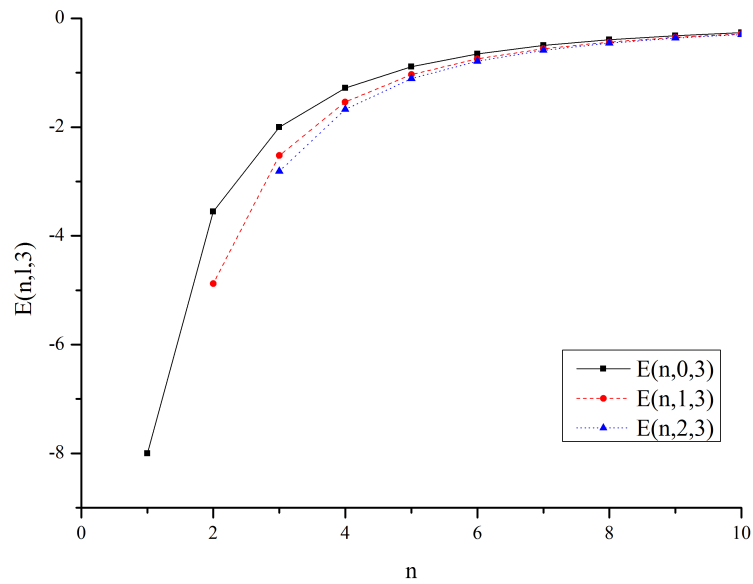


Figure 5: Variation of the energy when  $A = 1$ ,  $B = 8$  and  $D = 3$ . When  $n$  increases the energy increases as well. When  $l$  is increasing the energy decreases in each state.

For three dimensions the energy levels are shown in table 1 for some two atomic

molecules as nitrogen, carbon monoxide, nitrogen monoxide and CH [Berkdemir].

$n$	$l$	$N_2$	CO	NO	CH
0	0	0.054430	0.050823	0.041118	0.083214
1	0	0.162057	0.151287	0.122311	0.241123
	1	0.162546	0.151755	0.122724	0.244381
2	0	0.268229	0.250354	0.202274	0.389547
	1	0.268711	0.250816	0.202681	0.392611
	2	0.269675	0.251744	0.203494	0.398722
3	0	0.372972	0.348051	0.281033	0.529229
	1	0.373447	0.348507	0.281434	0.532115
	2	0.374398	0.349418	0.282235	0.53787
	3	0.375823	0.350785	0.283436	0.546467
4	0	0.476313	0.444403	0.358611	0.660844
	1	0.476779	0.444852	0.359006	0.663565
	2	0.477717	0.445751	0.359795	0.668992
	3	0.479124	0.447099	0.360978	0.677098
	4	0.480999	0.448895	0.362555	0.687842
5	0	0.578269	0.539434	0.435032	0.785001
	1	0.578732	0.539877	0.435421	0.787569
	2	0.579658	0.540764	0.436198	0.792692
	3	0.581046	0.542093	0.437364	0.800343
	4	0.582896	0.543865	0.438917	0.810487
	5	0.585208	0.546082	0.440858	0.823071

Table 1: Energy levels for two atomic molecules in eV for different values of  $n$  and  $l$  [Berkdemir]



## 4 Morse Potential

### 4.1 Expansion of the Wave Function

In this section the radial wave function with an anharmonic potential will be analysed. Since knowing from (44)  $R(r)$  consists in terms of  $r^\lambda$ . For getting more handsome expressions  $-\frac{D-1}{2}$  is taken away from the exponent. In equ. (78) this will be repaired by introducing  $r^\tau$ .

The wave equation

$$\Psi(\mathbf{r}) = r^{-\frac{D-1}{2}} R(r) Y_{l_{D-2} \dots l_1}^l \quad (75)$$

will be inserted in equ. (36). This yields

$$\left( \frac{d^2}{dr^2} - \frac{l(l+D-2) + (D-1)(D-3)/4}{r^2} \right) R(r) = -2(E - V(r)) R(r), \quad (76)$$

with  $\kappa$  as given in equ. (47) it becomes shorter

$$\left( \frac{d^2}{dr^2} - \frac{\kappa^2 - 1/4}{r^2} \right) R(r) = -2(E - V(r)) R(r). \quad (77)$$

With the ansatz

$$R(r) = r^\tau e^{-br} G(r), \quad b = \sqrt{-2E}, \quad E < 0, \quad (78)$$

inserted the radial Schrödinger equation becomes after arranging in orders of  $r$

$$\begin{aligned} & (\tau(\tau-1) - (\kappa^2 - 1/4)) G(r) + \left( 2\tau \frac{dG(r)}{dr} - 2b\tau G(r) \right) r \\ & + \left( \frac{d^2 G(r)}{dr^2} - 2b \frac{dG(r)}{dr} - 2V(r)G(r) \right) r^2 = 0. \end{aligned} \quad (79)$$

To determine  $\tau$  this equation is considered at the origin. The terms with  $r$  and  $r^2$  can be neglected. So it is obtained

$$\tau_{1,2} = \frac{1}{2} \pm \kappa. \quad (80)$$

Only  $\tau > 0$  is used. So the behaviour in equ. (78) at the infinity depends only on the exponential function. Otherwise there would be no term to describe the behaviour at the origin.

Expanding  $G(r)$  as standard series

$$G(r) = \sum_{k=0}^{\infty} \gamma_k r^k, \quad \gamma_0 \neq 0 \quad (81)$$

provides the radial wave function

$$R(r) = r^{1/2+\kappa} e^{-br} \sum_{k=0}^{\infty} \gamma_k r^k, \quad \gamma_0 \neq 0 \quad (82)$$

and the wave function is

$$\Psi(r) = r^{1+\kappa-D/2} e^{-br} Y_{l_{D-2} \dots l_1}^l \sum_{k=0}^{\infty} \gamma_k r^k, \quad \gamma_0 \neq 0. \quad (83)$$

In equ. (79) has to be inserted a potential to obtain the coefficients  $\gamma_k$ . Here the chosen potential is the Morse potential

$$V(r) = V_0 (e^{-2\beta r} - 2e^{-\beta r}), \quad (84)$$

where  $V_0 > 0$ . To make this expression more handsome there is used a transformation

$$\begin{aligned} e^{-2\beta r} &= \sum_{n=0}^{\infty} \frac{(-2\beta r)^n}{n!} = \sum_{n=0}^{\infty} (-1)^n 2^n \frac{(\beta r)^n}{n!} \\ e^{-\beta r} &= \sum_{n=0}^{\infty} \frac{(-\beta r)^n}{n!} = \sum_{n=0}^{\infty} (-1)^n \frac{(\beta r)^n}{n!} \\ \Rightarrow e^{-2\beta r} - 2e^{-\beta r} &= \sum_{n=0}^{\infty} (-1)^n (2^n - 2) \frac{\beta^n}{n!} r^n = \\ &= 2 \sum_{n=0}^{\infty} (-1)^n \frac{(2^{n-1} - 1) \beta^n}{n!} r^n = 2 \sum_{n=0}^{\infty} c_n r^n. \end{aligned} \quad (85)$$

So the Morse potential can be written as

$$V(r) = 2V_0 \sum_{n=0}^{\infty} c_n r^n. \quad (86)$$

The expressions for  $G(r)$ ,  $V(r)$  and  $\tau = \kappa + \frac{1}{2}$  are inserted in equ. (79). That yields

$$\sum_{k=0}^{\infty} (k(2\kappa + k)) \gamma_k r^k - \sum_{k=0}^{\infty} 2b(k + \kappa + 1/2) \gamma_k r^{k+1} - 4V_0 \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} c_l \gamma_k r^{l+k+2} \quad (87)$$

from which can be obtained

$$\begin{aligned} \gamma_1 &= b\gamma_0, \\ \gamma_2 &= \frac{b(2\kappa + 3)\gamma_1 + 4V_0\gamma_0 c_0}{4 + 4\kappa}. \end{aligned} \quad (88)$$

Finally can be obtained from equ. (87)

$$\gamma_n = \frac{b(2\kappa + 2n - 1)\gamma_{n-1} + 4V_0 S_{n,k}}{n(2\kappa + n)} \quad (89)$$

with

$$S_{n,k} = \sum_{l=0}^N c_l \gamma_{N-l}, \quad \text{where } N = n - 2 > 0. \quad (90)$$

In the case of the Kratzer potential there is a handsome formula to get the energy levels. But in the case of the Morse potential it would take a hard work to get them. The Morse potential can be mapped to the potential of the harmonic oscillator. It can be seen in figure 6 that the two potentials are similar only in the range very close to the minimum.

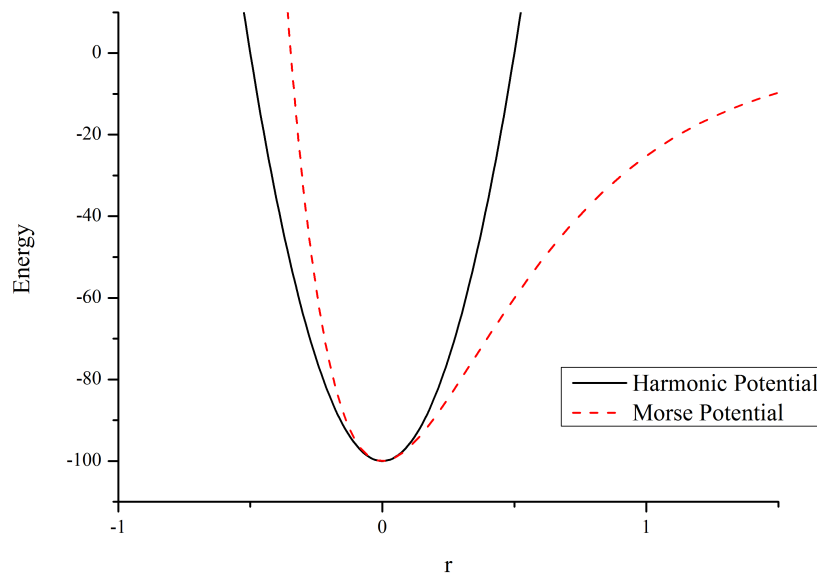


Figure 6: The Morse potential (red dashed line) can be approached by the harmonic potential (black line) in range very close to the minimum.

## 5 Summary

The introduced formalism which is necessary to handle wave equations in higher dimensions applied to two and three dimensions delivers the well known expressions for the hyperspherical coordinates, the Laplacian, the volume element and the angular momentum operator in polar coordinates.

The investigation of the Kratzer potential yields to expressions for the energy levels in dependence of the dimension and the quantum numbers  $n$  and  $l$ . If  $l$  equals to zero the energy levels have a minimum in two dimensions. For dimensions higher than 25 the energy levels are approximatively independent of the dimension. If  $l$  is greater than zero the energy level rises with the dimension for fixed  $n$ . Even in higher dimensions the energy levels are increasing if the dimension is fixed and the quantum number  $n$  is increasing. For fixed dimension and fixed quantum number  $n$  the energy is increasing with increasing quantum number  $l$ .

The Morse potential is very difficult to handle. In the range close to the minimum it can be mapped to the potential of the harmonic oscillator.

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Ich versichere durch meine Unterschrift, dass ich meine Bachelorarbeit *Theoretical Investigation of the Kratzer and Morse Potentials in Higher-Dimensional Quantum Mechanics* selbständig und ohne fremde Hilfe angefertigt habe, und dass ich alle von anderen Autoren wörtlich übernommenen Stellen, wie auch die, die sich an die Gedankengänge anderer Autoren eng anlehnenen Ausführungen meiner Arbeit besonders gekennzeichnet und die Quellen zitiert habe.

Münster, den 14. April 2014