Quantum Mechanics I

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Coding is easy, algebra is easy, calculus is easy, physics is imposible.

– Rajamani S. Narayanan

Preface

This book is written with my lack of knowledge in LaTeX and my notes token from Professor Rajamani S. Narayanan course on Quantum Mechanics at Florida International University. During this pages I am going to learn how to manage LaTeX as an useful tool while I am dealing with understand the world of the Quantum Mechanics.

I will start with some Classical Mechanics to understand how the Quantum Mechanics appeared in the first place.

I also want to thank to Abel Rosado who helps me and teaches me on how to use this template.

Adolfo Menéndez Rua

Contents

Preface **v**

Contents **vii**

1 Classical Mechanics **1**
1.1 The Two-Body Problem . . . 1
1.2 The Angular Momentum . . . 2
1.3 Cylindrical coordinates . . . 3
1.4 Potential wells . . . 5
1.5 Physical Examples . . . 5
1.6 Rotation and angular momentum . . . 8

2 Waves **9**
2.1 The wave function . . . 9
2.2 Energy and momentum . . . 9
2.3 P(x) function I: Definition and properties . . . 10
2.4 Fourier Series . . . 11
2.5 P(x) function II: $\psi(x)$ and $\tilde{\psi}(k)$ . . . 13
2.6 Free particle . . . 14
2.7 Examples . . . 17

3 Potentials V(x,y,z) **23**
3.1 Potential in 3 dimensions . . . 23
3.2 Discontinuous Functions . . . 24
3.3 Square Potential Well . . . 25
3.4 Examples . . . 30

4 Delta function potential **33**
4.1 Definition of the potential . . . 33
4.2 Solution . . . 33

5 Multiple potentials **37**
5.1 Definition . . . 37
5.2 Solution . . . 38
5.3 Solutions for N = 1,2 . . . 39
5.4 Solving for x as a circunference . . . 41
5.5 Solution for all the posible energies. . . . 44

6 Algebra: Linear vector space **47**
6.1 Definition of linear vector space . . . 47
6.2 Inequations . . . 48
6.3 Definitions in Wave Mechanicsand Operators . . . 49

7 Harmonic Oscilator **53**
7.1 Definition . . . 53
7.2 Solving the Wave Equation . . . 54
7.3 Temperature . . . 57

8 2-Dimensional Potential **59**
8.1 Classical Mechanics 59
8.2 Quantum Mechanics 62
8.3 Mixed Quantum states 69
8.4 The angular momentum 69

9 3-Dimensional Space **75**
9.1 Angular Momentum in 3 Dimensions 75
9.2 Angular Momentum as a vector operator 80
9.3 Matrix representation for j=1, 1/2, 2 83

Appendix **85**

Notation **87**

Alphabetical Index **89**

List of Figures

1.1 Two bodies interacting with some force . . . 1
1.2 Two-body problem with new coordinates . . . 2
1.3 Cylindrical coordinates . . . 3
1.4 Effective Potential . . . 5
1.5 Effective Potential for Earth-Sun . . . 5
1.6 Effective Potential for Electron-Proton . . . 6
1.7 Effective Potential for Electron-Proton (Electric Potential) . . . 7

2.1 Normal distribution for mean=0 and sigma=1, to simulate a experiment measured by different people . . . 10
2.2 P(x) and P(k) for $\sigma = 0.1$. . . . 15
2.3 P(x) and P(k) for $\sigma = 5$. . . . 15
2.4 Function $\sigma(t)$ for the Earth experiment . . . 17
2.5 Gif for P(x,t) of the Earth experiment . . . 18
2.6 Function $\sigma(t)$ for the Electron experiment . . . 18
2.7 Gif for P(x,t) of the Electron experiment . . . 19
2.8 Function $\sigma(t)$ for the Neutron decay . . . 19
2.9 Gif for P(x,t) of the Neutron decay . . . 20
2.10 Function $\sigma(t)$ for the Electron experiment . . . 21
2.11 Gif for P(x,t) of the Electron experiment . . . 21

3.1 Discontinuous function with a finite jump in x = 0 . . . 24
3.2 Square Potential Well . . . 25
3.3 α as a function of β for $\gamma = 5$ . . . 29
3.4 $\phi(x)$ and P(x) functions for gamma = 10 . . . 30
3.5 $\phi(x)$ and P(x) functions for gamma = 10 . . . 31
3.6 $\phi(x)$ and P(x) functions for gamma = 100 . . . 31
4.1 Delta function potential . . . 33

4.2 Solution for g=2.5 of phi(x) for the delta function potential. . . . 35
5.1 Multiple delta function potentials problem. . . . 37

5.2 Coefficients outside of the potentials near x=nd. . . . 37
5.3 Solutions for $(T^N)_{22} = 0$ for N=2 and d=2 . . . 40
5.4 Solutions for $(T^N)_{22} = 0$ for N=2 and d=0.5 . . . 40
5.5 alpha as a function of N for $d = 2$. . . . 41
5.6 x as a circunference . . . 41
5.7 Potential between -d/2 and d/2 . . . 42
5.8 Energy as a function of the number of potentials. . . . 43
5.9 Energy as a function of the distance between potentials. . . . 44
5.10 All the energies as a function of the number of potentials. . . . 45
5.11 All the energies as a function of the distance between potentials. . . . 45

7.1 Potential V(x) and some energy levels. . . . 57
7.2 Potential V(x) and some energy levels. . . . 58

8.1 $\beta(\tau)$ function for different values of alpha . . . 61

8.2 Orbital movement of the particle for different values of α 62
8.3 Probability distribution for the state $\psi_{0,0}(u,v)$ 66
8.4 Probability distribution for the state $\psi_{0,1}(u,v)$ 66
8.5 Probability distribution for the state $\psi_{1,0}(u,v)$ 67
8.6 Probability distribution for the state $\psi_{0,1}(r,\theta)$ 67
8.7 Probability distribution for the state $\psi_{1,0}(r,\theta)$ 68

List of Tables

Classical Mechanics 1

1.1 The Two-Body Problem

As it is showed in Figure 1.1 we have two bodies with masses m_1 and m_2 and they interact with a force unknown.

We can define their positions as: $\vec{r_1}$ and $\vec{r_2}$ and the separation between them as $\vec{r} = \vec{r_1} - \vec{r_2}$

I said that the force is unknown but we know:

- $F_{12} = -F_{21}$
- The force only depends on the distance between the two bodies and the direction is the line between them, i.e. $F = f(r)\hat{r}$ [1]
- The force can be defined as a central force so we can define a potential as: $f(r) = \frac{dv(r)}{dr}$

Using Newton 3rd Law we can explain the movement of this two objects by two equations:

$$m_1 \frac{d^2\vec{r_1}}{dt^2} = f(r)\hat{r} \tag{1.1}$$

$$m_2 \frac{d^2\vec{r_2}}{dt^2} = -f(r)\hat{r} \tag{1.2}$$

Let's add 1.1 and 1.2, this is going to be useful later.

$$m_1 \frac{d^2\vec{r_1}}{dt^2} + m_2 \frac{d^2\vec{r_2}}{dt^2} = 0 \tag{1.3}$$

We can not get anything from 1.1 and 1.2, so we are going to transform this equations into something we can use to resolve them. First, we define the center of mass and their derivatives among time:

$$r_{\vec{CM}} = \frac{m_1\vec{r_1} + m_2\vec{r_2}}{m_1 + m_2} \tag{1.4}$$

$$v_{\vec{CM}} = \frac{d}{dt} r_{\vec{CM}} = \frac{1}{m_1 + m_2}\left[m_1 \frac{d\vec{r_1}}{dt} + m_2 \frac{d\vec{r_2}}{dt}\right] \tag{1.5}$$

$$a_{\vec{CM}} = \frac{d}{dt} v_{\vec{CM}} = \frac{1}{m_1 + m_2}\left[m_1 \frac{d^2\vec{r_1}}{dt^2} + m_2 \frac{d^2\vec{r_2}}{dt^2}\right] \tag{1.6}$$

If we look at 1.6 we can see something equal to the left term on 1.3 so we can say that the acceleration of the center of mass is zero, i.e. $a_{\vec{CM}} = 0$.

1.1 The Two-Body Problem . . . 1
1.2 The Angular Momentum . . 2
1.3 Cylindrical coordinates . . . 3
1.4 Potential wells 5
1.5 Physical Examples 5
1.6 Rotation and angular momentum 8

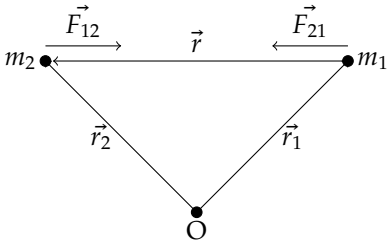

Figure 1.1: Two bodies interacting with some force at some time

1: $\hat{r} = \frac{\vec{r}}{|\vec{r}|}$

This mean that the center of mass moves with a constant velocity and we can define it's move as:

$$\vec{r_{CM}} = R_{CM} + V_{CM} \cdot t \tag{1.7}$$

Where R_{CM} and V_{CM} are constants defined by initial conditions. Knowing this we can make a change of the coordinates with the next assumption:

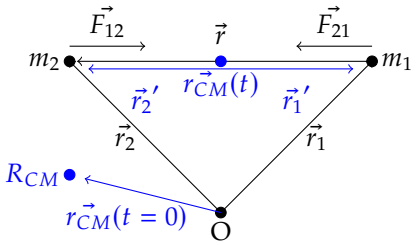

Figure 1.2: Two-body problem with the new coordinates

$$\vec{r_1} = \vec{r_1'} + \vec{r_{CM}} \tag{1.8}$$

$$\vec{r_2} = \vec{r_2'} + \vec{r_{CM}} \tag{1.9}$$

Now let's calculate the new center of mass $\vec{r'_{CM}}$ using 1.8 and 1.9

$$\begin{aligned} \vec{r'_{CM}} &= \frac{m_1\vec{r_1'} + m_2\vec{r_2'}}{m_1 + m_2} \\ &= \frac{1}{m_1 + m_2}\left[m_1(\vec{r_1} - \vec{r_{CM}}) + m_2(\vec{r_2} - \vec{r_{CM}})\right] \\ &= \vec{r_{CM}} - \frac{1}{m_1 + m_2}\left[\vec{r_{CM}}(m_1 + m_2)\right] \\ &= \vec{r_{CM}} - \vec{r_{CM}} = 0 \end{aligned} \tag{1.10}$$

[2]

2: The professor demonstrate the same but with the expression for $\vec{r_{CM}}$, this is just another way I prefer.

As it should be, our new center of mass is the origin for all time because our new referential system is moving with the center of mass. From this assumptions and using the definition of the new center of mass above we can get a new system of equations.

$$\begin{cases} m_1\vec{r_1'} + m_2\vec{r_2'} = 0 \\ \vec{r_1'} - \vec{r_2'} = \vec{r} \end{cases} \Rightarrow \begin{cases} \vec{r_1'} = \frac{m_2\vec{r}}{m_1+m_2} \\ \vec{r_2'} = \frac{-m_1\vec{r}}{m_1+m_2} \end{cases} \tag{1.11}$$

We use what we obtain from 1.11 in 1.1 and 1.2. We can do this because the force does not change in this coordinates because only depend on r and this magnitude is still the same, i.e. $\vec{r} = \vec{r'}$.

$$m\frac{d^2\vec{r}}{dt^2} = f(r)\vec{r} \tag{1.12}$$

We get the same equation from both equations.This expression will be useful to resolve the problem later.

m is the reduce mass define as: $m = \frac{m_1 m_2}{m_1+m_2}$

Normally we can use $m \approx m_2$ when $m_1 >> m_2$, some examples of this are Sun and Earth or proton and electron. With real values: $m_{S-E} = \frac{m_S m_E}{m_S+m_E} \approx 5.96998 \cdot 10^{24} kg m_E$, where $m_S = 2 \cdot 10^{30} kg, m_E = 5.97 \cdot 10^{24} kg$

1.2 The Angular Momentum

We define the angular momentum as:

$$\vec{L} = \vec{r} \times \vec{p} = m\vec{r} \times \frac{d\vec{r}}{dt} \tag{1.13}$$

We want to now how this quantity changes among time.

$$\frac{d\vec{L}}{dt} = m\frac{\vec{dr}}{dt} \times \frac{d\vec{r}}{dt} + m\vec{r} \times \frac{d^2\vec{r}}{dt^2} = 0 + \vec{r} \times f(r)\hat{r} = 0 \tag{1.14}$$

The law of the conservation of angular momentum says that the angular momentum of a system remains constant unless an external rotational force (torque) acts upon it.

As we just demonstrate the angular momentum vector is constant and we can redefine it as:

$$\vec{L} = L\hat{z} \tag{1.15}$$

The decision of L going through the $\hat{z}$ direction is going to be very resourceful.

1.3 Cylindrical coordinates

We need to choose a coordinate system to resolve the problem. Our best option is to choose cylindrical coordinates.

$$\begin{aligned} \vec{r} &= \rho\hat{\rho} + z\hat{z} \\ \frac{d\vec{r}}{dt} &= \frac{d\rho}{dt}\hat{\rho} + \rho\frac{d\phi}{dt}\hat{\phi} + \frac{dz}{dt}\hat{z} \end{aligned} \tag{1.16}$$

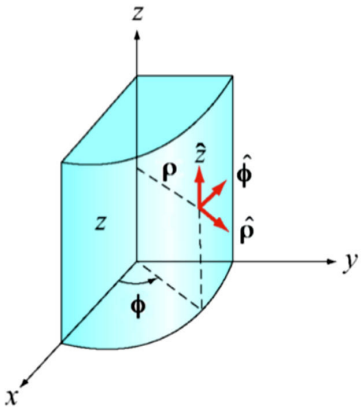

Figure 1.3: Cylindrical coordinates. https://www.researchgate.net/publication/334148643/figure/fig1/AS:775915730649091@1562004134358/Diagram-of-a-standard-cylindrical-coordinate-syste jpg

If we use 1.16 in 1.14 we can look at $\vec{L}$ components

$$\begin{aligned} \vec{L} =& m(\rho\hat{\rho} + z\hat{z}) \times \left(\frac{d\rho}{dt}\hat{\rho} + \rho\frac{d\phi}{dt}\hat{\phi} + \frac{dz}{dt}\hat{z}\right) = \\ & - mz\rho\frac{d\phi}{dt}\hat{\rho} + m\left(z\frac{d\rho}{dt} - \rho\frac{dz}{dt}\right)\hat{\phi} + m\rho^2\frac{d\phi}{dt}\hat{z} \end{aligned} \tag{1.17}$$

Using the definition in 1.15 and our new equation we get 4 different equations if we compare the angular momentum in each direction.

$$\begin{aligned} &1. \quad L \neq 0 \\ &2. \quad mz\rho\frac{d\phi}{dt} = 0 \\ &3. \quad m\left(z\frac{d\rho}{dt} - \rho\frac{dz}{dt}\right) = 0 \\ &4. \quad m\rho^2\frac{d\phi}{dt} = L \end{aligned} \tag{1.18}$$

This gives you a lot of information:

- $m \neq 0$

- $\rho \neq 0$
- $\frac{d\phi}{dt} \neq 0$
- $z = 0$
- $\frac{d\phi}{dt} = \frac{L}{m\rho^2}$

This equations not only give us a fixed value of z it also give us that in the system we choose the value for z is 0 for all time. We also can get a relation between the derivative of ϕ and ρ. We will use this later to resolve the problem.

If z=0 we can redefine $\vec{r}$ from 1.16.

$$\begin{aligned} \vec{r} &= \vec{\rho} = \rho\hat{\rho} \\ \frac{d^2\vec{\rho}}{dt^2} &= \left[\frac{d^2\rho}{dt^2} - \rho\left(\frac{d\phi}{dt}\right)^2\right]\hat{\rho} + \left[2\frac{d\rho}{dt}\frac{d\phi}{dt} + \rho\frac{d^2\phi}{dt^2}\right]\hat{\phi} \end{aligned} \tag{1.19}$$

We loose the therm that goes in the $\hat{\phi}$ direction because is zero. We can see this in two different ways:

- Now our force $F = f(r)\hat{r} = f(\rho)\hat{\rho}$ because 1.19 so the second derivative of $\vec{\rho}$ only can have a component in the $\hat{\rho}$ direction.
- If we calculate what we have in the $\hat{\phi}$ component using some notions in derivatives and 1.18 we would get 0 [3]

If we return to 1.12 with everything we learnt we can get something very interesting, an scalar equation.

$$m\left[\frac{d^2\rho}{dt^2} - \rho\left(\frac{d\phi}{dt}\right)^2\right] = f(\rho) \tag{1.20}$$

We get a scalar equation with two variables ρ and ϕ, but we can use 1.18 as before and reduce everything to a scalar equation with one variable.

$$m\left[\frac{d^2\rho}{dt^2} - \rho\frac{L^2}{m^2\rho^4}\right] = f(\rho) = -\frac{dv(\rho)}{d\rho} \tag{1.21}$$

We can put everything in one side of the equation and multiply both sides by a factor $\frac{d\rho}{dt}$

$$\begin{aligned} m\frac{d^2\rho}{dt^2}\frac{d\rho}{dt} - \frac{d}{dt}\left(\frac{L^2}{m\rho^3}\right) + \frac{d}{dt}\frac{dv(\rho)}{d\rho} &= 0 \\ \frac{d}{dt}\left(\frac{1}{2}m\left(\frac{d\rho}{dt}\right)^2 + \frac{L^2}{2m\rho^2} + v(\rho)\right) &= 0 \end{aligned} \tag{1.22}$$

We know that this magnitude inside the brackets is constant during the time. This magnitude is the total energy, E, and we can divide it three:

Linear Kinetic Energy $K = \frac{1}{2}m(\frac{d\rho}{dt})^2$
Angular Kinetic Energy $K_\alpha = \frac{L^2}{2m\rho^2}$

3: $2\frac{d\rho}{dt}\frac{d\phi}{dt} + \rho\frac{d^2\phi}{dt^2} = \frac{d}{dt}\left(\rho^2\frac{d\phi}{dt}\right) = \frac{d}{dt}\left(\frac{L}{m}\right) = 0$, because both L and m are constants.

Potential Energy $v(\rho) = \frac{-k}{r}$ [4]

4: This is what we usually use as potential energy because it appears in nature, for example, Newton Gravity Law and Coulomb Law

1.4 Potential wells

We are going to study the angular kinetic energy and the potential energy (both are functions of ρ), we call the addition of these two energies **Effective potential**

In Figure 1.4 we can see many things:

- The function have a minimum that is the lowest possible total energy because the linear kinetic energy is always greater or equal to 0, i. e. $K \geq 0$. This energy represents a circular motion.
- If we have a higher energy but still negative, the movement is an elliptical motion with two values that are the nearest and the furthest point in the ellipse.
- If the energy is positive the motion is no more a close orbit and we say that the motion is an hyperbola.
- If the total energy is 0, the motion is in the limit between a close and an open orbit and the movement is a parable.

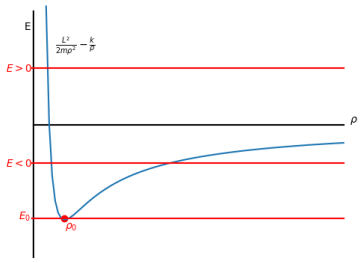

Figure 1.4: Effective Potential

In the next section we are going to give real values to this magnitudes.

1.5 Physical Examples

1. Earth-Sun problem: If we take the Earth and the Sun as our two bodies we need to know some values. We already know the reduce mass from the previous section. The k value of the potential energy is $k = GM_S m_E$, we know this value from Newton´s Gravitational Law.

- $m_E = 2 \cdot 1030kg$
- $M_S = 5.97 \cdot 10^{24} kg$
- $G = 6.67 \cdot 10^{11} Nm^2/kg^2$

The total energy of the system is:

$$E = \frac{1}{2}m\left(\frac{d\rho}{dt}\right)^2 + \frac{L^2}{2m\rho^2} + \frac{-GM_S m_E}{\rho} \tag{1.23}$$

We can see in Figure 1.5 that if we represent $U = K_\alpha + v(\rho)$ against ρ we get a similar function to the one in Figure 1.4, but we can see in the axis that we have large energies and distances. That is reasonable if we think that we are working with massive objects as planets.

We can calculated now the minimum energy the Earth-Sun system can have in which, the Earth would orbit by a circular motion.

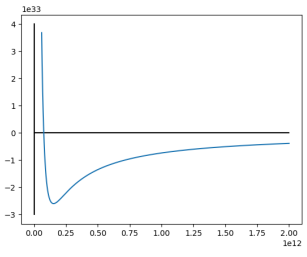

Figure 1.5: Effective Potential for Earth-Sun

To calculate this energy we need to calculate first the value of ρ for this minimum energy (ρ_{min}). This value can be found by matching the first derivative of the function U(ρ) to 0

$$\frac{dU}{d\rho} = \frac{d}{d\rho}\left[\frac{L^2}{2m\rho^2} + \frac{-GM_S m_E}{\rho}\right] = \frac{-L^2}{m\rho^3} + \frac{GM_S m_E}{\rho^2} \tag{1.24}$$

If we match 1.29 to 0 and solve for ρ we get ρ_{min}

$$\begin{aligned} \frac{-L^2}{m\rho^3} + \frac{GM_S m_E}{\rho^2} &= 0 \\ \frac{GM_S m_E^2 \rho - L^2}{m_E \rho^3} &= 0 \\ \rho_{min} &= \frac{L^2}{GM_S m_E^2} \end{aligned} \tag{1.25}$$

If we use 1.25 in 1.23 knowing that our minimum energy implies K = 0, we get the minimum energy possible.

$$E = -\frac{1}{2}\frac{G^2 M_S^2 m_E^3}{L^2} = -\frac{1}{2}\frac{GM_S m_E}{\rho_{min}} = \frac{1}{2}v(\rho_{min}) \tag{1.26}$$

If we look into the equation 1.26 we can demonstrate that the minimum energy is a half of the potential energy.

2. Electron-Proton problem: If we take a proton and an electron we can do the same as before knowing their masses. The problem is very similar, just with different conditions. The reduce mass is going to be the mass of the electron because it is much less than the mass of the proton.

- $m_e = 9.11 \cdot 10{-}31kg$
- $m_p = 1.67 \cdot 10^{-27}kg$
- $G = 6.67 \cdot 10^{11}kg$

The total energy of the system is:

$$E = \frac{1}{2}m\left(\frac{d\rho}{dt}\right)^2 + \frac{L^2}{2m\rho^2} + \frac{-GM_p m_e}{\rho} \tag{1.27}$$

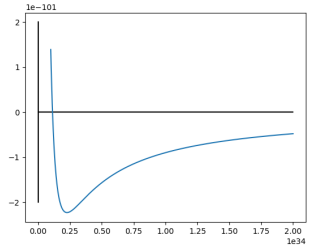

Figure 1.6: Effective Potential for Electron-Proton

We can see in Figure 1.6 that if we represent $U = K_\alpha + v(\rho)$ against ρ we get a similar function to Figure 1.4, but if we focus in the axis we can see that we have very low energies. That is reasonable if we think that we are working with particles that have very little mass.

I'm not going to do all we did before. In this case, because the energy is so low, is not interesting to study it. But there is another potential that affects electron and proton, the electric potential.

3. Electron-Proton problem with Electric Potential: In this case we need to define the charges of the proton and the electron. Also we need to define a new potential, where $k = \frac{Ze^2}{4\pi\epsilon_0}$ where Z is the atomic number, e is the charge of the electron [5] and ϵ_0 is the permittivity of free space.

- $e = 1.6 \cdot 10^{-19} \cdot 1030kg$
- $\epsilon_0 = 8.85 \cdot 10^{-12}kg$

5: This value was discovered by the Nobel Price Robert Andrews Millikan by his experiment called: Millikan oil drop experiment

The total energy of the system is:

$$E = \frac{1}{2}m\left(\frac{d\rho}{dt}\right)^2 + \frac{L^2}{2m\rho^2} + \frac{-Ze^2}{4\pi\epsilon_0\rho} \tag{1.28}$$

If we look at Figure 1.7 and compare it with Figure 1.6 we can see a high difference in the Energy scale. This means that the electrical force is much stronger than the gravitational force.

We can calculated now the minimum energy the Electron-Proton system can have in which, the electron would orbit by a circular motion around the proton.

To calculate this energy we need to calculate first the value of ρ for this minimum energy (ρ_{min}). This value can be found by matching the first derivative of the function in Figure 1.5 to 0

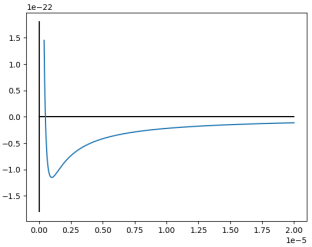

Figure 1.7: Effective Potential for Electron-Proton (Electric Potential)

$$\frac{dU}{d\rho} = \frac{d}{d\rho}\left[\frac{L^2}{2m\rho^2} + \frac{-Ze^2}{\rho}\right] = \frac{-L^2}{m\rho^3} + \frac{-Ze^2}{4\pi\epsilon_0\rho^2} \tag{1.29}$$

If we match 1.29 to 0 and solve for ρ we get ρ_{min}.

$$\begin{aligned} \frac{-L^2}{m\rho^3} + \frac{Ze^2}{4\pi\epsilon_0\rho^2} &= 0 \\ Ze^2m\rho - 4L^2\pi\epsilon_0 &= 0 \\ \rho_{min} &= \frac{4L^2\pi\epsilon_0}{Ze^2m} \end{aligned} \tag{1.30}$$

We can also get the square of the angular momentum as a function of ρ.

$$L^2 = \frac{m\rho_{min}Ze^2}{4\pi\epsilon_0} \tag{1.31}$$

Now, we have two different expressions for the minimum energy.

$$\begin{aligned} 1)E_{min} &= -\frac{Ze^2}{8\pi\epsilon_0\rho^2} \\ 2)E_{min} &= -\frac{Z^2e^4m}{2(4\pi\epsilon_0)^2}\frac{1}{L^2} \end{aligned} \tag{1.32}$$

Looking at the first expression we have the same as the Earth-Proton problem, we get that the minimum energy is half of the potential energy.

The second expression is even more interesting because after measure the length wave of light from an hydrogen atom, Bohr discovered that L was proportional to the energy level of the atom (n). Later they found that the relation is:

$$L = hn \tag{1.33}$$

h is known as the Plank constant.
$h \approx 6.63 \cdot 10^{-34}$

1.6 Rotation and angular momentum

To finished this chapter we are going to talk about something that is very interesting and purely mathematical.

We know that the rotation in 3D is not commutative and we also know that the definition of the module of $\vec{L}$ is

$$L^2 = |\vec{L}|^2 = L_x^2 + L_y^2 + L_z^2 \tag{1.34}$$

This means that we can have multiple solutions for L using rotations.

We define a vector |j,m > where j is the representation and m is the bases vector of the representation. Then we get this relations:

$$\begin{aligned} &1) L^2|j,m> = j(j+1)|j,m> \\ &2) L_z|j,m> = m|j,m> \end{aligned} \tag{1.35}$$

I'm not proving anything, we will talk about this later.

Waves 2

2.1 The wave function 9
2.2 Energy and momentum . . . 9
2.3 P(x) function I: Definition and properties 10
2.4 Fourier Series 11
2.5 P(x) function II: $\psi(x)$ and $\tilde{\psi}(k)$ 13
2.6 Free particle 14
2.7 Examples 17

Waves are some example of classical mechanics, where we have a function that propagates among time. During this chapter we will define their properties and their relation with quantum mechanics.

2.1 The wave function

We define a function that propagates in one dimension (x) among the time (t).

$$\psi(x,t) = e^{i(kx-\omega t)} \tag{2.1}$$

Where ω is the angular velocity of propagation and k is the wave number. We are working with complex numbers but the solution to the function can not be a complex number because it has a physical meaning.

We can define the phase as the function inside the exponential.

$$\phi(x,t) = kx - \omega t \tag{2.2}$$

If we set ϕ constant we will be "riding" the wave.

2.2 Energy and momentum

We are interested in see what happens among time and space in this function, so we are going to differentiate.

$$\begin{aligned} \frac{d}{dt}\psi(x,t) &= -i\omega e^{i(kx-\omega t)} \\ \frac{d}{dx}\psi(x,t) &= ike^{i(kx-\omega t)} \end{aligned} \tag{2.3}$$

We choose to work with one dimension but everything could have been done in three dimensions just using x and k as vectors.

Now we are going to do some assumptions.

$$\begin{aligned} E &= \hbar\omega = i\hbar\frac{d}{dt} \\ P &= \hbar k = -i\hbar\vec{\nabla} \end{aligned} \tag{2.4}$$

We can define the energy as some constant ($\hbar$) times the frequency. If we use the same constant and multiply it to the wave number we get something with units of momentum, so we can call it momentum.

The second term in both expression is what we call energy and momentum operator.

We now from classical mechanics that energy and momentum are related.

$$E = \frac{P \cdot P}{2m} + v \tag{2.5}$$

In the previous chapter we got the expression of the energy, with which we can get the position at any time if the are some initial conditions given.

In the same way, if $\psi(\vec{x}, 0)$ is given we can compute $\psi(\vec{x}, t)$ using the energy and momentum operators.

2.3 P(x) function I: Definition and properties

Experimentally describe a particle at rest. If we plot the position measure we will get different answers for the same experiment.

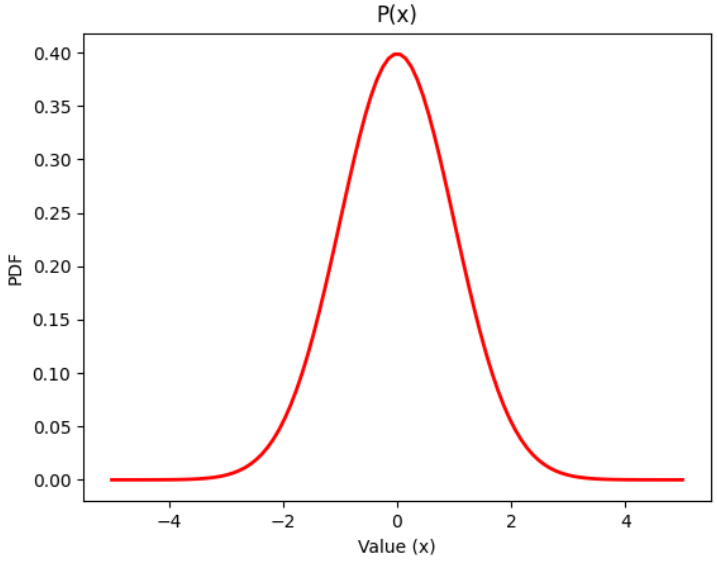

Figure 2.1: Normal distribution for mean=0 and sigma=1, to simulate a experiment measured by different people

*Uncertainty is not probability

In wave mechanics P(x) should be interpreted as $\psi^2(x, 0)$.

We can define P(x) as a Gaussian distribution with an undetermined constant.

$$P(x) = Ae^{-\frac{x^2}{2\sigma^2}} \tag{2.6}$$

We also make the next choice to define P(x):

$$\int_{-\infty}^{\infty} P(x)dx = 1 \tag{2.7}$$

We are going to ignore the constant for now to keep things simpler.

$$I = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx \tag{2.8}$$

$\Re[\alpha] > 0, \alpha \in \mathbb{C}$

We need to resolve the integral of P(x), but it is not a direct integral and is difficult to resolve it directly. Luckily we can use a trick to resolve this integral.

$$\begin{aligned} I^2 &= \left[\int_{-\infty}^{\infty} e^{-\alpha x^2} dx\right]\left[\int_{-\infty}^{\infty} e^{-\alpha y^2} dy\right] = \\ &= \int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2)} dx dy = \\ &= \int_0^{2\pi} d\theta \int_0^{\infty} r e^{-\alpha r^2} dr = \\ &= 2\pi \frac{-1}{2\alpha}\left[e^{-\alpha r^2}\right]_0^{\infty} = \frac{\pi}{\alpha} \end{aligned} \tag{2.9}$$

dxdy = rdrdθ

If we want 2.7 to be true we need to normalize it using the result from 2.9.

$$A = \sqrt{\frac{\alpha}{\pi}} \qquad where \qquad \alpha = \frac{1}{2\sigma^2} \tag{2.10}$$

We get that the final value of our P(x) function is:

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}} \tag{2.11}$$

We will continue with this later but first, we need to define Fourier Series.

2.4 Fourier Series

If we have a periodic function with length L so f(x) = f(x+L), then we can rewrite any function in this way:

$$f(x) = \sum_{k=0}^{N} \tilde{f}_k \psi_k(x) \tag{2.12}$$

Where $\psi_k(x)$ follow the next statements.

$$\begin{aligned} &1)\ \psi_k(x) = \frac{1}{\sqrt{L}} e^{i\frac{2\pi k}{L}x} \\ &2)\ \int_0^L \psi_k^{\star}(x)\psi_{k'}(x) = \delta_{k,k'} \end{aligned} \tag{2.13}$$

δ is a Dirac delta

Using Fourier analysis we can rewrite our wave function into:

$$\psi(x) = \sqrt{P(x)} = \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx} dk \tag{2.14}$$

If now we set some equations for $\psi(x)$.

$$\begin{aligned} &1)\ Dom[\psi(x)] = \left(\frac{-L}{2}, \frac{L}{2}\right) \\ &2)\ \psi(\frac{L}{2}) = \psi(\frac{-L}{2}) \\ &3)\ \psi(x) = e^{ikx} = e^{i\frac{2\pi n}{L}x} \end{aligned} \tag{2.15}$$

We defined a orthogonal function g_n.

$$\begin{aligned} g_n(x) &= \frac{1}{\sqrt{L}} e^{i\frac{2\pi}{L}nx} \\ \int_{\frac{-L}{2}}^{\frac{L}{2}} g_n^{\star}(x) g_l(x) dx &= \frac{1}{L} \int_{\frac{-L}{2}}^{\frac{L}{2}} e^{i\frac{2\pi x}{L}(l-n)} dx = \delta_{l,n} \end{aligned} \tag{2.16}$$

$\delta_{l,n}$ is called Kronecker delta, this function is 1 when l = n and 0 for any other values

We can use this function to rewrite $\psi(x)$

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} \tilde{\psi}_n g_n(x) \\ \psi(x) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \frac{2\pi}{L} e^{i\frac{2\pi n}{L}x} \tilde{\psi}_n \end{aligned} \tag{2.17}$$

The last expression in 2.17 is a Riemann sum so we can turn that expression into an integral.

$$\psi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx} dk \tag{2.18}$$

We can find also an expression for $\tilde{\psi}_n$.

$$\begin{aligned}
&\int_{\frac{-L}{2}}^{\frac{L}{2}} \psi(x) g_l^\star(x) dx = \\
&= \frac{1}{\sqrt{L}} \sum_{-\infty}^{\infty} \tilde{\psi}_n \int_{\frac{-L}{2}}^{\frac{L}{2}} g_n(x) g_l^\star(x) dx = \\
&= \frac{1}{\sqrt{L}} \sum_{-\infty}^{\infty} \tilde{\psi}_n \delta_{n,l} = \frac{1}{\sqrt{L}} \tilde{\psi}_l \qquad (2.19) \\
&\tilde{\psi}_l = \sqrt{L} \int_{\frac{-L}{2}}^{\frac{L}{2}} \psi(x) g_l^\star(x) dx \\
&\tilde{\psi}_l = \int_{\frac{-L}{2}}^{\frac{L}{2}} \psi(x) e^{-i\frac{2\pi l}{L}x} dx
\end{aligned}$$

If we extend to the limit where L approximate infinity we can get a general solution for $\tilde{\psi}(x)$.

$$\tilde{\psi}(k) = \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \qquad (2.20)$$

We have two different relations between $\psi(x)$ and $\tilde{\psi}(k)$, we need to make sure this two relations make sense together. To do this we are going to use 2.20 and 2.18.

$$\begin{aligned}
\psi(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \psi(y) e^{-iky} dy \right] e^{ikx} dk = \\
&= \int_{-\infty}^{\infty} \psi(y) \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} dk \right] dy \qquad (2.21) \\
\psi(x) &= \int_{-\infty}^{\infty} \psi(y) \delta(x-y) dy
\end{aligned}$$

The last equation we get from 2.21 is the definition of the Dirac delta function itself so we prove that both expressions we have are right.

2.5 P(x) function II: $\psi(x)$ and $\tilde{\psi}(k)$

We recover the equation 2.11 and know we get $\psi(x)$ remembering that $\psi^2(x) = P(x)$.

$$\psi(x) = \sqrt{P(x)} = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma^2}} \qquad (2.22)$$

We can also define $\tilde{\psi}(k)$ with 2.20.

$$\tilde{\psi}(k) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \int_{-\infty}^{\infty} e^{\frac{-x^2}{4\sigma^2} - ikx} dx \qquad (2.23)$$

This integral is not easy to resolve, but we can get something similar to 2.8 and we already know the solution for that integral.

$$\begin{aligned} &\frac{x^2}{4\sigma^2} + ikx = \frac{1}{4\sigma^2}[x^2 + 4i\sigma^2 kx] = \\ &= \frac{1}{4\sigma^2}[(x + 2i\sigma^2 k)^2 + 4\sigma^4 k^2] \\ &e^{\frac{-x^2}{4\sigma^2} - ikx} = e^{-\sigma^2 k^2} e^{-\frac{1}{4\sigma^2}(x+2i\sigma^2 k)^2} \end{aligned} \tag{2.24}$$

This expression can be used in 2.26 to resolve the integral doing a variable change ($\tau = x + 2i\sigma^2 k$).

$$\tilde{\psi}(k) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\sigma^2 k^2} \int_{-\infty}^{\infty} e^{-\frac{\tau^2}{4\sigma^2}} d\tau \tag{2.25}$$

We are not going to explain why $\infty + 2i\sigma^2 k = \infty$ and $-\infty + 2i\sigma^2 k = -\infty$, so the limits do not change. This can be prove with some complex analysis.

Now we can resolve this integral because we already know the solution from 2.8

$$\tilde{\psi}(k) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\sigma^2 k^2} \sqrt{4\sigma^2\pi} = 2^{\frac{3}{4}} \pi^{\frac{1}{4}} \sigma^{\frac{1}{2}} e^{-\sigma^2 k^2} \tag{2.26}$$

2.6 Free particle

If we set up the problem as a particle.

For t = 0:

- x = 0
- v = 0

Then x(t) = 0. Also if E or p are given instead of v we can resolve the problem for x(t)

If we interpret the free particle as a wave, using the knowledge from section 2.2 we will find a equation that describe the motion of the wave. First, we want to find a relation between w and k. We can get this equation using 2.4 and 2.5. Because we are working with a free particle $\nu = 0$

$$\omega = \frac{\hbar k^2}{2m} \tag{2.27}$$

The motion function can be found also using 2.4 and 2.5

$$\left(i\hbar \frac{d}{dt}\right)\psi = \frac{1}{2m}\left(-i\hbar \frac{d}{dx}\right)^2 \psi \tag{2.28}$$

We define P(x,0) as a gaussian function as we did in previous chapters.

$$P(x,0) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{2.29}$$

This P(x,t) function is what we called intensity of the wave, the question now is: if the wave is free ($\psi = \psi(x,t)$), what is P(x,t) ?

We know from the previous chapter the solutions for $\psi(x,0)$ and $\tilde{\psi}(x,0)$ when P(x,0) is a gaussian.

$$\psi(x,0) = \frac{1}{\sqrt[4]{2\pi\sigma^2}} e^{\frac{x^2}{4\sigma^2}} \tag{2.30}$$

$$\tilde{\psi}(k) = 2^{\frac{3}{4}} \pi^{\frac{1}{4}} \sigma^{\frac{1}{2}} e^{-\sigma^2 k^2} \tag{2.31}$$

If $\psi(x,0)$ is interpreted as amplitude at x, $\tilde{\psi}(k)$ can be interpreted as amplitude at k. Also, we can define a intensity of k where $P(k) = \tilde{\psi}^2(k)$

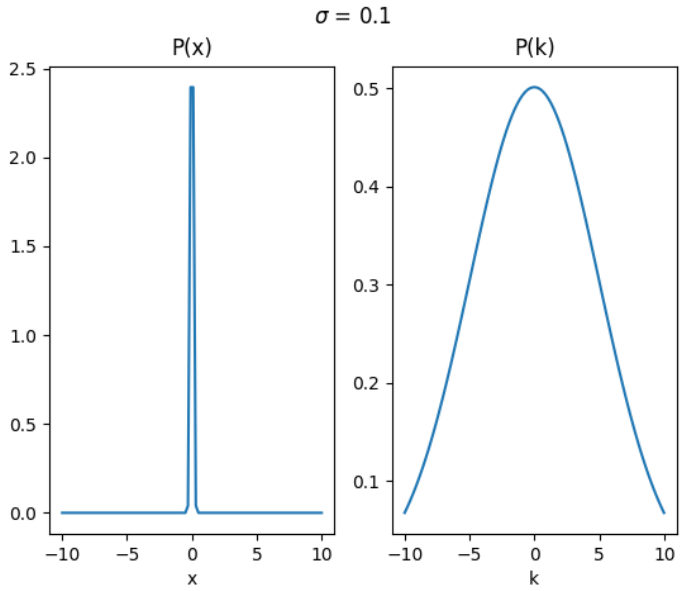

Figure 2.2: P(x) and P(k) for $\sigma = 0.1$.

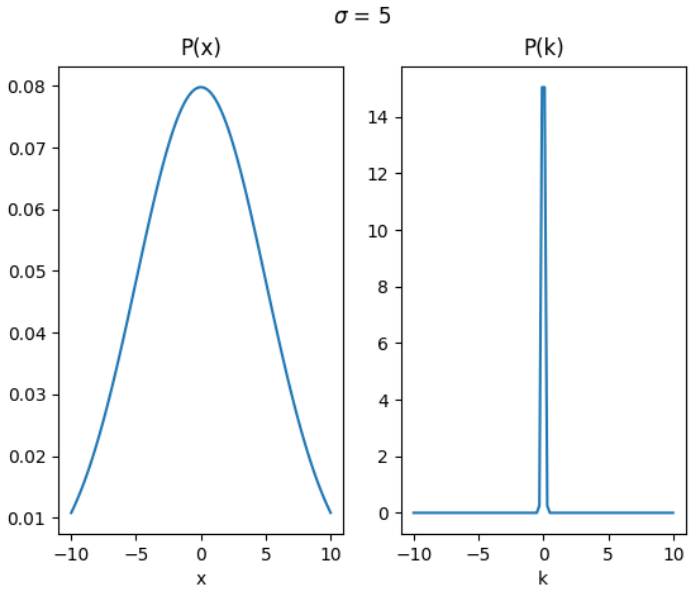

Figure 2.3: P(x) and P(k) for $\sigma = 5$.

In this page we can see two different figures. In Figure 2.2 we have a

very accurate result for the x value and a more deviated value for k while in Figure 2.3 is completely the opposite. This is a preamble to the uncertainty principle, however we still haven´t talk about quantum physics, this is just wave mechanics.

We need to get the expression among the time.

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} 2^{\frac{3}{4}}\pi^{\frac{1}{4}}\sigma^{\frac{1}{2}}e^{-\sigma^2k^2}e^{ikx}e^{-i\frac{\hbar k^2}{2m}t}dk \tag{2.32}$$

This integral is not easy to resolve so we need to work the exponent.

$$\begin{aligned}
&-\sigma^2k^2 - i\frac{\hbar k^2}{2m}t + ikx = \\
&= -(\sigma^2 + \frac{i\hbar t}{2m})k^2 + ikx = \\
&= -(\sigma^2 + \frac{i\hbar t}{2m})(k^2 - \frac{ikx}{\sigma^2 + \frac{i\hbar t}{2m}}) = \\
&= -(\sigma^2 + \frac{i\hbar t}{2m})(k - \frac{ix}{2(\sigma^2 + \frac{i\hbar t}{2m})})^2 + \frac{x^2}{4(\sigma^2 + \frac{i\hbar t}{2m})^2}
\end{aligned} \tag{2.33}$$

We get a similar exponent to the ones we work with where $\alpha = -(\sigma^2 + \frac{i\hbar t}{2m})$ and my variable is $\tau = k - \frac{ix}{2(\sigma^2+\frac{i\hbar t}{2m})}$

Using this to resolve 2.32 we can get a final expression for $\psi(x,t)$.

$$\begin{aligned}
\psi(x,t) &= \frac{1}{2\pi}2^{\frac{3}{4}}\pi^{\frac{1}{4}}\sigma^{\frac{1}{2}}\frac{\pi^{\frac{1}{2}}}{(\sigma^2 + \frac{i\hbar t}{2m})^{\frac{1}{2}}}e^{\frac{-x^2}{4(\sigma^2+\frac{i\hbar t}{2m})}} = \\
&= \left(\frac{\sigma^2}{2\pi(\sigma^2 + \frac{i\hbar t}{2m})^2}\right)^{\frac{1}{4}} e^{-\frac{x^2}{4(\sigma^2+\frac{i\hbar t}{2m})}}
\end{aligned} \tag{2.34}$$

We can calculate P(x,t) knowing ψ(x,t).

$$\begin{aligned}
P(x,t) &= \frac{\sigma}{\sqrt{2\pi}(\sigma^4 + \frac{\hbar^2t^2}{4m^2})^{\frac{1}{2}}}e^{\frac{-x^2}{4}\left(\frac{1}{\sigma^2+\frac{ikt}{2m}} + \frac{1}{\sigma^2-\frac{ikt}{2m}}\right)} = \\
&= \frac{1}{\sqrt{2\pi\sigma^2(1 + \frac{\hbar^2t^2}{4m^2\sigma^4})}}e^{\frac{-x^2}{2\sigma^2}\left(\frac{1}{1+\frac{k^2t^2}{4m^2\sigma^4}}\right)}
\end{aligned} \tag{2.35}$$

We can get the final result of P(x,t) from this equations.

$$P(x,t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}}e^{-\frac{x^2}{2\sigma^2(t)}} \tag{2.36}$$

$$\sigma(t) = \sigma\sqrt{1 + \frac{\hbar^2t^2}{4m^2\sigma^4}} \tag{2.37}$$

We define the characteristic time (τ) as a property of the experiment itself.

$$\tau = \frac{m\sigma^2}{\hbar} \tag{2.38}$$

2.7 Examples

As we did in the first chapter we want to get some real values for this equations. We will find and plot the P(x,t) and $\sigma(t)$ for 3 problems: the earth, the electron and a neutrino.

Earth problem: We want to measure the position of the planet earth. Our data for this problem is:

- $m = 5.97 \cdot 10^{24} kg$
- $\sigma_0 = 10\%$
- $\hbar = 1.05 \cdot 10^{-34} J/s$

We want to know the characteristic time first.

$$\tau = \frac{5.97 \cdot 10^{24} \cdot 0.1^2}{1.05 \cdot 10^{-34}} = 5.69 \cdot 10^{56} s \tag{2.39}$$

We can plot now in steps of τ the function $\sigma(t)$.

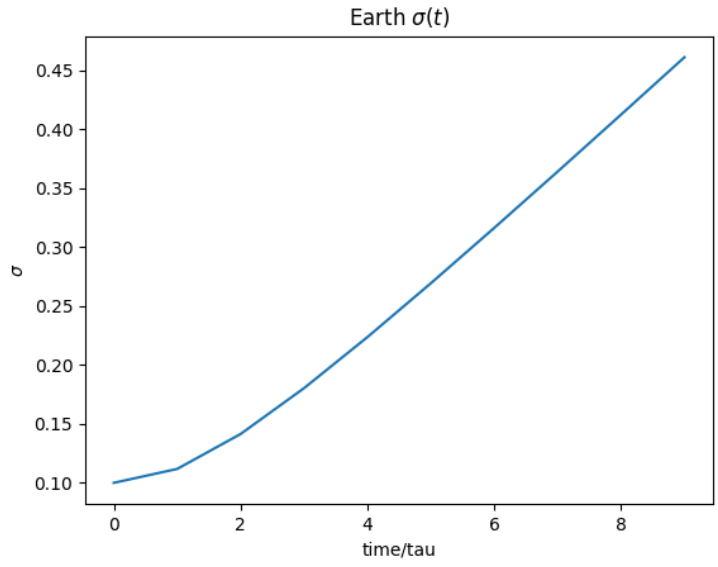

Figure 2.4: Function $\sigma(t)$ for the Earth experiment

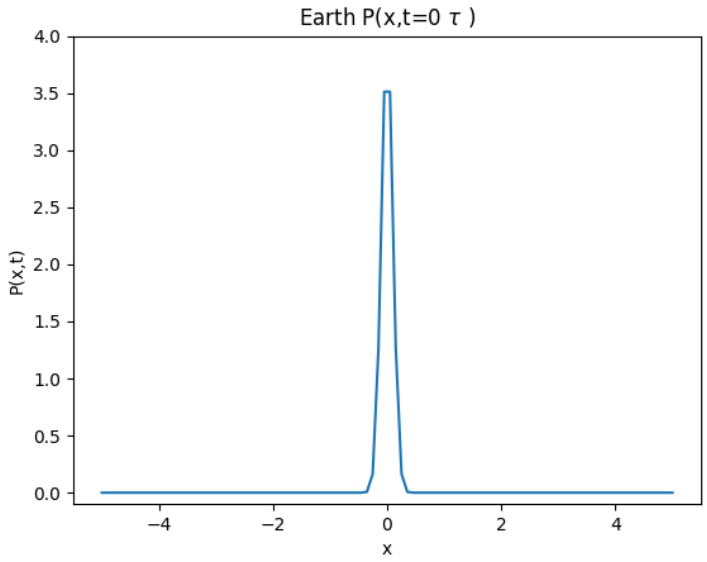

Figure 2.5: Gif for P(x,t) of the Earth experiment

Electron problem: We want to measure the position of an electron. Our data for this problem is:

- $m = 9.11 \cdot 10^{-31} kg$
- $\sigma_0 = 10\%$
- $\hbar = 1.05 \cdot 10^{-34} J/s$

We want to know the characteristic time first.

$$\tau = \frac{9.11 \cdot 10^{-31} \cdot 0.1^2}{1.05 \cdot 10^{-34}} = 86.76s \tag{2.40}$$

We can plot now in steps of τ the function $\sigma(t)$.

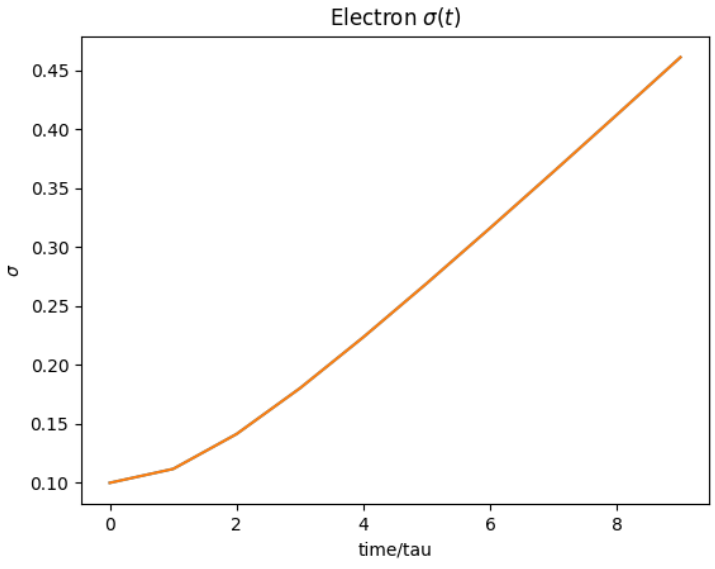

Figure 2.6: Function $\sigma(t)$ for the Electron experiment

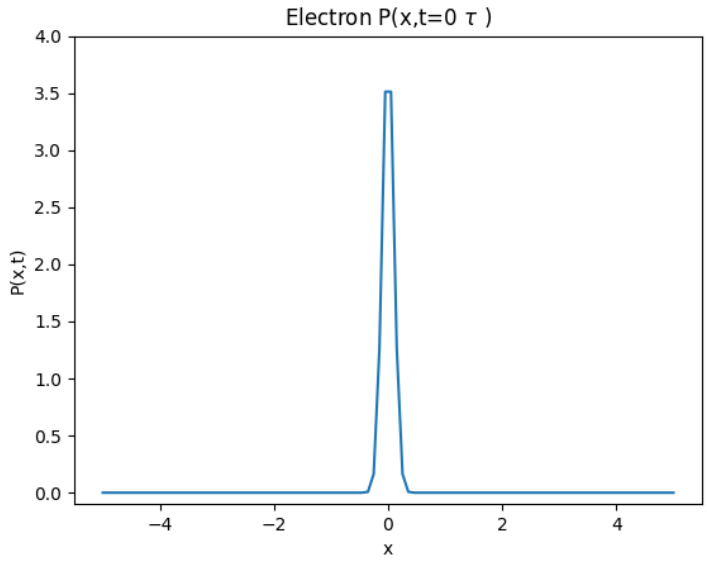

Figure 2.7: Gif for P(x,t) of the Electron experiment

At a first view the figures for the Earth and the Electron seems similar but we have to think that we are using the characteristic time as a step so the scale is completely different, while the electron functions evolve significantly in less than 100 seconds, the Earth function is changing in an order of 10^{56} seconds (MORE THAN THE AGE OF THE UNIVERSE!!).

Neutron problem: In this experiment we are going to measure the position of a neutron before it decays. A neutron has an average life time of 879 seconds. In this case because we know the scale of time we want to work with we won't calculate the characteristic time now. The data for this experiment is:

- $m = 1.67 \cdot 10^{-27} kg$
- $\sigma_0 = 10\%$
- $\hbar = 1.05 \cdot 10^{-34} J/s$

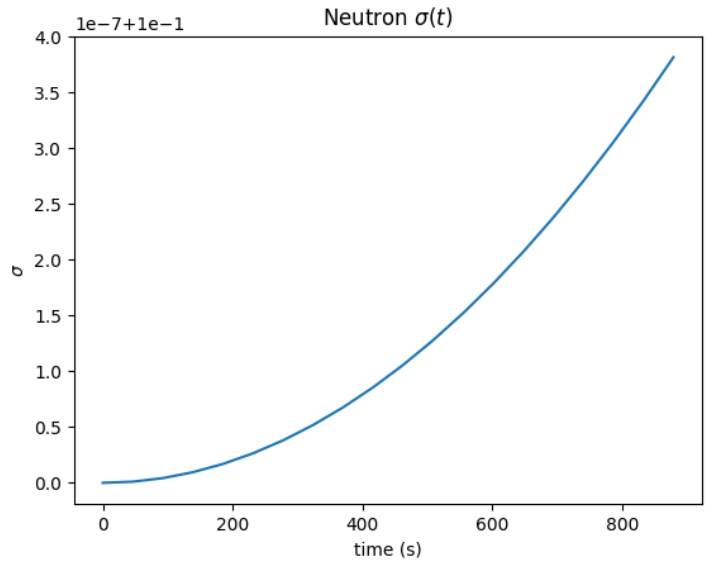

Figure 2.8: Function $\sigma(t)$ for the Neutron decay

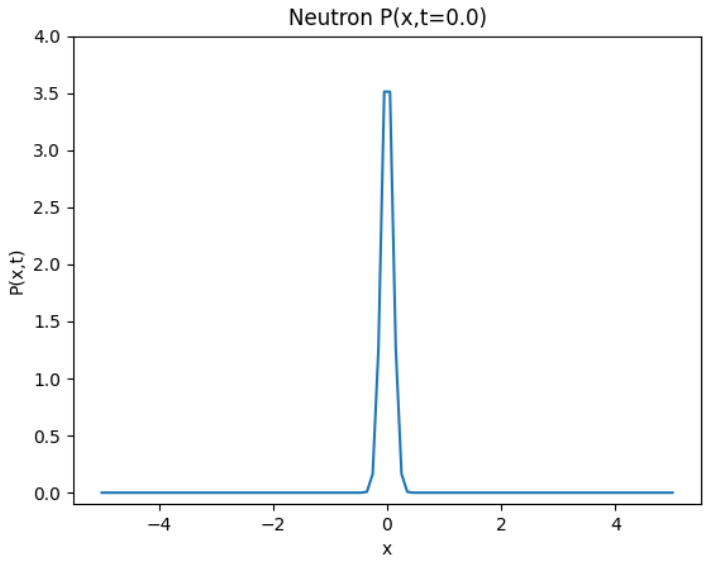

Figure 2.9: Gif for P(x,t) of the Neutron decay

In this case we can not appreciate a change in this scale of time. The neutron decays to fast to get an important change in his intensity. But how fast, is to fast? We can calculate the characteristic time to answer this question.

$$\tau = \frac{1.67 \cdot 10^{-27} 0.1^2}{1.05 \cdot 10^{-34}} = 1.59 \cdot 10^5 s \tag{2.41}$$

We can appreciate in this equation that the characteristic time is almost 10^3 times bigger than the decay time, that is why we don't get to see a change in the density function among time.

Extra problem: We want to do one more experiment. We can use this functions to know how much it would change the measure of a human. The data is:

- $m = 70kg$
- $\sigma_0 = 10\%$
- $\hbar = 1.05 \cdot 10^{-34} J/s$

We want to know the characteristic time first.

$$\tau = \frac{70 \cdot 0.1^2}{1.05 \cdot 10^{-34}} = 6.67 \cdot 10^{33} s \tag{2.42}$$

We can plot now in steps of τ the function $\sigma(t)$.

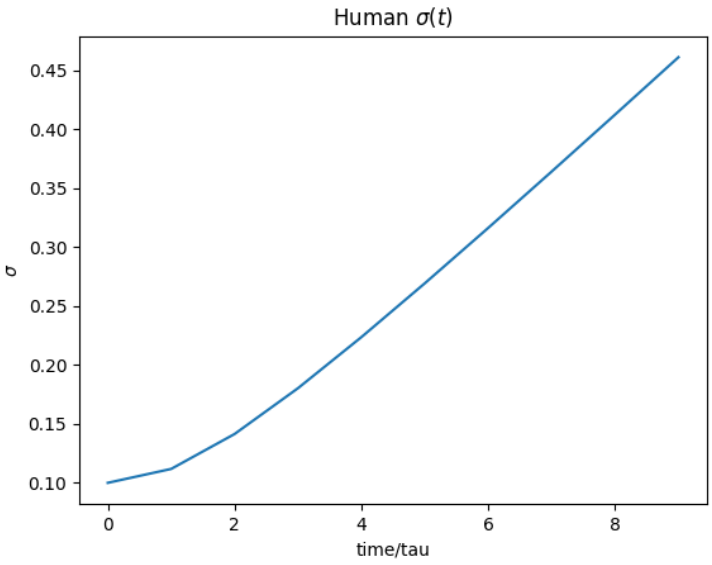

Figure 2.10: Function $\sigma(t)$ for the Electron experiment

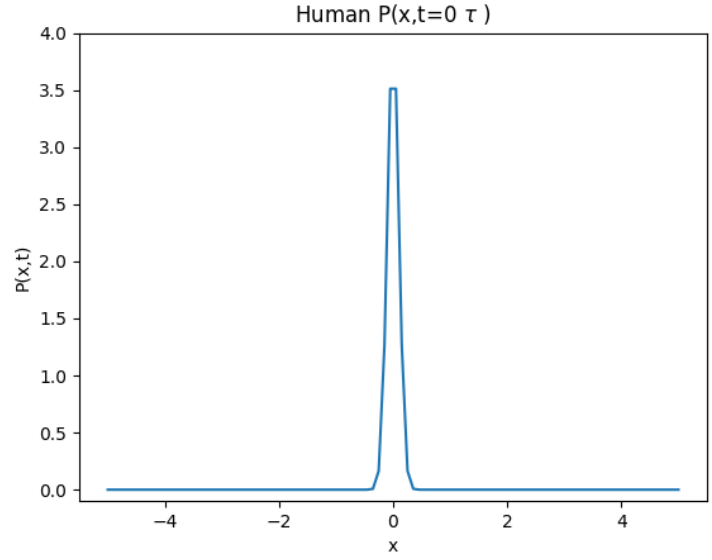

Figure 2.11: Gif for P(x,t) of the Electron experiment

Again we get something similar to the Earth and the Electron problems, but this time our step is an order of $10^{33}s$, this is still larger than the age of the universe.

A free particle is an easy example but we will start with something more difficult in the next chapter.

3 Potentials V(x,y,z)

In this chapter we will find the intensity and the ψ function of a particle under a potential.

3.1 Potential in 3 dimensions

First, we need to define our energy and our equations in 3D, this equations can be obtained from the second chapter generalizing to 3 dimensions.

$$\frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) = E \tag{3.1}$$

$$\left[-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + V(x, y, z) \right] \psi = i\hbar \frac{\partial}{\partial t} \psi \tag{3.2}$$

Where ψ is a function of space and time, i.e. $\psi = \psi(x, y, z, t)$. Before doing some operations with this equations we want to define a boundary for the intensity function. When we talk about this function in the second chapter we define a boundary in 2.7, we need to do the same but in 3 dimensions.

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(x, y, z) dx dy dz = 1 \tag{3.3}$$

For this equation to be satisfied we need to achieve this properties:

- $\lim_{x \to \infty} P(x, y, z) = 0 \; \forall y, z$
- $\lim_{y \to \infty} P(x, y, z) = 0 \; \forall x, z$
- $\lim_{z \to \infty} P(x, y, z) = 0 \; \forall x, y$

The intensity is define as $P(x, y, z, t) = \psi\psi^\star$. We have defined the intensity and we can continue now with Equation 3.2. To resolve this we will use the equation and it's conjugate and we will multiply for ψ or $\psi^\star$.

$$\begin{aligned} \psi^\star \left[-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + V \right] \psi &= i\psi^\star \hbar \frac{\partial}{\partial t} \psi \\ \psi \left[-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + V \right] \psi^\star &= -i\psi \hbar \frac{\partial}{\partial t} \psi^\star \end{aligned} \tag{3.4}$$

To continue we will subtract the first equation with the second one.

$$\begin{aligned}
&\frac{\hbar^2}{2m}\left[\psi\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi^\star-\psi^\star\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi\right]=i\hbar\left[\psi\frac{\partial}{\partial t}\psi^\star+\psi^\star\frac{\partial}{\partial t}\psi\right]\\
&\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial x}\left(\psi\frac{\partial}{\partial x}\psi^\star-\psi^\star\frac{\partial}{\partial x}\psi\right)+\frac{\partial}{\partial y}\left(\psi\frac{\partial}{\partial y}\psi^\star-\psi^\star\frac{\partial}{\partial y}\psi\right)+\right.\\
&\left.+\frac{\partial}{\partial z}\left(\psi\frac{\partial}{\partial z}\psi^\star-\psi^\star\frac{\partial}{\partial z}\psi\right)=i\hbar\left[\psi\frac{\partial}{\partial t}\psi^\star+\psi^\star\frac{\partial}{\partial t}\psi\right]\right.
\end{aligned}\tag{3.5}$$

If we integrate both sides we get that the left side is 0.

$$\begin{aligned}
&i\hbar\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\left[\psi\frac{\partial}{\partial t}\psi^\star+\psi^\star\frac{\partial}{\partial t}\psi\right]=0\\
&\frac{d}{dt}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\psi\psi^\star=0
\end{aligned}\tag{3.6}$$

This equation tell us that the total intensity must be constant among the time, so now we know the conditions of the intensity for space from 3.3 and for time.

3.2 Discontinuous Functions

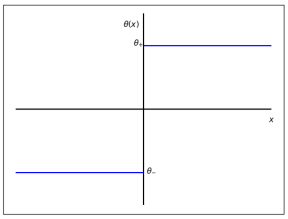

Figure 3.1: Discontinuous function with a finite jump in x = 0

We will work in one dimension only for now on to get things easier. Some potentials are discontinuous function, one of the most common example is the square well potential. We want to study this discontinuous functions and for that we will recover the delta function.

We want to prove that:

$$\frac{d\theta}{dx}=C\delta(x)\tag{3.7}$$

This equation is true if:

$$\int_{-\infty}^{\infty}f(x)\frac{d\theta}{dx}dx=f(0)C\tag{3.8}$$

Because of the definition of the delta function. To prove this and also to

get the value of C we need to operate carefully this integral.

$$\begin{aligned}
&\int_{-\infty}^{\infty}\left(\frac{d}{dx}[f(x)\theta(x)]-\theta(x)\frac{df}{dx}\right)dx = \\
&= \left[f(x)\theta(x)\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\theta}{dx}\theta(x)dx = \\
&= f(\infty)\theta_+ + f(-\infty)\theta_- + \theta_-\int_{-\infty}^{0}\frac{df}{dx}dx - \theta_+\int_{0}^{\infty}\frac{df}{dx}dx = \\
&= f(\infty)\theta_+ + f(-\infty)\theta_- + \theta_-(f(0)-f(-\infty)) - \theta_+(f(\infty)-f(0)) = \\
&= f(0)[\theta_- + \theta_+]
\end{aligned} \tag{3.9}$$

We prove that 3.7 is true and also that C is the "jump" distance in the discontinuous function.

3.3 Square Potential Well

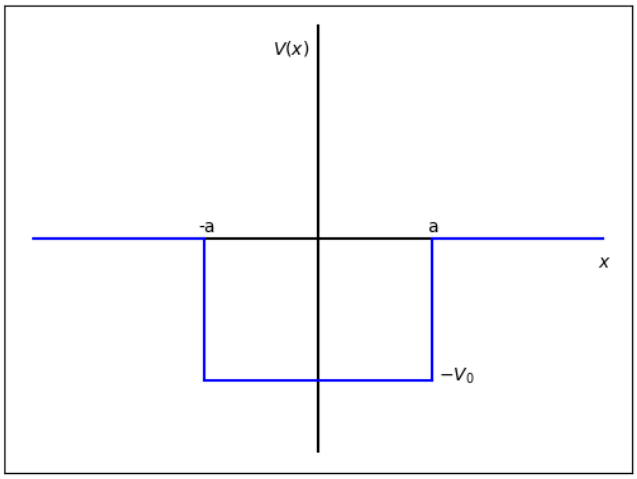

Figure 3.2: Square Potential Well

We have a potential as the one in Figure 3.2 and we want to study the intensity and the ψ function of a particle among space and time. First i have to define the potential.

$$f(x) = \frac{-dV}{dx} \tag{3.10}$$

In particle mechanics the problem will be solved with the equation of the energy.

$$E = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + V(x) = constant \tag{3.11}$$

In wave mechanics is more complex we will get the Schrödinguer Wave Equation for one dimension.

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{3.12}$$

Let's consider one solution to this equation.

$$\psi(x,t) = \phi(x)e^{-i\frac{E}{\hbar}t} \tag{3.13}$$

Where $\phi(x)$ is a real function, if we remember we solved $\phi(x)$ for the free particle problem and it was a exponential.

$$\phi(x) = e^{ikx} \tag{3.14}$$

This function does not fulfill equation 3.3.

$$\int_{-\infty}^{\infty}\phi^{\star}(x)\phi(x)dx = \infty \tag{3.15}$$

This means that we only have solutions if $V(x) \neq 0$.

Using our knowledge on the previous section we can get an expression for f(x).

$$f(x) = \frac{-dV}{dx} = -[(-V_0 - 0)\delta(-a) + (0 - (-V_0))\delta(a)] = V_0\delta(-a) - V_0\delta(a) \tag{3.16}$$

We want to redefine the energy, so we do not get stuck with the signs.

Energy = - E where E > 0

For a bound state $0 < E < V_0$ must be true. This is a bound state because is similar to the first chapter example when we said that a negative energy implies a closed orbit because the particle must be between the r_{min} and the r_{max} for the energy to be constant, this is exactly the same, but because is in one dimension the particle should bounce between the potential well in a classical approach.

We need now to rewrite the wave equation and the solution.

$$\psi(x,t) = \phi(x)e^{i\frac{E}{\hbar}t} \tag{3.17}$$

$$-E\phi(x) = \frac{-\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) \tag{3.18}$$

So the equation for the three different parts of the potential are:

$$\begin{aligned}
\frac{d^2\phi}{dx^2} &= \frac{2mE}{\hbar^2}\phi && where\ x < -a \\
\frac{d^2\phi}{dx^2} &= -\frac{2m(V_0 - E)}{\hbar^2}\phi && where\ -a < x < a \\
\frac{d^2\phi}{dx^2} &= \frac{2mE}{\hbar^2}\phi && where\ x > a
\end{aligned} \tag{3.19}$$

We need to resolve this equations. The solution to this equations are exponential for the first and the third intervals and an addition of a sine and a cosine function.

For the exponential functions we are going to define the exponent as α. Because the differential ecuation implies a second derivative this means that the exponential can be $-\alpha$ or $+\alpha$, this sign is going to depend on the equation 3.3. We are also going to define β as the argument of the sine and cosine functions.

$$\begin{aligned}
\alpha &= a\sqrt{\frac{2mE}{\hbar^2}} \\
\beta &= a\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \\
\gamma^2 &= \beta^2 + \alpha^2 = a^2\frac{2mV_0}{\hbar^2}
\end{aligned} \tag{3.20}$$

We have also defined gamma, that is a constant of the problem (does not depend on the energy) and is going to be useful to determine the values of α and β after we solve the equations.

We can solve now our differential equations.

$$\psi(x) = \begin{cases} Ae^{\frac{-\alpha}{a}x} & x > a \\ B\sin(\frac{\beta}{a}x) + C\cos(\frac{\beta}{a}x) & -a < x < a \\ De^{\frac{\alpha}{a}x} & x < -a \end{cases} \tag{3.21}$$

Now we need to use the boundary conditions. We already know that 3.3 must be true and we will use that condition later, but we also know that ϕ must be continuous because we define it as a continuous function and the first derivative must be continuous also because if not, then we will have Dirac's delta functions in the wave equation that can not cancel with anything. So we have two boundary conditions that will became 4 equations. But before we will do some changes in 3.21 to get easier

equations later.

$$\psi(x) = \begin{cases} Ae^{\frac{-\alpha}{a}x} & x > a \\ Be^{-\alpha}\sin(\frac{\beta}{a}x) + Ce^{-\alpha}\cos(\frac{\beta}{a}x) & -a < x < a \\ De^{\frac{\alpha}{a}x} & x < -a \end{cases} \tag{3.22}$$

The continuity conditions can be set now.

$$\begin{aligned} D &= -Bsin(\beta) + Ccos(\beta) \\ A &= Bsin(\beta) + Ccos(\beta) \\ D\alpha &= B\beta cos(\beta) + C\beta sin(\beta) \\ -A\alpha &= B\beta cos(\beta) - C\beta sin(\beta) \end{aligned} \tag{3.23}$$

This is a homogeneous system, so one of the solutions is A=B=C=D=0 but this solution is not allowed. If we solved for this we will get two equations that actually imply 4 equations.

$$\begin{aligned} C(\alpha cos(\beta) - \beta sin(\beta)) &= 0 \\ B(\alpha sin(\beta) + \beta cos(\beta)) &= 0 \end{aligned} \tag{3.24}$$

If B = C = 0, A and D will be 0 also and we already said that is not an option, so we have three possibilities. Let's try doing both parenthesis equal to 0 and add them multiplying by some factor.

$$\begin{aligned} &sin(\beta)(\alpha sin(\beta) + \beta cos(\beta)) + cos(\beta)(\alpha cos(\beta) - \beta sin(\beta)) = 0 \\ &\alpha sin^2(\beta) + \alpha cos^2(\beta) = 0 \end{aligned} \tag{3.25}$$

With our choice the solution is $\alpha = 0$ but α can not be 0, so we only have two choices both of them are right.

If we take a look at this dependency between α and β and we include our gamma equation to the chart we would see something interesting.

$$\begin{aligned} \alpha &= -\beta\cot(\beta) \\ \alpha &= \beta\tan(\beta) \\ \gamma^2 &= \alpha^2 + \beta^2 \end{aligned} \tag{3.26}$$

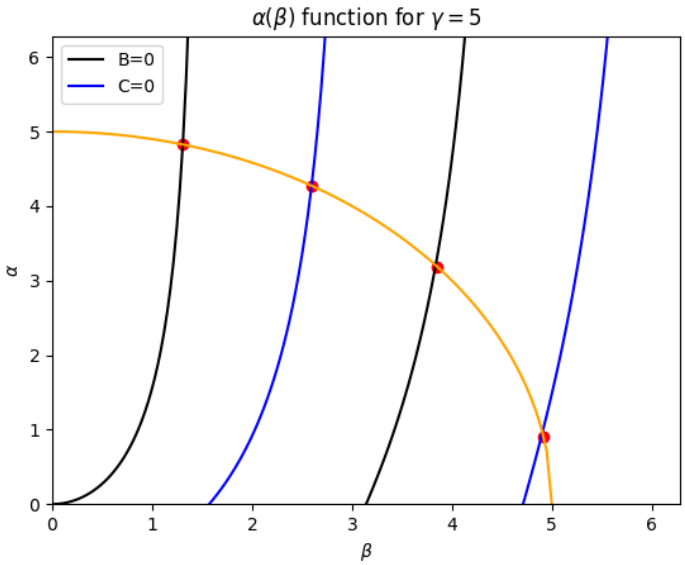

Figure 3.3: α as a function of β for $\gamma = 5$

This proves that the energy is quantized because only some values for α (that is a function of Energy) are possible.

And the solutions are:

Solution for C = 0

$$\begin{aligned} A &= Bsin(\beta) \\ B &= B \\ C &= 0 \\ D &= -Bsin(\beta) \end{aligned} \tag{3.27}$$

Solution for B = 0

$$\begin{aligned} A &= Ccos(\beta) \\ B &= 0 \\ C &= C \\ D &= Ccos(\beta) \end{aligned} \tag{3.28}$$

We still have one variable left to resolve, to do this we will need to use 3.3. We will resolve only for the case B = 0, the other one will turn the

same.

$$
\begin{aligned}
&\int_{-\infty}^{\infty} \phi^2(x)dx = \\
&= C^2 \left[cos^2(\beta) \int_{-\infty}^{-a} e^{\frac{2\alpha}{a}x} dx + e^{-2\alpha} \int_{-a}^{a} cos^2(\frac{\beta}{a}x)dx + cos^2(\beta) \int_{a}^{\infty} e^{-\frac{2\alpha}{a}x} dx \right] = \\
&= C^2 \left[cos^2(\beta) \frac{a}{2\alpha} \left[e^{\frac{2\alpha}{a}x} \right]_{-\infty}^{-a} + \frac{e^{-2\alpha}}{2} \left[\frac{a}{2\beta} sin(\frac{2\beta}{a}x) + x \right]_{-a}^{a} - cos^2(\beta) \frac{a}{2\alpha} \left[e^{\frac{2\alpha}{a}x} \right]_{a}^{\infty} \right] = \\
&C^2 a e^{-2\alpha} \left[\frac{cos^2(\beta)}{\beta \tan(\beta)} + \frac{sin(2\beta)}{2\beta} + 1 \right] = \\
&= C^2 a e^{-2\alpha} \left[\frac{1}{\alpha} + 1 \right] = 1
\end{aligned}
\tag{3.29}
$$

Now we need to resolve for C in the last step.

$$
C^2 = \frac{\alpha e^{2\alpha}}{a(1+\alpha)} \tag{3.30}
$$

If C=0 then, B^2 is equal to the expression above.

Now we can solve for everything in the problem for a given gamma.

3.4 Examples

We will plot some of the solutions for different gamma and for the largest gamma we will try to approach and explain a classical behaviour.

First example: In this case we will took gamma = 10, and plot two of the solutions, one for B=0 and the other one for C=0.

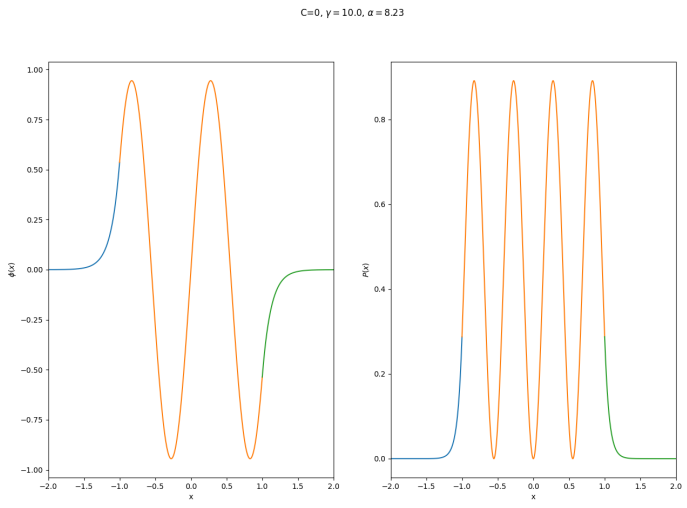

Figure 3.4: $\phi(x)$ and P(x) functions for gamma = 10

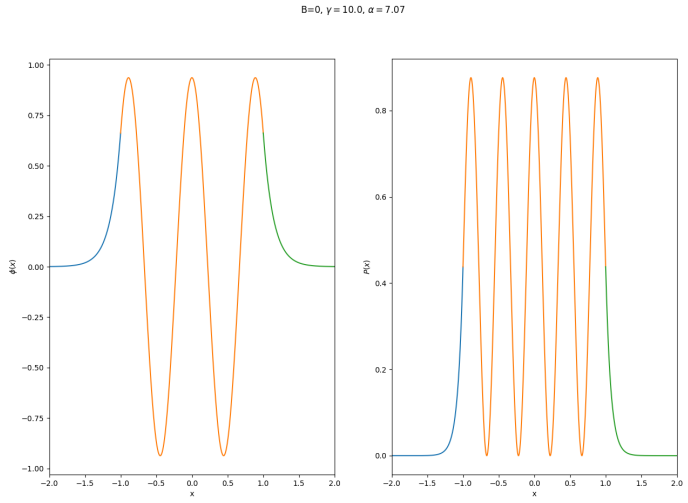

Figure 3.5: $\phi(x)$ and P(x) functions for gamma = 10

Now we will try to achieve a similar behaviour to the well-known particle approach, where all the probability is inside the square root potential and all of it is equally likely to have the particle. We can achieve this finding the P(x) function for a bigger gamma and a small alpha.

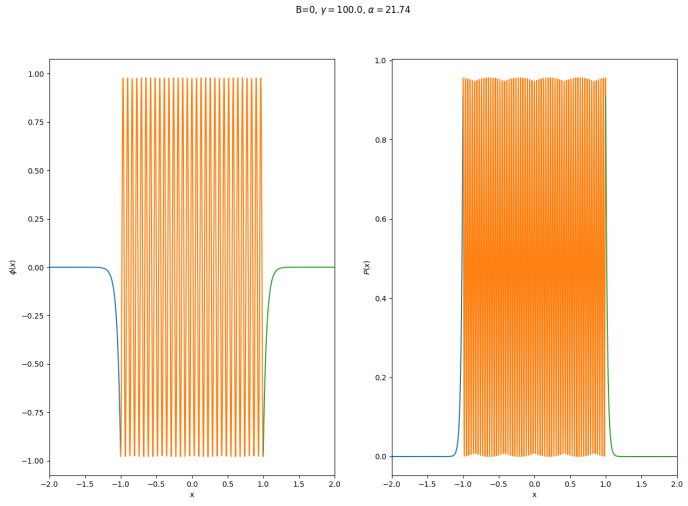

Figure 3.6: $\phi(x)$ and P(x) functions for gamma = 100

In Figure 3.6 we can see that we get what we expect for a particle behaviour but we still have that quantum behaviour because the integral outside of the square potential is not zero as it should be in the particle behaviour.

4 Delta function potential

We want to understand solids and their properties, for example why copper is a conductor and wood is not? For this and other questions we will propose our next problem, the delta function potential problem.

4.1 Definition of the potential . 33
4.2 Solution 33

4.1 Definition of the potential

We define our potential this time as

$$V(x) = -2C\delta(x) \tag{4.1}$$

Where $C = V_0 a$.

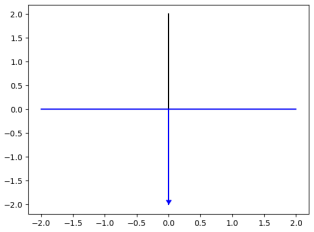

Figure 4.1: Delta function potential

Because we have delta functions in our equations we can not call them normal equations so we will use quotes to differentiate them from real equations.

$$'' + \frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + 2C\delta(x)\phi(x) = +E\phi(x)'' \tag{4.2}$$

4.2 Solution

The solution for this equation is:

$$\psi(x,t) = e^{i\frac{E}{\hbar}t}\phi(x) \tag{4.3}$$

Now we need to solve our equation for $\phi(x)$.

$$\begin{aligned} ''\frac{\partial^2\phi}{\partial x^2} + \frac{4mC}{\hbar^2}\delta(x)\phi(x) &= \frac{2mE}{\hbar^2}\phi(x)'' \\ ''\frac{\partial^2\phi}{\partial x^2} + \frac{4mV_0 a}{\hbar^2}\delta(x)\phi(x) &= \frac{2mE}{\hbar^2}\phi(x)'' \end{aligned} \tag{4.4}$$

We need to define two variables to resolve this equations, α and g (This variables are completely different to the variables in the previous chapter).

$$\begin{aligned} g &= \frac{2mV_0 a}{\hbar^2} \\ \alpha &= \sqrt{\frac{2mE}{\hbar^2}} \end{aligned} \tag{4.5}$$

As we did in the previous chapter we have to think about the continuity in $\phi(x)$. Can $\phi(x)$ be discontinuous? The answer is no. $\phi(x)$ is continuous because if it weren't continues the second derivative would look like the derivative of a delta function and the equations don't make sense with that assumption. However, in this case the first derivative of $\phi(x)$ must be discontinuous because we need the second derivative to go as a delta function.

We solve for $\phi(x) \neq 0$.

$$\frac{\partial^2 \phi(x)}{\partial x^2} = \alpha^2 \phi(x) \tag{4.6}$$

The solution to this differential equation is:

$$\phi(x) = \begin{cases} Ae^{\alpha x} & where \quad x \leq 0 \\ \\ Ae^{-\alpha x} & where \quad x \geq 0 \end{cases} \tag{4.7}$$

And the derivatives are going to be:

$$\frac{\partial \phi(x)}{\partial x} = \begin{cases} A\alpha e^{\alpha x} & where \quad x \leq 0 \\ \\ -A\alpha e^{-\alpha x} & where \quad x \geq 0 \end{cases} \tag{4.8}$$

$$''\frac{\partial^2 \phi(x)}{\partial x^2} = \begin{cases} A\alpha^2 e^{\alpha x} & where \quad x \leq 0 \\ \\ A\alpha^2 e^{-\alpha x} & where \quad x \geq 0 \end{cases} + B\delta(x)'' \tag{4.9}$$

To solve for A we are going to use the continuity conditions we mention before and the fundamental theorem of calculus.

$$\begin{gathered} \int_{-\infty}^{\infty} \frac{\partial^2 \phi(x)}{\partial x^2} dx = \left[\frac{\partial \phi}{\partial x}\right]_{x=-\infty} - \left[\frac{\partial \phi}{\partial x}\right]_{x=\infty} \\ A\alpha^2 \int_{-\infty}^{0} e^{\alpha x} dx + A\alpha^2 \int_{0}^{\infty} e^{-\alpha x} dx + B \int_{-\infty}^{-\infty} \delta(x) dx = 0 \\ A\alpha + A\alpha + B = 0 \\ B = -2A\alpha \end{gathered} \tag{4.10}$$

We want to integrate 4.4 for x=0 to remove the quotes.

$$\begin{gathered} A\alpha^2 \int_{-\infty}^{0} e^{\alpha x} dx + A\alpha^2 \int_{0}^{\infty} e^{-\alpha x} dx + = \int_{-\infty}^{\infty} \frac{\partial^2 \phi(x)}{\partial x^2} dx + 2g \int_{-\infty}^{\infty} \delta(x)\phi(x) dx \\ [\alpha A e^{\alpha x}]_{-\infty}^{0} - [\alpha A e^{\alpha x}]_{0}^{\infty} = 0 + 2g\phi(0) \\ 2\alpha A = 2gA \\ \alpha = g \end{gathered} \tag{4.11}$$

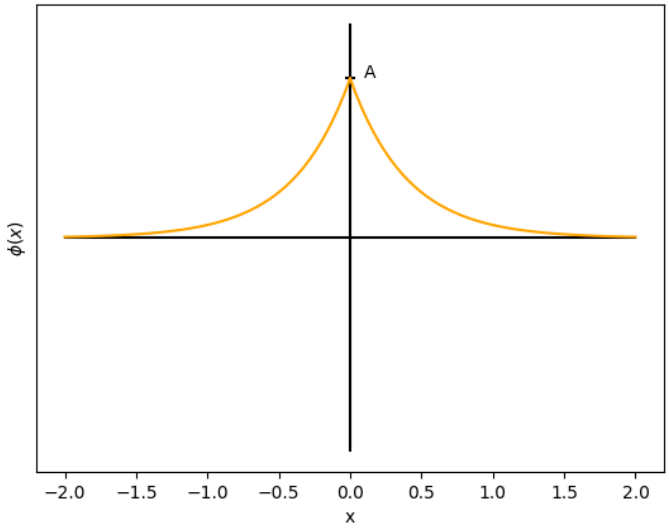

Figure 4.2: Solution for g=2.5 of phi(x) for the delta function potential.

In this case we only have one possible value for α so only one Energy level is possible. The solution to the problem is:

$$\phi(x) = \begin{cases} Ae^{gx} & x < 0 \\ Ae^{-gx} & x > 0 \end{cases} \tag{4.12}$$

$$P(x) = \begin{cases} A^2e^{2gx} & x < 0 \\ A^2e^{-2gx} & x > 0 \end{cases} \tag{4.13}$$

To solve for A we need to use the property from 3.3.

$$P(x) = \begin{cases} A^2e^{2gx} & x < 0 \\ A^2e^{-2gx} & x > 0 \end{cases} \tag{4.14}$$

$$\int_{-\infty}^{\infty} P(x)dx = 1$$

$$\frac{A^2}{g} = 1 \tag{4.15}$$

$$A^2 = g$$

We have finally solved the problem and the solution is:

$$\phi(x) = \begin{cases} \sqrt{g}e^{gx} & x < 0 \\ \sqrt{g}e^{-gx} & x > 0 \end{cases} \tag{4.16}$$

We will not do examples using this model because is not that usefull, but it will help us understand the next problem better.

Multiple potentials 5

5.1 Definition 37
5.2 Solution 38
5.3 Solutions for N = 1,2 39
5.4 Solving for x as a circunference 41
5.5 Solution for all the posible energies. 44

Until this moment we have only work with 1 potential well but if our goal is to understand solids and their properties we need to figure out how our quantum world works with multiple potential.

5.1 Definition

In this problem we will have N delta function potentials, as the one in the previous chapter, separated by a distance d, with a fix value for g of g=1. The potential can be defined as:

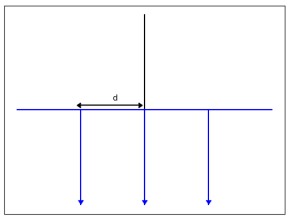

Figure 5.1: Multiple delta function potentials problem.

$$''V(x) = -2V_0 a \left[\sum_{n=1}^{N} \delta(x - nd)\right]'' \tag{5.1}$$

Using 5.1 we get the wave equation for this problem.

$$''\alpha^2\phi(x) = \frac{\partial^2\phi(x)}{\partial x^2} + 2g\left[\sum_{n=1}^{N} \delta(x - nd)\right]\phi(x)'' \tag{5.2}$$

Outside of the potentials the equation to solve will be the same as 4.6, our goal is going to be trying to find the relation between the A and B coefficients at both sides of a potential as we can see in Figure 5.2

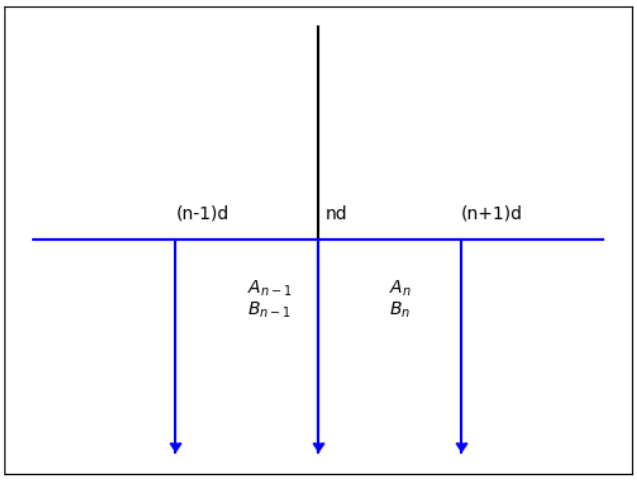

Figure 5.2: Coefficients outside of the potentials near x=nd.

5.2 Solution

We are adding the term $-nd \pm d/2$ in the exponential because it will make the math easier later.

Our potential at $x = nd$ will look like Figure 5.2 and the solution at the left and right side of the potential in x=nd will be:

$$\begin{aligned} \phi(x) &= A_{n-1}e^{-\alpha(x-[nd-\frac{d}{2}])} + B_{n-1}e^{\alpha(x-[nd-\frac{d}{2}])} \quad x < nd \\ \phi(x) &= A_n e^{-\alpha(x-[nd+\frac{d}{2}])} + B_n e^{\alpha(x-[nd+\frac{d}{2}])} \qquad x > nd \end{aligned} \tag{5.3}$$

First, if we look at the limits when n=1 and n=N we get the solutions from the previous chapter.

$$\begin{aligned} A_0 &= 0 \\ B_N &= 0 \end{aligned} \tag{5.4}$$

We will use the continuity of the function and its derivatives, as we already explain in Chapter 4, to relate the A and B coefficients.

The first condition is that $\phi(x)$ is continuous. To simplify we will use $v = e^{-\alpha\frac{d}{2}}$.

$$A_{n-1}v + \frac{B_{n-1}}{v} = \frac{A_n}{v} + B_n v \tag{5.5}$$

The second condition is our relation between the derivatives in $x = nd$ shown in 4.11

$$\begin{aligned} &[-\alpha A_{n-1}v + \alpha\tfrac{B_{n-1}}{v}] - [-\alpha\tfrac{A_n}{v} + \alpha B_n v] = 2[A_{n-1}v + \tfrac{B_{n-1}}{v}] \\ &A_{n-1}(-\alpha v - 2v) + B_{n-1}(\tfrac{\alpha}{v} - \tfrac{2}{v}) = -\alpha A_n\tfrac{1}{v} + \alpha B_n v \\ &-A_n\tfrac{1}{v} + B_n v = -vA_{n-1}(1+\tfrac{2}{\alpha}) + \tfrac{1}{v}B_{n-1}(1-\tfrac{2}{\alpha}) \end{aligned} \tag{5.6}$$

If we add and substract both conditions we will get the next equations:

$$\begin{aligned} B_n &= -\tfrac{1}{\alpha}A_{n-1} + \tfrac{1}{v^2}(1-\tfrac{1}{\alpha})B_{n-1} \\ A_n &= v^2(1+\tfrac{1}{\alpha})A_{n-1} + \tfrac{1}{\alpha}B_{n-1} \end{aligned} \tag{5.7}$$

We want to show this like a matrix.

$$\begin{pmatrix} A_n \\ \\ B_n \end{pmatrix} = \begin{bmatrix} v^2(1+\frac{1}{\alpha}) & \frac{1}{\alpha} \\ \\ -\frac{1}{v} & \frac{1}{v^2}(1-\frac{1}{\alpha}) \end{bmatrix} \begin{pmatrix} A_{n-1} \\ \\ B_{n-1} \end{pmatrix} \tag{5.8}$$

We will called this matrix T. Now we can relate any index with each other because T does not depend on n, i.e. $T = T(\alpha, d)$. Now we will

find the solutions for alpha using the relation between n=1 and n=N coefficients.

$$\begin{pmatrix} A_N \\ \\ B_N \end{pmatrix} = [T]^N \begin{pmatrix} A_0 \\ \\ B_0 \end{pmatrix} \tag{5.9}$$

To solve for alpha we will use 5.4.

$$\begin{pmatrix} A_N \\ \\ 0 \end{pmatrix} = \begin{bmatrix} (T^N)_{11} & (T^N)_{12} \\ \\ (T^N)_{21} & (T^N)_{22} \end{bmatrix} \begin{pmatrix} 0 \\ \\ B_0 \end{pmatrix} \tag{5.10}$$

For this equations to be true we get the condition, $(T^N)_{22} = 0$. This will give the solutions for alpha and will depend only on d.

However, the number of solutions for alpha will be dependent on N, i.e. the number of delta function potentials

5.3 Solutions for N = 1,2

Now that we have the general solution, we can try to get the simplest examples.

For N = 1 it will be extremely simple.

$$\frac{1}{v^2}(1 - \frac{1}{\alpha}) = 0 \tag{5.11}$$

Solving for α we get $\alpha = 1$ that exactly the value for g, this tell us that when N=1 we recover the solution from the previous chapter, wich make sense.

For N = 2 we need to square the matrix.

$$T^2 = \begin{bmatrix} v^2(1+\frac{1}{\alpha}) & \frac{1}{\alpha} \\ \\ -\frac{1}{\alpha} & \frac{1}{v^2}(1-\frac{1}{\alpha}) \end{bmatrix}^2 =$$

$$= \begin{bmatrix} v^2(1+\frac{1}{\alpha}) & \frac{1}{\alpha} \\ \\ -\frac{1}{\alpha} & \frac{1}{v^2}(1-\frac{1}{\alpha}) \end{bmatrix} \begin{bmatrix} v^2(1+\frac{1}{\alpha}) & \frac{1}{\alpha} \\ \\ -\frac{1}{\alpha} & \frac{1}{v^2}(1-\frac{1}{\alpha}) \end{bmatrix} = \tag{5.12}$$

$$= \begin{bmatrix} v^4(1+\frac{1}{\alpha})^2 - \frac{1}{\alpha^2} & \frac{1}{\alpha}[v^2(1+\frac{1}{\alpha}) + \frac{1}{v}(1-\frac{1}{\alpha})] \\ \\ -\frac{1}{\alpha}[v^2(1+\frac{1}{\alpha}) + \frac{1}{v}(1-\frac{1}{\alpha})] & -\frac{1}{\alpha^2} + \frac{1}{v^4}(1-\frac{1}{\alpha})^2 \end{bmatrix}$$

From the expresion of T_{22} we can get the solutions for alpha.

$$\begin{gathered} -\frac{1}{\alpha^2} + \frac{1}{v^4}(1-\frac{1}{\alpha})^2 = 0 \\ \pm\frac{1}{\alpha} = e^{\alpha d}(1-\frac{1}{\alpha}) \end{gathered} \tag{5.13}$$

We get two different solutions from this equation.

$$\begin{aligned} \alpha &= 1 + e^{-\alpha d} \\ \alpha &= 1 - e^{-\alpha d} \end{aligned} \tag{5.14}$$

If we plot both sides of the equations we can see two different results depending on d. If d is greater than 1 we will get two solutions if d is least than 1 we will only find one solution. This can be observe in Figure 5.3 and Figure 5.4.

As N increase with a fix d the number of alphas will increase until the discrete turns into a almost continuous behaviour. For an infinite N we will aproach a continuous energy range with posible energies. With N from 1 to 60 we can see the behaviour of the energy when d=2 and we can appreciate how the posible energies are more and more continuous for larger N.

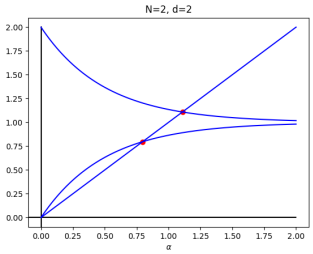

Figure 5.3: Solutions for $(T^N)_{22} = 0$ for N=2 and d=2

The solutions have been found using numerical analysis.

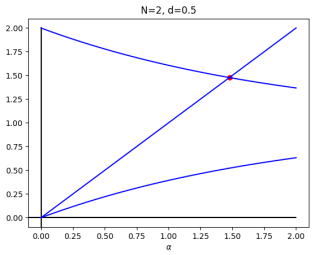

Figure 5.4: Solutions for $(T^N)_{22} = 0$ for N=2 and d=0.5

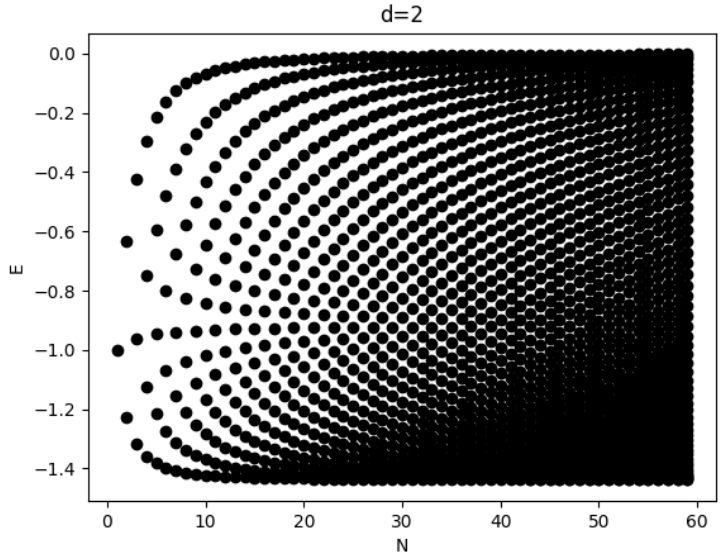

Figure 5.5: alpha as a function of N for $d = 2$.

5.4 Solving for x as a circunference

If we assume x axis is not a straight line, and instead it is inside a circunference of length L, like Figure 5.6, the math will look better and we will get some interesting new results.

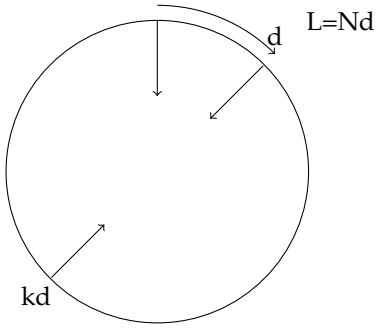

Figure 5.6: x as a circunference of distance L.

Because we have N potentials separated a distance d, we can say that $L = Nd$. When N is infinite we will have again that L is aproximately infinite and therefore the circunference will recover the straight line shape.

One of the consequences of this new aproach is that now E is not confined to only negative values. We know get a new wave equation where E is the energy.

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V(x)\phi(x) = E\phi(x) \tag{5.15}$$

We have to solve this equation with our boundaries as before, but we have new boundaries as a result of our transformation. We can use the rotation simetry to say that now our function is periodic. This give us new conditions:

$$\begin{array}{c} \phi(x+L) = \phi(x) \\ \frac{d\phi}{dx}(x+L) = \frac{d\phi}{dx}(x) \\ V(x+L) = V(x) \end{array} \tag{5.16}$$

We want to go even further and solve problems where $V(x)$ is periodic in d instead of L, i.e. $V(x+d) = V(x)$.

In this case we say, and it can be prove, that $\phi(x)$ is quasi-periodic.

$$\phi(x+d) = C\phi(x) \tag{5.17}$$

After the N potentials $\phi(x)$ must be the same again according to 5.16.

$$\phi(x + Nd) = C^N \phi(x) = \phi(x + L) = \phi(x) \tag{5.18}$$

This means that $C^N = 1$ and this lead us to N solutions for C.

$$C = e^{i\frac{2\pi}{N}k} \quad k = 0, 1, 2, ..., N-1 \tag{5.19}$$

We will solve the problem between d/2 and -d/2 as we can see in Figure 5.7

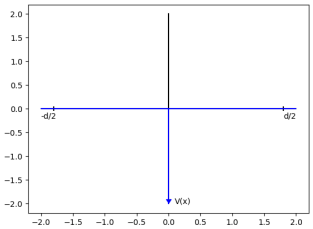

Figure 5.7: Potential between -d/2 and d/2

Outside of the potential the wave equation is:

$$\frac{d^2\phi(x)}{dx^2} = \begin{cases} \alpha^2\phi(x) & E < 0 \\ \beta^2\phi(x) & E > 0 \end{cases} \tag{5.20}$$

The solution fo this equations is the same as the one in Chapter 4, but we will change the notation, intead of terms of n we will called the coefficients A_L, B_L and A_R, B_R, for left and right of the potential.

Let's resume all the conditions.

$$\begin{aligned} &I) && \phi(d/2) = C\phi(-d/2) \\ &II) && \tfrac{\phi}{dx}(d/2) = C\tfrac{\phi}{dx}(-d/2) \\ &III) && \phi(x = 0^-) = \phi(x = 0^+) \\ &IV) && \left.\tfrac{d\phi}{dx}\right|_{x=0^-} - \left.\tfrac{d\phi}{dx}\right|_{x=0^+} = 2\phi(0) \end{aligned} \tag{5.21}$$

We have to solve for this conditions. We will use $v = e^{d\alpha/2}$ to simplify the math.

$$\begin{aligned} &I + II && B_R = \tfrac{C}{v^2} B_L \\ &I - II && A_R = Cv^2 A_L \\ &III => && (Cv^2 - 1)A_L = (1 - \tfrac{C}{v^2})B_L \\ &IV => && [-A_L\alpha + B_L\alpha] - [-A_R\alpha + B_R\alpha] = 2[A_L + B_L] \end{aligned} \tag{5.22}$$

Combining the four expresions we can get the equation to solve alpha for.

$$\cos\left(\frac{2\pi k}{N}\right) = \cosh(\alpha d) - \frac{1}{\alpha}\sinh(\alpha d) \tag{5.23}$$

If d and N are given we can get $\alpha(k)$.

To see the behaviour of the function with N we can fixed d and try to get all the solutions for alpha. We can see in Figure 5.8 how the energy range became continuous when N increase to infinite.

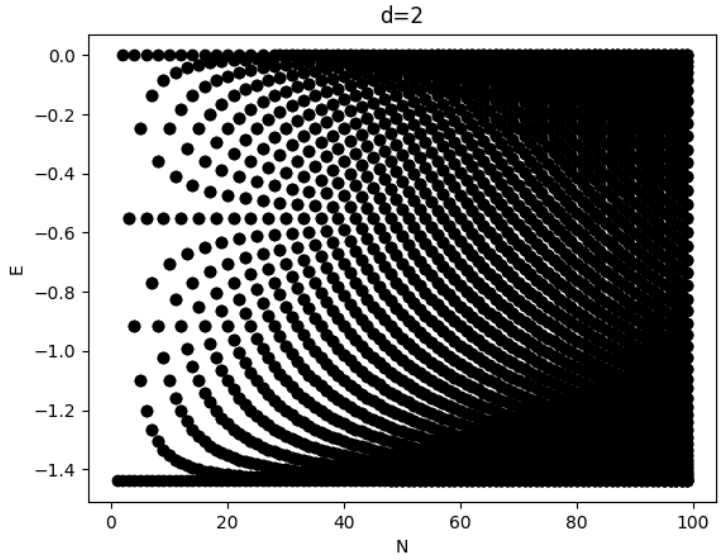

Figure 5.8: Energy as a function of the number of potentials.

In the other hand, if we want to see the behaviour of the function with d, we have to do before a numerical analisis of the function in the right side. First, we want to find the limit for $\alpha \to 0$. We will need to use Taylor expansion to solve it.

$$\begin{aligned} &\lim_{\alpha\to 0}(\cosh(\alpha d) - \tfrac{1}{\alpha}\sinh(\alpha d)) = \\ &= \cosh(0) - \lim_{\alpha\to 0}\tfrac{1}{\alpha}\tfrac{e^{\alpha d}-e^{-\alpha d}}{2} = \\ &= 1 - \lim_{\alpha\to 0}\tfrac{1}{\alpha}\tfrac{2\alpha d + o(\alpha^2)}{2} = 1 - d \end{aligned} \tag{5.24}$$

Now we want to see how the monotony of the function behaves, so we have to look at the derivative of the function. We will use taylor expansion again.

$$\begin{aligned} &\tfrac{d}{dx}\left[\cosh(\alpha d) - \tfrac{1}{\alpha}\sinh(\alpha d)\right] = \\ &= \left(\alpha + \tfrac{1}{\alpha^2}\right)\sinh(\alpha d) - \tfrac{d}{\alpha}\cosh(\alpha d) \approx \\ &\approx \alpha d^2(1 - \tfrac{d}{3}) + o(\alpha^3) \end{aligned} \tag{5.25}$$

If d is greater than 3 the function decreases first and then it increases until infinity. If d is less than 3 the function increases for all α. Is not important for us where the minimum is located, the key aspect is that if d is greater than 3 we get solutions for bigger alphas of the equation because the left function is confine in [-1,1].

In Figure 5.9 we can see that for a fixed value of N we can get all the energies depending on the distance. If we take a look into the maximum

energy we can see that for values of d greater than 2, this value starts to decrease.

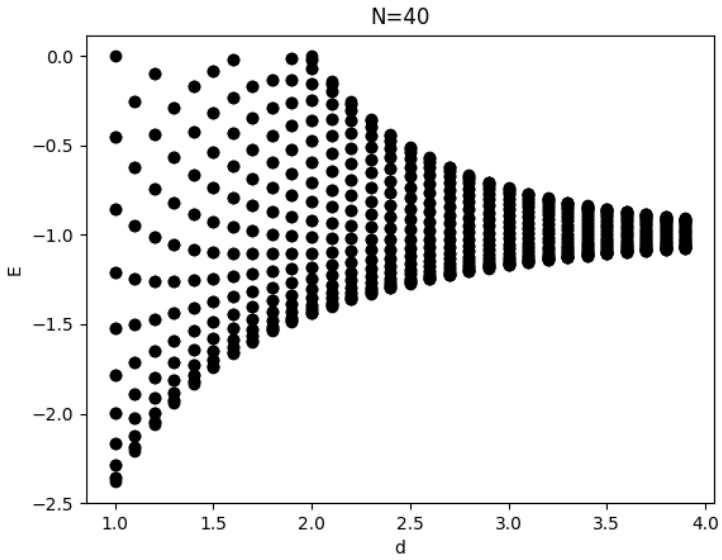

Figure 5.9: Energy as a function of the distance between potentials.

5.5 Solution for all the posible energies.

This is not the end of the chapter because as we already said, we have also positive energies. Solving for the second equation in 5.20 we get a similar equation to 5.23 but where $\beta = i\alpha$.

$$\cos\left(\frac{2\pi k}{N}\right) = \cos(\beta d) - \frac{1}{\beta}\sinh(\beta d) \tag{5.26}$$

Plotting all the solutions together, the positive and the negative ones, we can see how the energy levels behaves depending on the other two parameters, d and N. Moreover we can also see the gaps between the different energy levels.

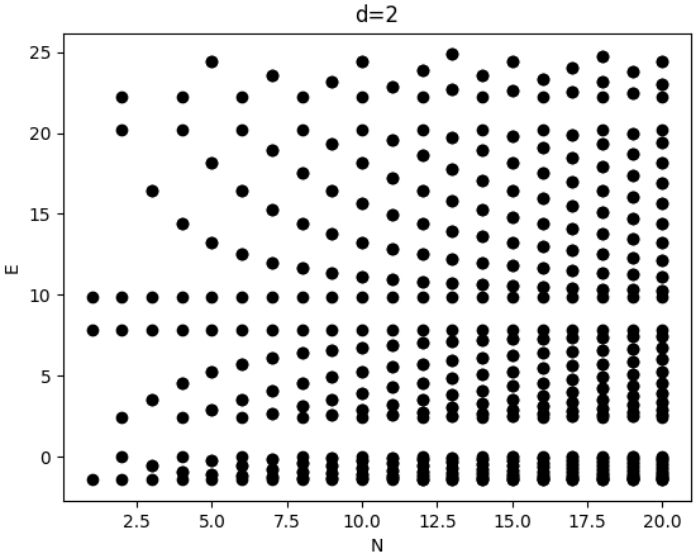

Figure 5.10: All the energies as a function of the number of potentials.

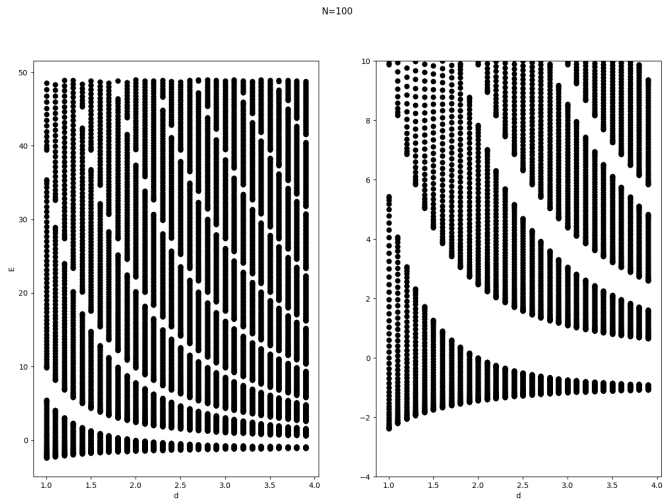

Figure 5.11: All the energies as a function of the distance between potentials.

In the figures above is appreciated how the energy levels are well define and the distance between them remain constant when we increase N.However while d goes to ifinite the width of the energy levels is decreasing.

There are more complicated problems that could be solved using this way of thinking. In this book we proposed the reader to solve this problem adding a new parameter, a, that is the distance between two potentials. Where d is still quasiperiodic and is the distance between this two pairs and the next pair.

Algebra: Linear vector space 6

This chapter will explain and define some mathematic concepts we will used to solve problems with more complicated.

6.1 Definition of linear vector space 47
6.2 Inequations 48
6.3 Definitions in Wave Mechanicsand Operators 49

6.1 Definition of linear vector space

A linear vector space is a space where each element of the space is a entry in the space. We will follow the notation for quantum mechanics, where:

- $|v\rangle$ Dirac notation for a vector
- $\langle v|$ Conjugate of the vector
- $\langle v \,|\, v\rangle$ Inner product

We can use n-special vector to write down all vector of a space n-dimensional.

$$e_i e_j = \delta_{i,j} \tag{6.1}$$

This vectors are called unit vectores, with them we can write any vector as:

$$|v\rangle = \sum_{i=1}^{n} v_i |e_i\rangle \tag{6.2}$$

We can get any elemnt of v usign this definitions.

$$\langle e_j \,|\, v\rangle = \sum_{i=1}^{n} v_i \langle e_j \,|\, e_i\rangle = v_j \tag{6.3}$$

All this operations can be done because every linear vector must follow:

$$\langle v \,|\, (a|w\rangle + b|w\rangle)\rangle = a\langle v \,|\, w\rangle + b\langle v \,|\, w\rangle \tag{6.4}$$

As we have a definition for $|v\rangle$, we wat one for $\langle v|$.

$$\langle v| = \sum_{i=1}^{n} v_i^* \langle e_i| \tag{6.5}$$

We can know prove that the inner product is greater or equal to 0.

$$\langle v \,|\, v\rangle = (\sum_{i=1}^{n} v_i^* \langle e_i|)(\sum_{j=1}^{n} v_j |e_j\rangle) = \sum_{i,j=1}^{n} v_i^* v_j \langle e_i \,|\, e_j\rangle = \sum_{i,j=1}^{n} v_i^* v_i \geq 0 \tag{6.6}$$

And also we have proved that the inner product can only be 0 if $|v\rangle = 0$, and it is called null vector.

Other property of the inner product:

$$\langle w \mid v\rangle = (\langle v \mid w\rangle)^* \tag{6.7}$$

We can define a unit vector in direction v as:

$$|\hat{v}\rangle = \frac{1}{\sqrt{\langle v \mid v\rangle}}|v\rangle \tag{6.8}$$

6.2 Inequations

In two dimensional space the inner product is given by the angle between the two vectors.

$$\begin{gathered}\vec{v_1}\cdot\vec{v_2} = \sqrt{\vec{v_1}\cdot\vec{v_1}}\sqrt{\vec{v_2}\cdot\vec{v_2}}\cos(\theta) \\ (\vec{v_1}\cdot\vec{v_2})(\vec{v_2}\cdot\vec{v_1}) = (\vec{v_1}\cdot\vec{v_1})(\vec{v_2}\cdot\vec{v_2})\cos^2(\theta) \leq (\vec{v_1}\cdot\vec{v_1})(\vec{v_2}\cdot\vec{v_2})\end{gathered} \tag{6.9}$$

This is known as Schwarz Inequation and can be generalize to every number of dimensions.

$$\langle w \mid v\rangle\langle v \mid w\rangle \leq \langle v \mid v\rangle\langle w \mid w\rangle \tag{6.10}$$

Now we want a relation between the sum of an inner product and it's conjugate.

$$\langle w \mid v\rangle + \langle v \mid w\rangle \leq 2\sqrt{\langle v \mid v\rangle\langle w \mid w\rangle} \tag{6.11}$$

Using 6.11 and 6.10 we can get the Triangle Inequality.

$$\begin{gathered}(\langle w| + \langle v|)(|w\rangle + |v\rangle) = \langle w \mid w\rangle + \langle v \mid v\rangle + \langle v \mid w\rangle + \langle w \mid v\rangle \\ (\langle w| + \langle v|)(|w\rangle + |v\rangle) \leq \sqrt{\langle w \mid w\rangle}^2 + \sqrt{\langle v \mid v\rangle}^2 + 2\sqrt{\langle w \mid w\rangle}\sqrt{\langle v \mid v\rangle} \\ \sqrt{(\langle w| + \langle v|)(|w\rangle + |v\rangle)} \leq \sqrt{\langle w \mid w\rangle} + \sqrt{\langle v \mid v\rangle} \\ Norm(|w\rangle + |v\rangle) \leq Norm(|w\rangle) + Norm(|v\rangle)\end{gathered} \tag{6.12}$$

6.3 Definitions in Wave Mechanicsand Operators

In our physical aproach $|e_i\rangle$ is a normalize function in one or more dimension, $\langle e_i|$ is the conjugate of the function and $\langle e_i \mid e_j\rangle$ is the inner product, define as an integral over all space.

We can rewrite the wave equations for each energy, E_i.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\phi_i(x) = [E_i]\phi_i(x) \tag{6.13}$$

Where the left part in brackets is a linear operator in our vector space and is acting an element giving as a result a proportionality with him self.

We have introduced a new concept, the linear operatorr. We say an operator is linear if:

$$\begin{gathered} A|v\rangle = |w\rangle \\ A(\alpha_1|v_1\rangle + \alpha_2|v_2\rangle) = \alpha_1 A|v_1\rangle + \alpha_2 A|v_2\rangle \end{gathered} \tag{6.14}$$

Where α_1, α_2 are complex numbers. As we did with vectors we have to established some rules.

$$A|e_i\rangle = \sum_j |e_j\rangle A_{ji} \tag{6.15}$$

Given A and the vectors that define our space, $|e_i\rangle$, we can find A_{ij}.

$$\langle e_k|(A|e_i\rangle) = \langle e_k|(\sum_j |e_j\rangle A_{ji}) = \sum_j (\langle e_k \mid e_j\rangle) Aji = \sum_j \delta_{kj} A_{ji} = A_{ki} \tag{6.16}$$

One consequence of this result is the matrix multiplication acting on components.

$$\begin{gathered} |w\rangle = A|v\rangle = A\sum_i v_i|e_i\rangle = \sum_i v_i \sum_j |e_j\rangle A_{ji} = \sum_j \sum_i A_{ji} v_i |e_j\rangle = \sum_j w_i |e_j\rangle \\ w_j = \sum_i A_{ji} v_i \end{gathered} \tag{6.17}$$

We can aply more than one operator to a vector.

$$\begin{gathered} |w\rangle = A(B|v\rangle) \\ w_j = \sum_i (A_{ji}(B|v\rangle)_i) = \sum_k \sum i A_{ji} B_{ik} v_k = \sum_k (AB)_{jk} v_k \end{gathered} \tag{6.18}$$

In general A and B do not commute.

$$|x\rangle = (AB - BA)|v\rangle \tag{6.19}$$

We call that difference of the multiplication of the operators, a commutator. It has the property:

$$\begin{gathered}[A, \alpha B + \beta C]|v\rangle = (A(\alpha B + \beta C) - (\alpha B + \beta C)A)|v\rangle = \\ = (\alpha AB + \beta AC - \alpha BA - \beta CA)|v\rangle = \\ = (\alpha(AB - BA) + \beta(AC - CA))|v\rangle\end{gathered} \tag{6.20}$$

This mean that:

$$[A, \alpha B + \beta C] = \alpha[A, B] + \beta[A, C] \tag{6.21}$$

There is also a rule with the product of two operators.

$$\begin{gathered}[A, BC] = ABC - BCA - BAC + BAC = \\ = (AB - BA)C + B(AC - CA) = \\ = [A, B]C + B[A, C]\end{gathered} \tag{6.22}$$

We called operator adjunt to A to $A^\dagger$ if:

$$\begin{gathered}A|v\rangle = |w\rangle \\ \langle A|^\dagger = \langle w|\end{gathered} \tag{6.23}$$

$A^\dagger$ is the transpose complex conjugate of the operator A.

$$A^\dagger = (A^\star)^T = (A^T)^\star \tag{6.24}$$

If $A = A^\dagger$ A is called hermitian

If $A = -A^\dagger$ A is called anti-hermitian

We define the identity operator, I, as:

$$(I)_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \tag{6.25}$$

If $AA^\dagger = I$ we say that A is a unitary operator.

We can also prove that $(AB)^\dagger = (B^\dagger A^\dagger)$.

$$(AB)^\dagger = ((AB)^T)^* = (B^T A^T)^* = (B^T)^*(A^T)^* = B^\dagger A^\dagger \tag{6.26}$$

Considering a hermitian operator H that satisfy:

$$H|h_i\rangle = h_i|h_i\rangle \tag{6.27}$$

Where $|h_i\rangle$ is an eigenvector such that the action of the operator on it, returns a vector proportional to itself with h_i as the proportionality (eigenvalue).

We can prove that the eigenvalue is a real number.

$$\begin{aligned} \langle h_i|H^\dagger &= h_i^*\langle h_i| \\ \langle h_i|H^\dagger &= h_i^*\langle h_i| \\ \langle h_i|H|h_i\rangle &= h_i\langle h_i \mid h_i\rangle \\ \langle h_i|H|h_i\rangle &= h_i^*\langle h_i \mid h_i\rangle \end{aligned} \tag{6.28}$$

We can also prove that the different eigenvectors are orthogonal.

$$\begin{aligned} \langle h_j|H|h_i\rangle &= h_j\langle h_i \mid h_j\rangle \\ \langle h_j|H|h_i\rangle &= h_i\langle h_i \mid h_j\rangle \\ (h_i - h_j)\langle h_j \mid h_i\rangle &= 0 \end{aligned} \tag{6.29}$$

If $h_i \neq h_j$ then the eigenvectors are orthogonal. In one dimensional problems we don't have problems because the eigenvalues are unique, we will talk about what happen when they are equal later when we introduce more dimensions.

It can be prove that the set of eigenvectors form a base.

$$PROVE\langle h_i \mid h_i\rangle = 1 NOTPROVEYET \tag{6.30}$$

Coming back to physics with all this properties we will define our inner product and our operator.

$$\langle\psi(x)|A|\phi(x)\rangle = \int_{-\infty}^{\infty}\psi^*(x)\left[\frac{d^2}{dx^2}\phi(x)\right]dx \tag{6.31}$$

Where our inner product is the integral of the product of the functions and the operator is the second derivative. We can prove that in this inner product our operator is hermitian with the limits $\phi(\pm\infty) = 0$ and $\psi(\pm\infty) = 0$.

$$\begin{aligned} &\textstyle\int_{-\infty}^{\infty}\psi^*(x)\left[\frac{d^2}{dx^2}\phi(x)\right]dx = \int_{-\infty}^{\infty}\frac{d}{dx}\left[\psi^*\frac{d}{dx}\phi\right] - \frac{d\psi^*}{dx}\frac{d\phi}{dx}dx = \\ &\psi^*\frac{d\phi}{dx}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\psi^*}{dx}\frac{d\phi}{dx}dx = -\int_{-\infty}^{\infty}\frac{d}{dx}\left(\frac{d\psi^*}{dx}\phi\right) - \frac{d^2\psi^*}{dx^2}\phi dx = \\ &= \frac{d\psi^*}{dx}\phi\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\left[\frac{d^2\psi^*}{dx^2}\right]^2\phi dx \end{aligned} \tag{6.32}$$

We have proved that:

$$\langle\psi(x)|\left(\frac{d^2}{dx^2}|\phi\rangle\right) = \left(\langle\psi(x)|\frac{d^2}{dx^2}\right)|\phi\rangle \tag{6.33}$$

This means that the operator is hermitian. And it will be also hermitian if we multiply by a real number and add a real number thats why we can

say that our operator for the Schrödinger wave equation is hermitian if V(x) is real.

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]|E_i\rangle = E_i|E_i\rangle \tag{6.34}$$

We will need also to explore how the operator d/dx behaves.

$$\int_{-\infty}^{\infty}\psi^*(x)\left[\tfrac{d}{dx}\phi(x)\right]dx = \int_{-\infty}^{\infty}\tfrac{d}{dx}\left[\psi^*\phi\right] - \left(\tfrac{d\psi^*}{dx}\right)\phi dx =$$

$$\psi^*\phi\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\left(-\tfrac{d}{dx}\psi^*\right)\phi dx = \int_{-\infty}^{\infty}\left(-\tfrac{d}{dx}\psi^*\right)\phi dx \tag{6.35}$$

$$\left(\tfrac{d}{dx}\right)^{\dagger} = -\tfrac{d}{dx}$$

We have proved that this operator is anti-hermitian.

Harmonic Oscilator 7

We want to use the algebra we learnt in the previous chaoter, for that we will try to solve the problem where the potential V(x), is a one dimensional harmonic oscilator potential.

7.1 Definition 53
7.2 Solving the Wave Equation 54
7.3 Temperature 57

7.1 Definition

The potential for an harmonic oscilator in one dimension is given by the expresion:

$$V(x) = \frac{1}{2}kx^2 \quad k > 0 \tag{7.1}$$

This potential comes from a force, $F(x) = -kx$, so the units of k are kg/s^2. Because of this we can say that:

$$\omega = \sqrt{\frac{k}{m}} \tag{7.2}$$

Using Newton 3rd Law we can say:

$$\frac{d^2x}{dt^2} = -\omega^2 x \tag{7.3}$$

Solving this equation we get:

$$\begin{aligned} x(t) &= A\sin(\omega t) + B\cos(\omega t) \\ v(t) &= A\omega\cos(\omega t) - B\omega\sin(\omega t) \end{aligned} \tag{7.4}$$

If we define some initial conditions such as $x(0) = x_0$ and $v(0) = 0$, we can solve the coeficients, in this case $B = x_0$ and $A = 0$.

$$\begin{aligned} x(t) &= x_0\cos(\omega t) \\ v(t) &= -x_0\omega\sin(\omega t) \end{aligned} \tag{7.5}$$

And we can define two energies, a potential energy and a kinetic energy. The total energy is going to be the addition of the other two.

$$\begin{aligned} P.E(t) &= \frac{1}{2}k(x(t))^2 = \frac{1}{2}kx_0^2 cos^2(\omega t) \\ K.E(t) &= \frac{1}{2}m(v(t))^2 = \frac{1}{2}m\omega^2 x_0^2 sin^2(\omega t) \\ T.E(t) &= P.E + K.E = \frac{1}{2}kx_0^2 = constant > 0 \end{aligned} \tag{7.6}$$

The total energy turn to be constant among time and positive.

7.2 Solving the Wave Equation

The Schrödinger wave equation gets the shape:

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right]\phi(x) = E\phi(x) \tag{7.7}$$

Firstly, we will simplify the equation using natural units. We will make a change of variables $x = by$ and try to get the equation for $\phi(bx) = \chi(y)$.

$$\begin{gathered}\frac{-\hbar^2}{2mb^2}\frac{d^2\chi(y)}{dy^2} + \frac{1}{2}kby^2\chi(y) = E\chi(y) \\ \frac{\hbar^2}{2mb^2} = \frac{1}{2}kb^2 \\ b^2 = \frac{\hbar^2}{m\omega}\end{gathered} \tag{7.8}$$

Now that we have the factor to turn into natural units we can rewrite our wave equation. We will also use the definition of the energy given in the second chapter, $E = \hbar\omega$.

$$\begin{gathered}-\frac{1}{2}\hbar\omega\frac{d^2\chi(y)}{dy^2} + \frac{1}{2}\hbar\omega y^2\chi(y) = \alpha(\hbar\omega)\chi(y) \\ -\frac{1}{2}\frac{d^2\chi_n}{dy^2} + \frac{1}{2}y^2\chi_n = \alpha_n\chi_n\end{gathered} \tag{7.9}$$

We want to find α_n and it's associate χ_n for every n. We will define the hermitian operator H from the previous equation.

$$\begin{gathered}-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2\,]\chi_n = [\alpha_n]\chi_n \\ H\chi_n = [\alpha_n]\chi_n\end{gathered} \tag{7.10}$$

We define the operator a using what we propose in the end of the previous chapter.

$$\begin{gathered}a = \frac{1}{\sqrt{2}}\left(\frac{d}{dy} + y\right) \\ a^\dagger = \frac{1}{\sqrt{2}}\left(\left(\frac{d}{dy}\right)^\dagger + (y)^\dagger\right) = \frac{1}{\sqrt{2}}\left(-\frac{d}{dy} + y\right) \\ (a^\dagger a)f(y) = \left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2 - \frac{1}{2}\right)f(y)\end{gathered} \tag{7.11}$$

We will called $a^\dagger a$ a new operator N, i. e. $N = a^\dagger a$. This operator is hermitian.

$$aa^\dagger - a^\dagger a = \left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2 + \frac{1}{2}\right) - \left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2 - \frac{1}{2}\right) = 1 \tag{7.12}$$

This resolut is interesting for many reason but one of them is that it prove that a can not be represented as a finite matrix.

Summarizing what we have done so far with this operators:

$$\begin{array}{c} \left[a, a^\dagger\right] = 1 \\ [N, a] = -a \\ \left[N, a^\dagger\right] = a^\dagger \end{array} \tag{7.13}$$

If we go again to the wave equation we have:

$$\begin{array}{c} [a^\dagger a + \frac{1}{2} = \alpha]\chi \\ N\chi = \left(\alpha - \frac{1}{2}\right)\chi \\ aN\chi = \left(\alpha - \frac{1}{2}\right)a\chi \\ N[a\chi] = \left(\alpha - 1 - \frac{1}{2}\right)a\chi \end{array} \tag{7.14}$$

$a\chi$ is an eigenvector with eigenvalue $(\alpha - 1)$

We can prove that χ have infinite solutions.

$$\begin{array}{c} a^\dagger N\chi = \left(\alpha - \frac{1}{2}\right)a^\dagger\chi \\ (Na^\dagger - a^\dagger)\chi = \left(\alpha - \frac{1}{2}\right)a^\dagger\chi \\ N(a^\dagger\chi) = \left(\alpha + 1 - \frac{1}{2}\right)(a^\dagger\chi) \end{array} \tag{7.15}$$

If χ has finite solutions, a has to be a finite matrix, and we prove that is not allowed.

$$\int_{-\infty}^{\infty} f^*(a^\dagger a f)dx = \int_{-\infty}^{\infty} (af)^*(af)dx \geq 0 \tag{7.16}$$

Now we know that $\alpha \geq \frac{1}{2}$, so the solutions have a minimum where $\alpha = \frac{1}{2}$.

We can search now for our first solution.

$$\begin{array}{c} a\chi_0 = 0 => \\ => \left(\frac{d}{dy} + \frac{1}{2}\right)\chi_0 = 0 \\ \left(aa^\dagger + \frac{1}{2}\right)\chi_0 = \frac{1}{2}\chi_0 \end{array} \tag{7.17}$$

The first two lines represent the lowest solution and the last one is the next solution. With this we get that:

$$\alpha = n + \frac{1}{2} \tag{7.18}$$

Now we want to calculate χ_0.

$$\begin{array}{c} a\chi_0 = 0 \\ \chi_0 = Ae^{-\frac{y^2}{2}} \end{array} \tag{7.19}$$

We need to find the value for A to normalize the solution.

$$\begin{gathered}\int_{-\infty}^{\infty} \chi_0 \chi_0 dx = 1 \\ A^2 \int_{-\infty}^{\infty} e^{-y^2} dx = 1 \\ A = \frac{1}{\pi^{\frac{1}{4}}}\end{gathered} \tag{7.20}$$

Our final expresion for χ_0 is:

$$\chi_0 = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{y^2}{2}} \tag{7.21}$$

From this we can say that:

$$N\chi_n = n\chi_n \tag{7.22}$$

We want to normalize χ_n so we will ad a normalization factor C, where $a^\dagger \chi_n = C\chi_{n+1}$

$$\begin{gathered}C^2 \int_{-\infty}^{\infty} \chi_{n+1}^2 dy = \int_{-\infty}^{\infty} (a^\dagger \chi_n)(a^\dagger \chi_n) dy = \int_{-\infty}^{\infty} = \\ = \int_{-\infty}^{\infty} \chi_n (a a^\dagger \chi_n) dy = \int_{-\infty}^{\infty} \chi_n n \chi_n dy + \int_{-\infty}^{\infty} \chi_n^2 dy = n + 1 \\ C = \sqrt{n+1}\end{gathered} \tag{7.23}$$

We want to redifine χ_n as:

$$\chi_n = \frac{H_n(y)}{\sqrt{2\pi}} e^{\frac{-y^2}{2}} \tag{7.24}$$

We want to find $\mathrm{H}_{n+1} using the previous two equations.$

$$\begin{gathered}a^\dagger \chi_n = C\chi_{n+1} = \sqrt{1+n}\chi_{n+1} \\ \frac{1}{\sqrt{2}} \left(-\frac{d}{dx} + y\right) \frac{H_n(y)}{\sqrt{2\pi}} e^{\frac{-y^2}{2}} = \sqrt{n+1} \frac{H_{n+1}}{\sqrt{2\pi}} e^{\frac{-y^2}{2}} \\ \frac{1}{\sqrt{2(n+1)}} \left[-H'(y) e^{\frac{-y^2}{2}} + yH(y) e^{\frac{-y^2}{2}} + yH(y) e^{\frac{-y^2}{2}}\right] = H_{n+1} e^{\frac{-y^2}{2}} \\ H_{n+1} = \frac{1}{\sqrt{2(n+1)}} \left[-H_n'(y) + 2yH_n(y)\right]\end{gathered} \tag{7.25}$$

Whre H_0 is define as $H_0 = 1$.

Because χ_n is normalized we can say that $H_n(y)$ are orthonormal polynomials under a Gaussian width.

$$\begin{aligned} \frac{1}{2\pi}\int_{-\infty}^{\infty}\chi_n(y)\chi_m(y)dy &= \delta_{nm} \\ \frac{1}{2\pi}\int_{-\infty}^{\infty}H_n(y)H_m(y)e^{\frac{-y^2}{2}}dy &= \delta_{nm} \end{aligned} \tag{7.26}$$

We called this functions Hermite polynomials.

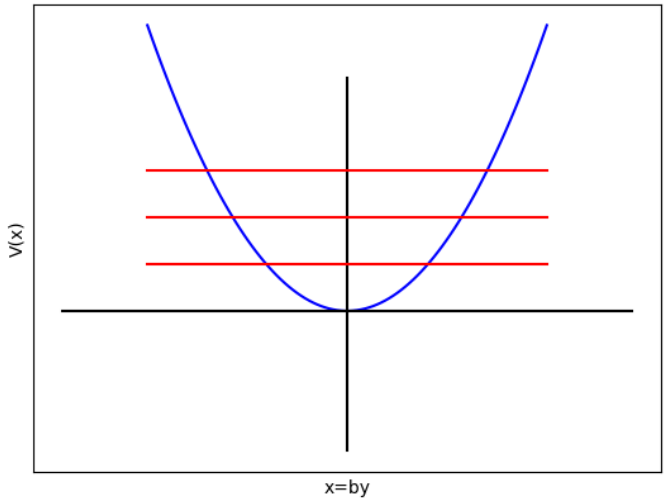

Figure 7.1: Potential V(x) and some energy levels.

We can see the solution for the problem in the figure above, where the distance of the gaps between the energies is always $\hbar\omega$.

7.3 Temperature

We have solved our potential, but we want to think now about a problem wiht multiple of this potentials. Firstly, we assume we are talking about an ideal gas wich means the particles don't talk one with each others. We want to answer the question; At a temperature, T what is the probablity that the energy is $\left(n+\frac{1}{2}\right)\omega$

We want to relate $K_bT <-> \left(n+\frac{1}{2}\right)\omega$. We have Boltzmann equation that say:

$$P_n = Ne^{\frac{-(n+1/2)\hbar\omega}{k_BT}} \tag{7.27}$$

It is a negative exponential where the fall of depend on T

Because it is a probablity for a fixed N we should have $\sum_{n=0}^{N}P_n = 1$ when N goes to ∞.

The average energy, E, will be define as:

$$E = \sum_{n=0}^{\infty} E_n P_n \tag{7.28}$$

If we called $\beta = \hbar\omega/k_B T$ we can get the average energy as:

$$\frac{E}{k_B T} = \frac{\beta(1 + e^{-\beta})}{2(1 - e^{-\beta})} \tag{7.29}$$

The behaviour of this function can be seen in the plot below.

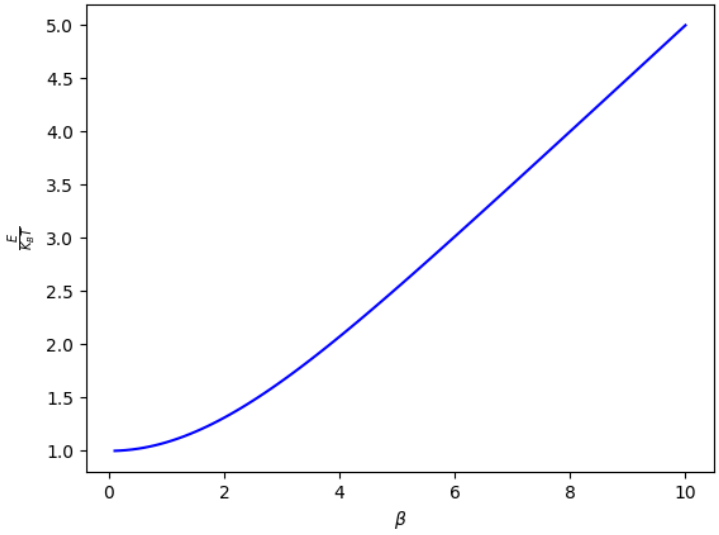

Figure 7.2: Potential V(x) and some energy levels.

If T goes to infinite the average energy goes to $E = K_B T$ and if T goes to 0 the average energy goes to $E = \frac{\hbar\omega}{2}$.

We will retur to the topic of temperature in future chapters.

2-Dimensional Potential 8

8.1 Classical Mechanics 59
8.2 Quantum Mechanics 62
8.3 Mixed Quantum states . . . 69
8.4 The angular momentum . . 69

We will worked with the harmonic oscilator again, but this time in 2 spatial dimensions.

8.1 Classical Mechanics

As we did in chapter 1 we want to understand first the behaviour of the classical mechanics for the problem.

The potential V(x,y) is:

$$V(x,y) = \frac{1}{2}k(x^2+y^2) = \frac{1}{2}k\rho^2 \tag{8.1}$$

The math becomes easier if we used polar coordinates as we did in Chapter 1. In this coordinates the energy is:

$$E = \frac{1}{2}m\left(\frac{\partial\rho}{\partial t}\right)^2 + \frac{L^2}{2m\rho^2} + \frac{1}{2}k\rho^2 \tag{8.2}$$

We are going to solve for the change among time in ρ to solve the problem.

$$\begin{aligned} \frac{\partial\rho}{\partial t} &= \sqrt{\frac{2}{m}\left(E - \frac{L^2}{2m\rho^2} - \frac{1}{2}k\rho^2\right)} \\ \frac{\partial\rho}{\partial t} &= \sqrt{\frac{k}{m\rho^2}\left(\frac{2E}{k}\rho^2 - \frac{L^2}{mk} - \rho^4\right)} \end{aligned} \tag{8.3}$$

Using equation 7.2 we can turn the previous equation into:

$$\frac{\rho}{\omega}\frac{\partial\rho}{\partial t} = \sqrt{\frac{2E}{m^2\omega^2}\rho^2 - \frac{L^2}{m\omega^2} - \rho^4} \tag{8.4}$$

We are going to change the variable ρ to u, where $u = \rho^2$. Solving for u the equation turns into:

$$\begin{aligned} \frac{1}{2\omega}\frac{\partial u}{\partial t} &= \sqrt{-\frac{L^2}{m\omega^2} + \frac{2E}{m^2\omega^2}u - u^2} \\ \frac{1}{2\omega}\frac{\partial u}{\partial t} &= \sqrt{\left(\frac{E^2}{m^2\omega^4} - \frac{L^2}{m^2\omega^2}\right) - \left(u - \frac{E}{m\omega}\right)^2} \\ \frac{1}{2\omega}\frac{\partial u}{\partial t} &= \sqrt{\frac{1}{m^2\omega^4}\left(E^2 - L^2\omega^2\right) - \left(u - \frac{E}{m\omega^2}\right)^2} \end{aligned} \tag{8.5}$$

The function inside of the square root needs to be positive, which make us say than the left parenthesis is greater than the right one that is always greater than 0, i. e. :

$$\begin{gathered}(E^2 - L\omega^2) \geq 0 \\ E \geq L\omega\end{gathered} \tag{8.6}$$

We know now that there is a minimum energy, which energy is $E = L\omega$. Whenthe energy is at it's minimum is easy to get u(t):

$$\begin{gathered}u(t) = \frac{E}{m\omega^2} = constant \\ \frac{\partial u}{\partial t} = 0\end{gathered} \tag{8.7}$$

To analize the rest of the solution for the Energy we are going to change some of the variables by some unitless variables.

$$\begin{gathered}E = \alpha L\omega \\ u = \beta \frac{E}{m\omega^2} \\ \omega t = \tau\end{gathered} \tag{8.8}$$

From the previous analysis of the minimum energy we can say that $\alpha \geq 1$. Now that we have our new parameters well define we can rewrite the expression we have been working with.

$$\begin{gathered}\frac{\alpha L}{m\omega}\frac{1}{2}\frac{\partial \beta}{\partial \tau} = \sqrt{\frac{L^2\omega^2}{m^2\omega^4}[\alpha^2 - 1] - \frac{\alpha^2 L^2}{m^2\omega^2}[\beta - 1]^2} \\ \frac{1}{2}\frac{\partial \beta}{\partial \tau} = \sqrt{\left(1 - \frac{1}{\alpha^2}\right) - (\beta - 1)^2}\end{gathered} \tag{8.9}$$

Knowing that alpha is a fixed constant we can solve this equation. But first i will make the math simpler by saying $A = \left(1 - \frac{1}{\alpha^2}\right)$

$$\frac{\partial \beta}{2\sqrt{A - (\beta - 1)^2}} = \partial \tau \tag{8.10}$$

To solve the integral we have to define the limits; for τ as it is a measure of time is going to start at $\tau = 0$ and end in a general τ, but for β it can start at any arbitrary $\beta \geq 0$, so we will say that β goes from β_0 to a general β.

$$\int_{\beta_0}^{\beta} \frac{\partial \beta'}{2\sqrt{A - (\beta - 1)^2}} = \int_0^{\tau} \partial \tau' \tag{8.11}$$

This integral can be solved directly if we change the variable beta and the constant A by $f = \beta - 1$ and $A = B^2$.

$$\begin{aligned}
\int_{f_0+1}^{f+1} \frac{\partial f'}{2\sqrt{A-f'^2}} &= \int_0^\tau \partial\tau' \\
\int_{f_0+1}^{f+1} \frac{\partial f'}{2\sqrt{A(1-\frac{f'^2}{A}}} &= \int_0^\tau \partial\tau' \\
\int_{f_0+1}^{f+1} \frac{B\partial f'}{2\sqrt{(1-\frac{f'^2}{B^2}}} &= \int_0^\tau \partial\tau'
\end{aligned} \tag{8.12}$$

This last integral can be solved directly and it will give us the result for $f(\tau)$ and then we can recover the solution for $\beta(\tau)$.

$$\begin{aligned}
\arcsin(\tfrac{f+1}{B}) - \arcsin(\tfrac{f_0}{B}) &= 2\tau \\
\beta(\tau) &= B\sin\left(2\tau + \arcsin\left(\tfrac{\beta_0}{B}\right)\right) \\
\beta(\tau) &= \sqrt{1-\tfrac{1}{\alpha^2}}\sin\left(2\tau + \arcsin\left(\frac{\beta_0}{\sqrt{1-\frac{1}{\alpha^2}}}\right)\right)
\end{aligned} \tag{8.13}$$

This is our final solution for β, from this solution we can get $\rho(t)$ by undoing the changes of variables in 8.8.

We can not forget about the other variable, the angle ϕ. To solve for phi we will used the definition of the angular momentum.

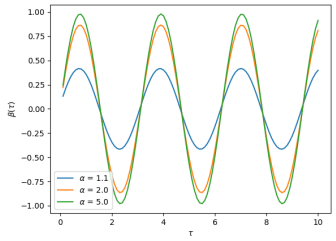

Figure 8.1: $\beta(\tau)$ function for different values of alpha

$$\begin{aligned}
L &= m\rho^2\frac{\partial\phi}{\partial t} \\
\frac{\partial\phi}{\partial t} &= \frac{L}{m\rho^2} \\
\frac{\partial\phi}{\partial\tau} &= \frac{1}{\alpha\beta(\tau)}
\end{aligned} \tag{8.14}$$

We want to find the solution for $\beta(\phi)$.

$$\frac{\partial\beta}{\partial\phi} = \frac{\frac{\partial\beta}{\partial\tau}}{\frac{\partial\phi}{\partial\tau}} = 2\alpha\beta\sqrt{\left(1-\tfrac{1}{\alpha^2}-(\beta-1)^2\right)} \tag{8.15}$$

Solving this equation we end up with:

$$\beta(\phi) = 1 + \sqrt{\left(1-\tfrac{1}{\alpha^2}\right)}\sin\left(\tfrac{1}{\alpha}\tan(\phi)\right) \tag{8.16}$$

We can turn beta into rho by undoing the changes of variables in 8.8.

$$\rho(\phi) = \sqrt{\beta(\phi)\frac{E}{m\omega^2}} = \sqrt{\beta(\phi)\alpha} \tag{8.17}$$

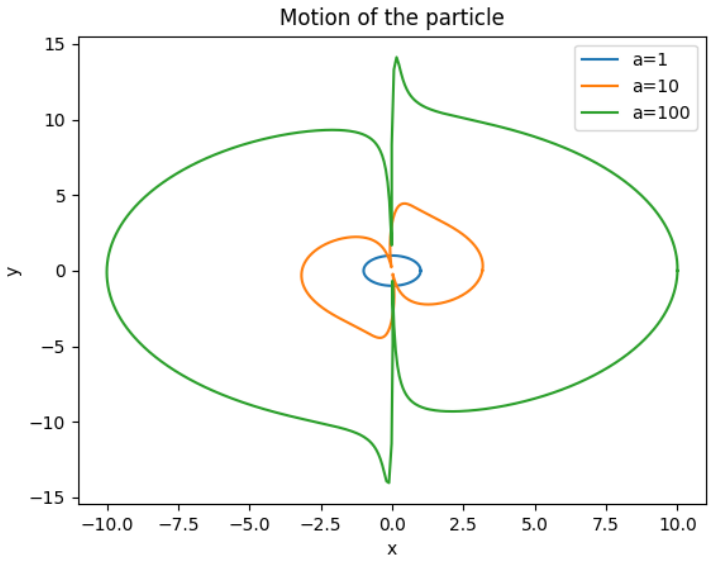

Figure 8.2: Orbital movement of the particle for different values of α

In the figure below we can see the orbital movement of the particle for different values of α.

8.2 Quantum Mechanics

We are going to solve the problem using the Schrödinger wave equation.

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right]+\frac{1}{2}m\omega^2(x^2+y^2)\phi=E\phi \tag{8.18}$$

In this case we are not going to solve the problem in polar coordinates, we are going to solve it in cartesian coordinates. First, we have to set the equation to natural units.

$$\begin{gathered} x=bu \\ y=bv \\ b^2=\frac{\hbar}{m\omega} \\ \phi(x=bu,y=bv)=\psi(u,v) \end{gathered} \tag{8.19}$$

Our wave equation now is:

$$-\frac{1}{2}\hbar\omega\left[\frac{\partial^2\psi}{\partial u^2}+\frac{\partial^2\psi}{\partial v^2}\right]+\frac{1}{2}\hbar\omega(u^2+v^2)\psi=E\psi \tag{8.20}$$

As we did in the classical aproach we are going to change the energy by $E = \alpha\hbar\omega$. The wave equation now looks like:

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\right) + \frac{1}{2}(u^2 + v^2)\right]\psi = \alpha\psi \tag{8.21}$$

As we did in one dimension we can use some operators to solve this equation. We are going to define this as:

$$\begin{aligned} a_u &= \frac{1}{\sqrt{2}}\left[\frac{\partial}{\partial u} + u\right] \\ a_v &= \frac{1}{\sqrt{2}}\left[\frac{\partial}{\partial v} + v\right] \\ a_u^\dagger &= \frac{1}{\sqrt{2}}\left[-\frac{\partial}{\partial u} + u\right] \\ a_v^\dagger &= \frac{1}{\sqrt{2}}\left[-\frac{\partial}{\partial v} + v\right] \end{aligned} \tag{8.22}$$

It can be proved that $aa^\dagger$ is an hermitian operator of χ for any of the variables; u,v.

We have also similar relations to the ones we had in one dimension.

$$\begin{aligned} \left[a_u, a_u^\dagger\right] &= 1 \\ \left[a_v, a_v^\dagger\right] &= 1 \\ \left[a_u, a_v\right] &= 0 \\ \left[a_u^\dagger, a_v^\dagger\right] &= 0 \\ N_u &= a_u^\dagger a_u \\ N_v &= a_v^\dagger a_v \\ \left[N_u, a_u^\dagger\right] &= a_u^\dagger \\ \left[N_u, a_u\right] &= -a_u \\ \left[N_v, a_v^\dagger\right] &= a_v^\dagger \\ \left[N_v, a_v\right] &= -a_v \end{aligned} \tag{8.23}$$

The commutator of any two cross operators is 0. With this we end up with the following equation:

$$\left[N_u + N_v\right]\psi = (\alpha - 1)\psi \tag{8.24}$$

Which means that $\alpha \geq 1$, as it was in classical mechanics. We can use the

operators $a_u^\dagger$ or $a_v^\dagger$ to get the next level of energy for the equation.

$$\begin{gathered}
[N_u + N_v + 1]\,(a^\dagger\psi) = \left[a^\dagger N_u + a^\dagger + a^\dagger N_v\right] \\
[N_u + N_v + 1]\,(a^\dagger\psi) = a^\dagger[N_u + N_v + 1]\psi \\
[N_u + N_v + 1]\,(a^\dagger\psi) = (\alpha + 1 - 1)a^\dagger\psi
\end{gathered} \tag{8.25}$$

The operator $a^\dagger$ could be either of the two posible operators, and the result is the same. We can say that the operator $a^\dagger$ is giving us the next level of energy for the equation, α increases by one.

There is an $\alpha = 1$, which is the minimum energy for the system, which means that there is a lower energy state ψ_0 where:

$$[N_u + N_v]\,\psi_0(u,v) = 0 \tag{8.26}$$

So:

$$a_u\psi_0(u,v) = 0 a_v\psi_0(u,v) = 0 \tag{8.27}$$

There must be a function $\psi_0(u,v)$ that satisfies this two equations. Let's try to solve it.

$$\begin{gathered}
\left(\frac{\partial}{\partial u} + u\right)\psi_0(u,v) = 0 \\
\left(\frac{\partial}{\partial v} + v\right)\psi_0(u,v) = 0
\end{gathered} \tag{8.28}$$

The solution for this equation is:

$$\begin{gathered}
\ln\psi_0(u,v) + \tfrac{1}{2}u^2 = f(v) \\
\ln\psi_0(u,v) + \tfrac{1}{2}v^2 = f(u) \\
\psi_0(u,v) = Ae^{-\frac{1}{2}(u^2+v^2)}
\end{gathered} \tag{8.29}$$

Where A is the normalization factor than can be calculated by:

$$\begin{gathered}
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_0^2(u,v)dudv = 1 \\
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}A^2e^{-u^2-v^2}dudv = 1 \\
A^2\int_{-\infty}^{\infty}e^{-u^2}du\int_{-\infty}^{\infty}e^{-v^2}dv = 1 \\
A^2\left(\sqrt{\pi}\right)^2 = 1 \\
A = \tfrac{1}{\sqrt{\pi}}
\end{gathered} \tag{8.30}$$

This is the solution for the ground state of the system. We can now use the operator $a^\dagger$ to get the next level of energy even for u or for v, both

states will have the same energy but different functions, i.e. $\alpha = 2$ have two states $\psi_{1,0}$ and $\psi_{0,1}$.

$$\begin{aligned}
\psi_0 &= \tfrac{1}{\sqrt{\pi}} e^{-\frac{1}{2}(u^2+v^2)} \\
\psi_{1,0} &= A_{1,0} a_u^\dagger \psi_0 = A_{1,0} \tfrac{1}{\sqrt{2}} \left[-\tfrac{\partial}{\partial u} + u \right] \psi_0 = A_{1,0} \sqrt{\tfrac{2}{\pi}} u e^{-\frac{u^2+v^2}{2}} \\
\psi_{0,1} &= A_{0,1} a_v^\dagger \psi_0 = A_{0,1} \tfrac{1}{\sqrt{2}} \left[-\tfrac{\partial}{\partial v} + v \right] \psi_0 = A_{0,1} \sqrt{\tfrac{2}{\pi}} v e^{-\frac{u^2+v^2}{2}}
\end{aligned} \tag{8.31}$$

To determine the normalization coeficient we have to use the same procedure as before.

$$A_{1,0}^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{1,0}^2(u,v) du dv = \tfrac{2}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^2 e^{-(u^2+v^2)} du dv \tag{8.32}$$

To solve this integral we are going to use polar coordinates.

$$\begin{aligned}
A_{1,0}^2 &= \tfrac{2}{\pi} \int_0^{\infty} r dr \int_0^{2\pi} r^2 \sin^2(\theta) e^{-r^2} d\theta = \\
&= \tfrac{2}{\pi} \int_0^{\infty} r^3 e^{-r^2} dr \int_0^{2\pi} \sin^2(\theta) d\theta = \tfrac{2}{\pi} \tfrac{1}{2} \pi = 1
\end{aligned} \tag{8.33}$$

Which means that $A^2 = 1$, so $A = e^{i\phi}$, but we are only interested in the real part of the function, so $A = 1$. We can do the same for $\psi_{0,1}$.

This variables are called Hidden Variables in quantum mechanics. They are not observable, but they have become important for new physics, for example in the field of quantum computation.

We can continue this process to get the next levels of energy. The final results fo the next level are:

$$\begin{aligned}
\psi_{2,0} &= \tfrac{2u^2-1}{2\sqrt{\pi}} e^{-\frac{u^2+v^2}{2}} \\
\psi_{0,2} &= \tfrac{2v^2-1}{2\sqrt{\pi}} e^{-\frac{u^2+v^2}{2}} \\
\psi_{1,1} &= \tfrac{uv}{\sqrt{2\pi}} e^{-\frac{u^2+v^2}{2}}
\end{aligned} \tag{8.34}$$

The solutions can be visualized in the following figures.

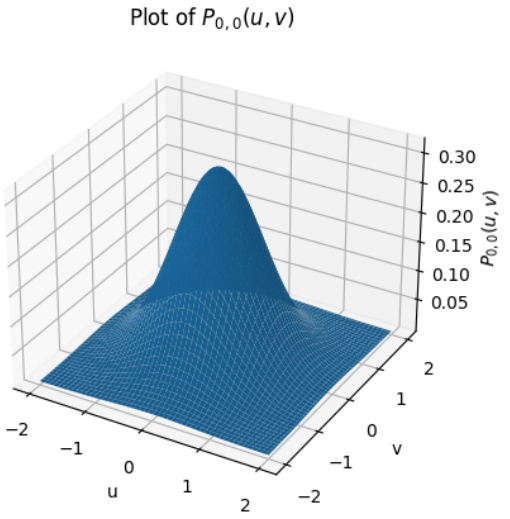

Figure 8.3: Probability distribution for the state $\psi_{0,0}(u,v)$

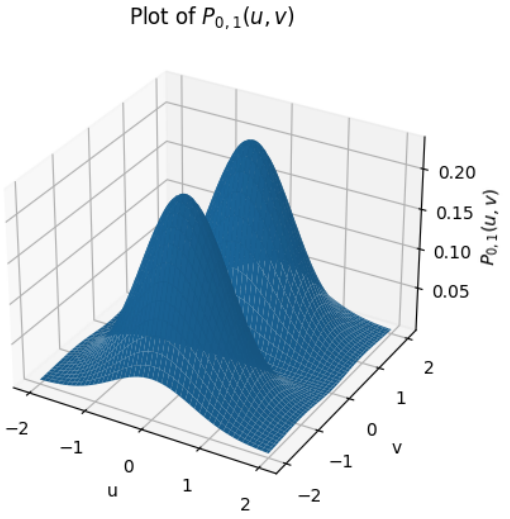

Figure 8.4: Probability distribution for the state $\psi_{0,1}(u,v)$

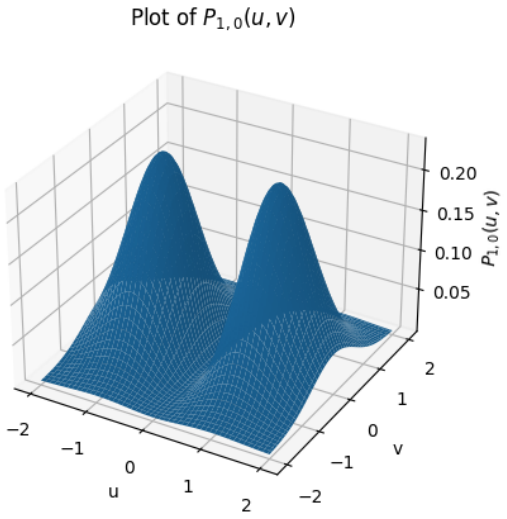

Figure 8.5: Probability distribution for the state $\psi_{1,0}(u,v)$

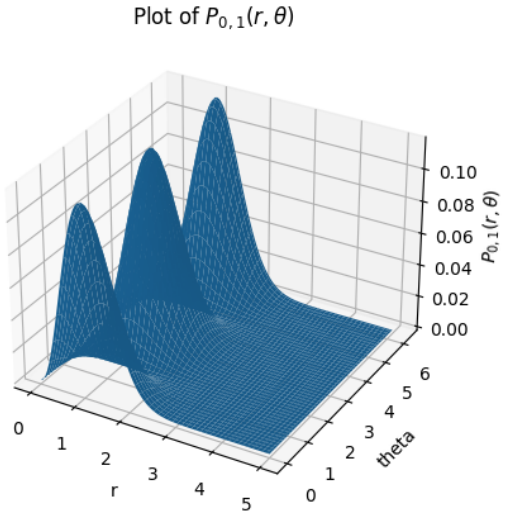

Figure 8.6: Probability distribution for the state $\psi_{0,1}(r,\theta)$

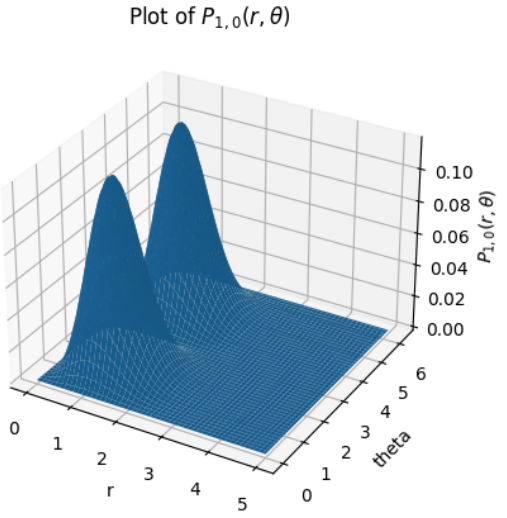

Figure 8.7: Probability distribution for the state $\psi_{1,0}(r,\theta)$

8.3 Mixed Quantum states

Given $\alpha = 2$ and the density Probability of a mixed state ψ, we can say that:

$$\psi = C_{1,0}\psi_{1,0} + C_{0,1}\psi_{0,1} \tag{8.35}$$

Where $C_{1,0}$ and $C_{0,1}$ are real numbers, (to keep it simpler). If the probability density is normalized we found:

$$\begin{gathered}
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^{\star}(u,v)\psi(u,v)dudv = 1 \\
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(C_{1,0}\psi_{1,0} + C_{0,1}\psi_{0,1}\right)^{\star}\left(C_{1,0}\psi 1,0 + C_{0,1}\psi 0,1\right)dudv = 1 \\
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(C_{1,0}^{2}\psi_{1,0}^{*}\psi 1,0 + C_{0,1}^{2}\psi_{0,1}^{*}\psi 0,1\right)dudv = 1 \\
C_{1,0}^{2} + C_{0,1}^{2} = 1
\end{gathered} \tag{8.36}$$

This means that the sum of the square of the coefficients is going to be 1.

We can transform the probability into any system, we are going to choose the probability in terms of r and θ

$$\begin{gathered}
P(r,\theta) = \psi^{\star}(r,\theta)\psi(r,\theta) = \left(C_{1,0}\psi_{1,0}^{*} + C_{0,1}\psi_{0,1}^{*}\right)^{\star}\left(C_{1,0}\psi 1,0 + C_{0,1}\psi 0,1\right) \\
P(r,\theta) = \frac{2}{\pi}\left(C_{1,0}^{2}\sin^{2}\theta + 2C_{1,0}C_{0,1}\sin\theta\cos\theta + C_{0,1}\cos^{2}\theta\right) \\
P(r,\theta) = \frac{2}{\pi}\left(\frac{1}{2} + \frac{C_{0,1}^{2}-C_{1,0}^{2}}{2}\cos 2\theta + C_{1,0}C_{0,1}\sin 2\theta\right)
\end{gathered} \tag{8.37}$$

This means than knowing the probability depending on the angle θ we can get the coefficients $C_{1,0}$ and $C_{0,1}$, i.e. how the state is distributed in terms of the pure quantum states.

8.4 The angular momentum

As we did in the classical mechanics we are going to solve the problem in polar coordinates.

We need to transform the variables and derivatives into a polar system.

$$\begin{gathered}
u = r\cos\theta \qquad\qquad v = r\sin\theta \\
du = (dr)\cos\theta - r\sin\theta d\theta \quad dv = (dr)\sin\theta + r\cos\theta d\theta
\end{gathered} \tag{8.38}$$

We will rename $\psi(u,v)$ to $\chi(r,\theta)$ and we want to know how the derivatives behave for χ.

$$\begin{aligned}
\frac{\partial}{\partial u}\chi &= \left[\left(\frac{\partial}{\partial\theta}\right)_r\left(\frac{\partial\theta}{\partial u}\right)_v + \left(\frac{\partial}{\partial r}\right)_\theta\left(\frac{\partial r}{\partial u}\right)_v\right]\chi = \\
&= \left(\frac{-\sin\theta}{r}\frac{\partial}{\partial\theta} + \cos\theta\frac{\partial}{\partial r}\right)\chi \\
\frac{\partial}{\partial v}\chi &= \left[\left(\frac{\partial}{\partial\theta}\right)_r\left(\frac{\partial\theta}{\partial v}\right)_u + \left(\frac{\partial}{\partial r}\right)_\theta\left(\frac{\partial r}{\partial v}\right)_u\right]\chi = \\
&= \left(\frac{\cos\theta}{r}\frac{\partial}{\partial\theta} + \sin\theta\frac{\partial}{\partial r}\right)\chi
\end{aligned} \tag{8.39}$$

We need to the second derivative.

$$\begin{aligned}
\frac{\partial^2}{\partial u^2}\chi &= \left(\frac{-\sin\theta}{r}\frac{\partial}{\partial\theta} + \cos\theta\frac{\partial}{\partial r}\right)\left(\frac{-\sin\theta}{r}\frac{\partial}{\partial\theta} + \cos\theta\frac{\partial}{\partial r}\right)\chi = \\
&= \left(\frac{\sin^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\sin^2\theta}{r}\frac{\partial}{\partial r} + \cos^2\theta\frac{\partial^2}{\partial r^2}\right)\chi \\
\frac{\partial^2}{\partial v^2}\chi &= \left(\frac{\cos\theta}{r}\frac{\partial}{\partial\theta} + \sin\theta\frac{\partial}{\partial r}\right)\left(\frac{\cos\theta}{r}\frac{\partial}{\partial\theta} + \sin\theta\frac{\partial}{\partial r}\right)\chi = \\
&= \left(\frac{\cos^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\cos^2\theta}{r}\frac{\partial}{\partial r} + \sin^2\theta\frac{\partial^2}{\partial r^2}\right)\chi
\end{aligned} \tag{8.40}$$

Our wave equation now looks like:

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right) + \frac{1}{2}r^2\right]\chi = \alpha\chi \tag{8.41}$$

If we compare this equation with the one we had for classical mechanics we can see a relation between the different energies in classical mechanics and these terms.

- $\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)$ is the kinetic energy in the radial direction.
- $\frac{1}{2}\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$ is the angular kinetic energy.
- $\frac{1}{2}r^2$ is the potential energy.

As we did in classical mechanics we are going to define the angular momentum as the operator: $L_z = \frac{\partial}{\partial\theta}$.

We want to know how this operator behaves with the operator H and the wave function.

$$\begin{aligned}
(HL_z)\chi &= \frac{-1}{2}\frac{\partial^3\chi}{\partial r^2\partial\theta} - \frac{1}{2r}\frac{\partial^2\chi}{\partial r\partial\theta} + \frac{1}{2r^2}\frac{\partial^3\chi}{\partial\theta^3} + \frac{1}{2}r^2\frac{\partial\chi}{\partial\theta} \\
(L_zH)\chi &= \frac{-1}{2}\frac{\partial^3\chi}{\partial r^2\partial\theta} - \frac{1}{2r}\frac{\partial^2\chi}{\partial r\partial\theta} + \frac{1}{2r^2}\frac{\partial^3\chi}{\partial\theta^3} + \frac{1}{2}r^2\frac{\partial\chi}{\partial\theta}
\end{aligned} \tag{8.42}$$

As we can see both operations are the same, this proves that the two operators commute.

$$[H, L_z] = 0 \tag{8.43}$$

If $H\chi = \alpha\chi$:

$$H(L_z\chi) = L_z(H\chi) = \alpha(L_z\chi) \tag{8.44}$$

Wich means that $L_z\chi$ is an eigenvector of the operator H with the same eigenvalue α. The eigenspace can be defined by eigenvectors of H and by eigenvectors of H and L_z at the same time.

We can found now the eigenvectors of L_z.

$$L_z\chi = l\chi \tag{8.45}$$

The solution for this differential equation is:

$$\chi = R(r)e^{l\theta} \tag{8.46}$$

Because the function χ is periodic in θ we can say that $l = im$.

$$\chi = R(r)e^{im\theta} \tag{8.47}$$

We didn't assume anything, we proved that because the operator commute the function can be described as above. This two operators commute because the force is a central force wich means that $V(r)$ is only a function of r.

$$\begin{aligned} H\chi_{\alpha,m} &= \alpha\chi_{\alpha,m} \\ L_z\chi_{\alpha,m} &= im\chi_{\alpha,m} \end{aligned} \tag{8.48}$$

Now we have to solve the wave equation for the radial function, $R(r)$.

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2} - r^2 + 2\alpha\right] R(r) = 0 \tag{8.49}$$

If we look at the results in Section 3, we can see that there is an exponential factor in the solution. We will take that out to make math simpler.

$$\begin{aligned} R(r) &= e^{-\frac{r^2}{2}}P(r) \\ \frac{dR}{dr} &= \left(\frac{dP}{dr} - rP\right)e^{\frac{-r^2}{2}} \\ \frac{d^2R}{dr^2} &= \left(\frac{d^2P}{dr^2} - 2r\frac{dP}{dr} + (r^2-1)P\right)e^{\frac{-r^2}{2}} \end{aligned} \tag{8.50}$$

If we substitute this into 8.49:

$$\begin{aligned} &\left[\frac{d^2P}{dr^2} - 2r\frac{dP}{dr} + (r^2-1)P + \frac{1}{r}\frac{dP}{dr} - P - \frac{m^2P}{r^2} - r^2P + 2\alpha P\right]e^{\frac{-r^2}{2}} = 0 \\ &\frac{d^2P}{dr^2} + \left(\frac{1}{r} - 2r\right)\frac{dP}{dr} + \left(2\alpha - 2 - \frac{m^2}{r^2}\right)P = 0 \end{aligned} \tag{8.51}$$

We expect P(r) to be a polinomic function, but for a polinome to be normalizable must be finite wich means having a finite number of terms. Let's assume $P(r)\ r^{\beta}$ for $r \to 0$. Near $r = 0$ the derivatives will be:

$$\begin{gathered} \frac{dP}{dr}\ r^{\beta-1} \\ \frac{d^2P}{dr^2}\ r^{\beta-2} \end{gathered} \tag{8.52}$$

If we substitute this into the equation we get:

$$\begin{gathered} \beta(\beta-1)r^{\beta-2} + \left(\frac{1}{r} - 2r\right)\beta r^{\beta-1} + (2\alpha - 2 - \frac{m^2}{r^2})r^{\beta} = 0 \\ \left[\beta(\beta-1) + \beta - m^2\right] r^{\beta-2} + (2\alpha - 2 - 2\beta)r^{\beta} = 0 \\ \beta(\beta-1) + \beta - m^2 = 0 \Rightarrow \beta = \beta^2 = m^2 \Rightarrow \beta = |m| \end{gathered} \tag{8.53}$$

β has to be positive. We can redefine $P(r)$ as:

$$\begin{gathered} P(r) = r^{|m|}U(r) \\ \frac{dP}{dr} = |m|r^{|m|-1}U(r) + r^{|m|}\frac{dU}{dr} \\ \frac{d^2P}{dr^2} = |m|(|m|-1)r^{|m|-2}U(r) + 2|m|r^{|m|-1}\frac{dU}{dr} + r^{|m|}\frac{d^2U}{dr^2} \\ \left(\frac{1}{r} - 2r\right)\frac{dP}{dr} = |m|r^{|m|-2}U(r) - 2|m|r^{|m|-1}\frac{dU}{dr} - 2r^{|m|+1}\frac{dU}{dr} \\ \left(2\alpha - 2 - \frac{m^2}{r^2}\right)P = (2\alpha-2)r^{|m|}U(r) - m^2r^{|m|-2}U(r) \end{gathered} \tag{8.54}$$

If we substitute this into the differential equation we get:

$$\begin{gathered} (2\alpha - 2 - 2|m|)r^{|m|}U(r) + \left[(2|m|+1)r^{|m|-1} - 2r^{|m|+1}\right]\frac{dU}{dr} + r^{|m|}\frac{d^2U}{dr^2} = 0 \\ \frac{d^2U}{dr^2} + \left(\frac{2|m|+1}{r} - 2r\right)\frac{dU}{dr} + 2(\alpha - 1 - |m|)U = 0 \end{gathered} \tag{8.55}$$

This differential equation can be solved using Frobenius Method. We are going to assume that U(r) is an "infinite" polinomic function.

$$\begin{gathered} U(r) = \sum_{n=0}^{\infty} u_n r^n \\ \frac{dU}{dr} = \sum_{n=0}^{\infty} n u_n r^{n-1} \\ \frac{d^2U}{dr^2} = \sum_{n=0}^{\infty} n(n-1)u_n r^{n-2} \\ \left(\frac{2|m|+1}{r} - 2r\right)\frac{dU}{dr} = \frac{(2|m|+1)u_1}{r} + \sum_0^{\infty}(2|m|+1)u_{n+2}(n+2)r^n - \sum_0^{\infty} 2u_n n r^n \\ 2(\alpha - 1 - |m|)U = \sum_0^{\infty} 2(\alpha - 1 - |m|)u_n r^n \end{gathered} \tag{8.56}$$

Substituying:

$$0 = \frac{2|m|+1}{r}u_1 + \sum_0^\infty \left[u_{n+2}\left((n+2)(2|m|+1) + (n+2)(n+1)\right) + u_n\left((\alpha - 1 - |m|) - 2n\right)\right] r^n \tag{8.57}$$

This has to be 0 for every r, but also the first term has to be null, for the function to exist in $r = 0$.

$$u_1 = 0$$

$$u_{n+2}\left[(n+2)(2|m|+1) + (n+2)(n+1)\right] + u_n\left[(\alpha - 1 - |m|) - 2n\right] = 0$$

$$u_{n+2} = \frac{2[1+|m|+n-\alpha]}{(n+2)(2|m|+n+2)}u_n; n \geq 0 \tag{8.58}$$

All the odd terms are going to be 0. We need this to be finite so we have to arrange a value N for when all the greater terms are 0, i.e. $u_{N+2} = 0$. This implies:

$$2[1 + |m| + N - \alpha] = 0 \Rightarrow \alpha = 1 + |m| + N \tag{8.59}$$

We know that N has to be even. We can represent alpha with this new parameters N and m.

N	m	α	$\chi(r,\theta)$
0	0	1	$\chi(r,\theta) = u_0 e^{\frac{-r^2}{2}}$
0	+1	2	$\chi(r,\theta) = u_0 r e^{\frac{-r^2}{2}} e^{i\theta}$
0	-1	2	$\chi(r,\theta) = u_0 r e^{\frac{-r^2}{2}} e^{i\theta}$
2	0	3	$\chi(r,\theta) = u_0(1-r^2) e^{\frac{-r^2}{2}}$
0	+2	3	$\chi(r,\theta) = u_0 r^2 e^{\frac{-r^2}{2}} e^{2i\theta}$
0	-2	3	$\chi(r,\theta) = u_0 r^2 e^{\frac{-r^2}{2}} e^{2i\theta}$

This gave us pretty much every understandment on harmonic oscilators. We will get more into the angular momentum in the next chapter.

9 3-Dimensional Space

9.1 Angular Momentum in 3 Dimensions 75
9.2 Angular Momentum as a vector operator 80
9.3 Matrix representation for j=1, 1/2, 2 83

We've been working with harmonic oscilators and gravitational potentials but there are other interesting potentials that we are going to mention here.

- Electric Potential $V(r) = \frac{\alpha}{r}$, $\alpha > 0$
- Confining Potential $V(r) = kr$
- Higgs Potential $V(r) = \frac{\alpha}{r} e^{-mr}$

There are others like: Reed Potential, Cornell Potential,...

9.1 Angular Momentum in 3 Dimensions

We can also have potentials that doesn't come from central forces. In those cases we have to look carefully at the angular momentum.

$$\vec{L} = \vec{r} \times \vec{p} \tag{9.1}$$

$$\begin{aligned} L_x &= yp_z - zp_y \\ L_y &= zp_x - xp_z \\ L_z &= xp_y - yp_x \end{aligned} \tag{9.2}$$

Using our knowledge from equation 2.4 we can say,

$$\begin{aligned} L_x &= -i\hbar(y\tfrac{\partial}{\partial z} - z\tfrac{\partial}{\partial y}) \\ L_y &= -i\hbar(z\tfrac{\partial}{\partial x} - x\tfrac{\partial}{\partial z}) \\ L_z &= -i\hbar(x\tfrac{\partial}{\partial y} - y\tfrac{\partial}{\partial x}) \end{aligned} \tag{9.3}$$

This three components of the angular momentum and the angular momentum itself are hermitian operators. We want to see how they commute between them.

$$\begin{aligned} (L_xL_y)\psi &= -\hbar^2(y\tfrac{\partial}{\partial z} - z\tfrac{\partial}{\partial y})(z\tfrac{\partial}{\partial x} - x\tfrac{\partial}{\partial z})\psi = \\ &= -\hbar^2\left[y\left(\tfrac{\partial\psi}{\partial x} + z\tfrac{\partial^2\psi}{\partial x\partial z}\right) - yx\tfrac{\partial^2\psi}{\partial z^2} - z^2\tfrac{\partial^2\psi}{\partial x\partial y} - zx\tfrac{\partial^2\psi}{\partial y\partial z}\right](a) \\ (L_yL_x)\psi &= -\hbar^2(z\tfrac{\partial}{\partial x} - x\tfrac{\partial}{\partial z})(y\tfrac{\partial}{\partial z} - z\tfrac{\partial}{\partial y})\psi = \\ &= -\hbar^2\left[zy\tfrac{\partial^2\psi}{\partial x\partial z} - xy\tfrac{\partial^2\psi}{\partial z^2} - z^2\tfrac{\partial^2\psi}{\partial x\partial y} + x\tfrac{\partial\psi}{\partial y} + xz\tfrac{\partial^2\psi}{\partial z\partial y}\right](b) \\ (a) - (b) &= [L_x, L_y] = i\hbar L_z \end{aligned} \tag{9.4}$$

In the same way it can be prooved that:

$$\begin{aligned}[L_y, L_z] &= i\hbar L_x \\ &= i\hbar L_y\end{aligned} \tag{9.5}$$

These 3 operators are closed under conmmutation, wich means that the conmmutation of any two of them give us the third one.

We our going to use the Levi-Civita epsilon to write the angular momentum in a more compact way.

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{9.6}$$

Levi-Civita epsilon has a lot of application in linear algebra. For example it can be used to determine the determinant of a matrix.

Now using the properties from 6.22 we want to calculate the conmmutation between L_i and L_i^2.

$$\begin{gathered}[L_i, L_i^2] = [L_i, L_i]L_i + L_i[L_i, L_i] = 0 \\ \left[L_i, L_j^2\right] = \left[L_i, L_j\right] L_j + L_j[L_i, L_j] = i\hbar\left(L_kL_j\right) + i\hbar\left(L_jL_k\right) = i\hbar(L_kL_j + L_jL_k) \\ \left[L_i, L_k^2\right] = [L_i, L_k]L_k + L_k[L_i, L_k] = -i\hbar\left(L_jL_k\right) - i\hbar\left(L_kL_j\right) = -i\hbar(L_kL_j + L_jL_k) \\ \left[L_i, L_i^2 + L_j^2 + L_k^2\right] = [L_i, L] = 0\end{gathered} \tag{9.7}$$

This means that the angular momentum and the square of the angular momentum commute. We can simultaneously diagonalize them because they commute, so a base wher both are diagonalizable can be found.

$$\begin{aligned}L^2|l, m\rangle &= \hbar^2 l^2|l, m\rangle \\ L_3|l, m\rangle &= \hbar m|l, m\rangle\end{aligned} \tag{9.8}$$

We choose this notation for the eigenvalues to make the connection with the eigenvalues. Also we choose the notation 1,2,3 instead of x,y,z. These changes are just for convenience.

In general terms:

$$\begin{gathered}\left[L^2, L_c\right] = \left[\sum_{n=1}^3 L_a^2, L_c\right] = \sum_{n=1}^3 [L_aL_a, L_c] = \\ = \sum_{n=1}^3 (L_a[L_a, L_c] + [L_a, L_c]L_a) = \\ = i\hbar \sum_{a,b=1}^3 \epsilon_{acb}L_aL_b + i\hbar \sum_{a,b=1}^3 \epsilon_{acb}L_bL_a = \\ i\hbar \left(\sum_{a,b=1}^3 \epsilon_{acb}\epsilon_{bca}\right) L_aL_b = 0\end{gathered} \tag{9.9}$$

We can use the Levi-Civita epsilon to change the order of the indices.

Going back to equation 9.8 we can say

$$\begin{aligned}
\langle l,m|L_a^2|l,m\rangle = (\langle l,m|L_1)(L_a|l,m\rangle) = (L_a|l,m\rangle)^\dagger(L_a|l,m\rangle) \geq 0 \\
\langle l,m|L_1^2+L_2^2|l,m\rangle \geq 0 \\
\langle l,m|L_1^2+L_2^2+L_3^2-L_3^2|l,m\rangle \geq 0 \\
\langle l,m|L^2|l,m\rangle - \langle l,m|L_3^2|l,m\rangle \geq 0 \\
\hbar^2 l^2\langle l,m\,|\,l,m\rangle - \hbar^2 m^2\langle l,m\,|\,l,m\rangle \geq 0 \\
\hbar^2(l^2-m^2) \geq 0 \\
l^2 \geq m^2
\end{aligned} \tag{9.10}$$

This result means that the proyectionof the angular momentum in the z direction is less or equal to the total angular momentum, as one would expected.

We want to create new operators L_+ and L_- that are going to be useful to us.

$$\begin{aligned}
L_+ = L_1 + iL_2 \\
L_- = L_1 - iL_2
\end{aligned} \tag{9.11}$$

With the next properties:

$$\begin{aligned}
L_+^\dagger = L_- \\
L_-^\dagger = L_+
\end{aligned} \tag{9.12}$$

As every time, when we have a new operator we want to know it commutes with the rest.

$$\begin{aligned}
[L_3,L_+] = [L_3,L_1] + i\,[L_3,L_2] = i\hbar L_2 - ii\hbar L_1 = \hbar L_1 + i\hbar L_2 = \hbar L_+ \\
[L_3,L_-] = [L_3,L_1] - i\,[L_3,L_2] = i\hbar L_2 + ii\hbar L_1 = -\hbar L_1 + i\hbar L_2 = -\hbar L_- \\
[L_+,L_-] = [L_1+iL_2,L_1-iL_2] = [L_1,L_1] + [L_2,L_2] - i\,[L_1,L_2] + i\,[L_2,L_1] = 2\hbar L_3 \\
\left[L^2,L_+\right] = \left[L^2,L_1\right] + i\left[L^2,L_2\right] = 0 \\
\left[L^2,L_-\right] = \left[L^2,L_1\right] - i\left[L^2,L_2\right] = 0
\end{aligned} \tag{9.13}$$

With this new operators we can get the next eigenvectors for m without changing l.

$$L^2(L+|l,m\rangle) = L_+L^2|l,m\rangle = L_+\hbar^2l^2|l,m\rangle = \hbar^2l^2(L_+|l,m\rangle) \tag{9.14}$$

This means that $L_+|l,m\rangle$ is an eigenvector of L^2 with the same eigenvalue $\hbar^2l^2$.

$$L_3(L_+|l,m\rangle) = (\hbar L_+ + L_+L_3)|l,m\rangle = \hbar(m+1)(L_+|l,m\rangle) \tag{9.15}$$

This implies that $L_+|l,m\rangle$ is an eigenvector of L_3 with eigenvalue $\hbar(m+1)$, i.e, $L_+|l,m\rangle \propto |l,m+1\rangle$. We can do the same for L_-.

$$\begin{gathered} L^2(L_-|l,m\rangle) = L_-\hbar^2l^2|l,m\rangle = \hbar^2l^2(L_-|l,m\rangle) \\ L_3(L_-|l,m\rangle) = (-\hbar L_- + L_-L_3)|l,m\rangle = \hbar(m-1)(L_-|l,m\rangle) \end{gathered} \tag{9.16}$$

This implies that $L_-|l,m\rangle$ is an eigenvector of L^2 with eigenvalue $\hbar^2l^2$ and of L_3 with eigenvalue $\hbar(m-1)$, i.e, $L_-|l,m\rangle \propto |l,m-1\rangle$.

We can use L_+ and L_- to get all the eigenvalues of L_3, but there is a limit because for a fixed l, m can only take values from -l to l as we proved in 9.10. This can only happen if the next eigenvalue is 0.

$$\begin{gathered} L_+|l,m_{max}\rangle = 0 \\ L_-|l,m_{min}\rangle = 0 \end{gathered} \tag{9.17}$$

We are going to solve for the maximum values of m multiplying by L_-.

$$\begin{gathered} L_-L_+|l,m_{max}\rangle = 0 \\ (L_1 - iL_2)(L_1 + iL_2)|l,m_{max}\rangle = 0 \\ |l,m_{max}\rangle = 0 \\ |l,m_{max}\rangle = 0 \\ (\hbar^2l^2 - \hbar^2m_{max}^2 - \hbar^2m_{max})|l,m_{max}\rangle = 0 \\ \hbar^2l^2 - \hbar^2m_{max}^2 - \hbar^2m_{max} = 0 \\ l^2 = m_{max}^2 + m_{max} \end{gathered} \tag{9.18}$$

Which implies than the maximum m is less than l, this can only happen because L^2 and L_3 are operators. We can do the same for the minimum

value of m.

$$\begin{gathered} L_+L_-|l, m_m in\rangle = 0 \\ (L_1 + iL_2)(L_1 - iL_2)|l, m_m in\rangle = 0 \\ |l, m_m in\rangle = 0 \\ |l, m_m in\rangle = 0 \\ (\hbar^2 l^2 - \hbar^2 m_{min}^2 + \hbar^2 m_{min})|l, m_{min}\rangle = 0 \\ \hbar^2 l^2 - \hbar^2 m_{min}^2 + \hbar^2 m_{min} = 0 \\ l^2 = m_{min}^2 - m_{min} \end{gathered} \tag{9.19}$$

If we compare the limits of m we end up with the next result.

$$m_{max}^2 + m_{max} = m_{min}^2 - m_{min} \tag{9.20}$$

This expresion have two solutions:

$$\begin{gathered} m_{max} = m_{min} - 1 \\ m_{max} = -m_{min} \end{gathered} \tag{9.21}$$

The first solution can be discarted because it would imply that m_{max} is less than m_{min}. The second solution is the real one. We know that m increases or decreases by a factor of 1, so we can say that:

$$m_{max} = m_{min} + I \tag{9.22}$$

Where I is an non-negative integer. If we used what we know about the limits of m we can say that:

$$\begin{gathered} m_{max} = -m_{max} + I \\ m_{max} = \frac{I}{2} \end{gathered} \tag{9.23}$$

This means that L_z is quantized, i. e., only some proyections of the angular momentum in the z axis are allowed. We are going to start labeling the eigenfunctions as $|j, m\rangle$ where j is defined by:

$$\begin{gathered} j = m_{max} \\ l^2 = j(j+1) \end{gathered} \tag{9.24}$$

Where j can be the natural numbers or half of them, i.e., j = 0, 1/2, 1, 3/2... Now our eigenfunctions follow:

$$L^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$$
$$L_3|j,m\rangle = \hbar m|j,m\rangle \tag{9.25}$$

For m = j, j-1, j-2,..., -j. The j,m pair make a completeset of (orthogonal) eigenvectors. Following what we know from 6.29:

$$\langle j_1, m_1 \mid j_1, m_2\rangle = 0 \text{ if } m_1 \neq m_2$$
$$\langle j_1, m_1 \mid j_2, m_1\rangle = 0 \text{ if } j_1 \neq j_2 \tag{9.26}$$

We also set the normalization condition:

$$\langle j, m \mid j, m\rangle = 1 \tag{9.27}$$

From now we will move on to what an experimentalist will measure.

9.2 Angular Momentum as a vector operator

We can interpret the angular momentum as:

$$\vec{L} = L_1\hat{i} + L_2\hat{j} + L_3\hat{k} \tag{9.28}$$

In a classical way we know that the angular mometum is conserved, so we can say that all the angular momentum is in one direction.

$$\vec{L}x\vec{L} = (L_2L_3 - L_3L_2)\hat{i} + (L_3L_1 - L_1L_3)\hat{j} + (L_1L_2 - L_2L_1)\hat{k} \tag{9.29}$$

In classical mechanics that product is 0 because the components are numbers but in a quantum way they are operators that doesn't commute, in this case the cross product is:

$$\vec{L}x\vec{L} = i\hbar\vec{L} \tag{9.30}$$

This is the operator equation. On an experiment we can measure the angular momentum of the electron in hydrogen. Assume it is in one state ψ.

$$\int_{-\infty}^{\infty} dxdydz\psi^\star(x,y,z)O\psi(x,y,z) = \text{ Measurement of O} \tag{9.31}$$

We are going to make a distintion between the angular momentum $\vec{L}$, and the measured angular momentum, $\vec{l}$.

$$\begin{gathered}\vec{l} = \langle s|\vec{L}|s\rangle \\ \vec{l} = \langle s|L_1|s\rangle\hat{i} + \langle s|L_2|s\rangle\hat{j} + \langle s|L_3|s\rangle\hat{k}\end{gathered} \tag{9.32}$$

With the next properties:

$$\begin{gathered}\vec{l}x\vec{l} = 0 \\ \vec{l}\cdot\vec{l} = (\langle s|L_1|s\rangle)^2 + (\langle s|L_2|s\rangle)^2 + (\langle s|L_3|s\rangle)^2 \geq 0\end{gathered} \tag{9.33}$$

We want to know the value of this dot product.

$$\begin{gathered}\langle j,m|L_3|j,m\rangle = \hbar m\langle j,m\,|=\rangle\hbar m \\ \langle j,m|L_3^2|j,m\rangle = \hbar^2m^2 = (\langle j,m|L_3|j,m\rangle)^2 \\ \langle j,m|L^2|j,m\rangle = \hbar^2 j(j+1) \\ \langle j,m|L_1^2 + L_2^2|j,m\rangle = \hbar^2(j(j+1) - m^2)\end{gathered} \tag{9.34}$$

To get the value of $\langle j,m|L_1|j,m\rangle$ we have to use the definition of L_+ and L_-.

$$\begin{gathered}\langle j,m|L_1|j,m\rangle = \langle j,m|L_+|j,m\rangle + \langle j,m|iL_-|j,m\rangle = \\ = N_+\langle j,m\,|\,j,m+1\rangle + N_-\langle j,m\,|\,j,m-1\rangle = 0\end{gathered} \tag{9.35}$$

The same argument can be done for L_2. Because of this we can say that:

$$\begin{cases} l_1 = 0 \\ l_2 = 0 \\ l_3 = \hbar m \\ l^2 = ? \end{cases} \tag{9.36}$$

We have two definitions if we consider l^2 as the measure of L^2 is going to be $l^2 = \hbar^2 j(j+1)$, but if we consider l^2 as the square of the measure L we get $\hbar^2m^2$. This is exactly the same as talking about the square of the mean or taking about the variance, so we are familiarize with this concepts from chapter 2.

We said before that the operators L_+ and L_- are proportional to the next or the previous eigenfunctions. Now we want to find the exact value of

the proportionality constant.

$$
\begin{aligned}
{}_{+}|j,m\rangle &= n_{+,j,m}|j,m+1\rangle \\
L_{-}|j,m\rangle &= n_{-,j,m}|j,m-1\rangle \\
\langle j_1,m_1\,|\,j_2,m_2\rangle &= \delta_{j_1,j_2}\delta_{m_1,m_2}
\end{aligned}
\tag{9.37}
$$

We can always find real positive values for both n_+ and n_-. We want them to be like this because we are going to take the conjugate of the expresion above.

$$
\begin{aligned}
\langle j,m|L_{-} &= n_{+,j,m}\langle j,m+1| \\
(\langle j,m|L_{-})(L_{+}|j,m\rangle) &= n^2_{+,j,m}\langle j,m+1\,|\,j,m+1\rangle \\
\langle j,m|(L_1-iL_2)(L_1+iL_2)|j,m\rangle &= n^2_{+,j,m} \\
\langle j,m|L_1^2+L_2^2-\hbar L_3|j,m\rangle &= n^2_{+,j,m} \\
\hbar^2 j(j+1)-\hbar^2m^2-\hbar^2m\langle j,m\,|\,j,m\rangle &= n^2_{+,j,m} \\
\hbar^2[j(j+1)-m(m+1)] &= n^2_{+,j,m}
\end{aligned}
\tag{9.38}
$$

We have finally reach the value of $n_{+,j,m}$. We can write now:

$$
L_{+}|j,m\rangle = \hbar\sqrt{j(j+1)-m(m+1)}|j,m+1\rangle \tag{9.39}
$$

It is easy to prove from this that $L_{+}|j,j\rangle = 0$, as we wanted. We can do the same for L_{-}.

$$
\begin{aligned}
\langle j,m|L_{+} &= n_{-,j,m}\langle j,m-1| \\
(\langle j,m|L_{+})(L_{-}|j,m\rangle) &= n^2_{-,j,m}\langle j,m-1\,|\,j,m-1\rangle \\
\langle j,m|(L_1+iL_2)(L_1-iL_2)|j,m\rangle &= n^2_{-,j,m} \\
\langle j,m|L_1^2+L_2^2+\hbar L_3|j,m\rangle &= n^2_{-,j,m} \\
\hbar^2 j(j+1)-\hbar^2m^2+\hbar^2m\langle j,m\,|\,j,m\rangle &= n^2_{-,j,m} \\
\hbar^2[j(j+1)-m(m-1)] &= n^2_{-,j,m}
\end{aligned}
\tag{9.40}
$$

We can write now:

$$
L_{-}|j,m\rangle = \hbar\sqrt{j(j+1)-m(m-1)}|j,m+1\rangle \tag{9.41}
$$

And for $m = -j$ we get 0 again, as we wanted. Knowing L_+ and L we can get the values for all the three components of the angular momentum.

$$\begin{aligned} L_1 &= \tfrac{L_+ + L_-}{2} \\ L_2 &= \tfrac{L_+ - L_-}{2i} \end{aligned} \tag{9.42}$$

The components of $\vec{L}$ acting on $|j, m\rangle$ are:

$$\begin{aligned} L_1|j,m\rangle &= \tfrac{\hbar}{2}(\sqrt{j(j+1) - m(m+1)}|j, m+1\rangle + \sqrt{j(j+1) - m(m-1)}|j, m-1\rangle) \\ L_2|j,m\rangle &= \tfrac{\hbar i}{2}(\sqrt{j(j+1) - m(m+1)}|j, m+1\rangle - \sqrt{j(j+1) - m(m-1)}|j, m-1\rangle) \\ L_3|j,m\rangle &= \hbar m|j,m\rangle \end{aligned} \tag{9.43}$$

Using the knowledge from chapter 6, if we want to get the excat values for every component of the three operators we can apply 6.16.

$$\begin{aligned} (L_1)_{j_1 m_1, j_2, m_2} &= \langle j_1, m_1|L_1|j_2, m_2\rangle = \tfrac{\hbar}{2}[\sqrt{j_2(j_2+1) - m_2(m_2+1)}\delta_{j_1 j_2, m_1 m_2+1} + \sqrt{j_2(j_2+1) - m_2(m_2-1)}\delta_{j_1 j_2, m_1 m_2-1}] \\ (L_2)_{j_1 m_1, j_2, m_2} &= \langle j_1, m_1|L_2|j_2, m_2\rangle = \tfrac{-\hbar i}{2}[\sqrt{j_2(j_2+1) - m_2(m_2+1)}\delta_{j_1 j_2, m_1 m_2+1} - \sqrt{j_2(j_2+1) - m_2(m_2-1)}\delta_{j_1 j_2, m_1 m_2-1}] \\ (L_3)_{j_1 m_1, j_2, m_2} &= \langle j_1, m_1|L_3|j_2, m_2\rangle = \hbar m_2 \delta_{j_1 j_2, m_1 m_2} \end{aligned} \tag{9.44}$$

We can see at first sight that L_3 has to be a diagonal matrix, while L_1 and L_2 can only have non-zero values on the secondary diagonals. In the next section we will get the values of the matrix for some j.

9.3 Matrix representation for j=1, 1/2, 2

The case for j=0 is a trivial case. We are going to start with j=1, where the set of values for m is m=1,0,-1. We are going to define the matrices as:

$$L_a = \begin{bmatrix} (L_a)_{-1,-1} & (L_a)_{-1,0} & (L_a)_{-1,1} \\ (L_a)_{0,-1} & (L_a)_{0,0} & (L_a)_{0,1} \\ (L_a)_{1,-1} & (L_a)_{1,0} & (L_a)_{1,1} \end{bmatrix} \tag{9.43}$$

Where the subindixes of the components represent m_1 and m_2. We can use the expresions from to get the matrix representation of the angular momentum.

$$L_1 = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, L_2 = \frac{i\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, L_3 = \hbar\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{9.44}$$

Appendix

Notation

The next list describes several symbols that will be later used within the body of the document.

c Speed of light in a vacuum inertial frame

h Planck constant

Greek Letters with Pronunciations

Character	Name	Character	Name
α	alpha *AL-fuh*	ν	nu *NEW*
β	beta *BAY-tuh*	ξ, Ξ	xi *KSIGH*
γ, Γ	gamma *GAM-muh*	o	omicron *OM-uh-CRON*
δ, Δ	delta *DEL-tuh*	π, Π	pi *PIE*
ϵ	epsilon *EP-suh-lon*	ρ	rho *ROW*
ζ	zeta *ZAY-tuh*	σ, Σ	sigma *SIG-muh*
η	eta *AY-tuh*	τ	tau *TOW (as in cow)*
θ, Θ	theta *THAY-tuh*	υ, Υ	upsilon *OOP-suh-LON*
ι	iota *eye-OH-tuh*	ϕ, Φ	phi *FEE, or FI (as in hi)*
κ	kappa *KAP-uh*	χ	chi *KI (as in hi)*
λ, Λ	lambda *LAM-duh*	ψ, Ψ	psi *SIGH, or PSIGH*
μ	mu *MEW*	ω, Ω	omega *oh-MAY-guh*

Capitals shown are the ones that differ from Roman capitals.

Alphabetical Index

preface, v