On the Quantization of Inertia

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Abstract

We study the Klein-Gordon equation (KG) in Newtonian and Schwarzschild space-times to describe the behavior of a scalar particle in an inertial system. We obtain a general Schrödinger equation immerse in these geometries and focus on the gravitational quantum effects. We give some examples where it is possible to study the energy levels, effective potential and the wave function of the systems, these results contain the gravitational effects due to the curvature of space-time.

Abstract (Spanish)

Se estudia la ecuación de Klein-Gordon (KG) en las métricas Newtoniana y de Schwarzschild para describir el comportamiento de una partícula escalar en un sistema inercial. Obteniendo una ecuación general de Schrödinger, la cual está inmersa en dichas geometrías, centrándonos en los efectos cuántico-gravitacionales. A partir de diversos ejemplos donde se estudian los niveles de energía, potencial efectivo, función de onda del sistema, inluyendo los efectos gravitacionales debido a la curvatura del espacio-tiempo.

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Contents

1 Introduction

In this last century, *General Relativity* (GR) and *Quantum Mechanics* (QM), the two pillars of modern physics, have been developed and verified independently with great precision, while quantum physics can describe successfully the behavior of tiny particles such as atoms and electrons, moreover relativity is very accurate for forces at cosmic scales. However, in some cases, the two theories produce incompatible results and there are different definitions for the same concept, an example could be the concept of force, in Einstein's theory the interaction is manifested by the curvature of space-time, in contrast, in quantum theory for the other interactions, such electromagnetism, the exchange of particles is which causes the interactions, this idea of QM on interaction has been extended to have a *Grand Unification Theory* where it is possible to make compatible three of the four fundamental interactions, such as weak and strong nuclear interaction and electromagnetism interaction, this theory gave rise to *Standard Model* of elemental particles, for this model was combined QM with Special Relativity, i.e, relativistic effect of QM in flat space. Gravity is not yet a interaction of Standard Model, but if it is, the mediator particle would be called 'graviton', a massless particle with spin 2.

One of the most important problems in theoretical and fundamental physics is to have an *Unify Theory* where the principal theories in physics, General Relativity and Quantum Mechanics, can be compatible. In the last decades, it has proposed some theories to be *Everything Theory*, these theories contain different ideas to solve the incompatibility between GR and QM, nevertheless the experimental verification of these candidates and their theoretical problems are so complex, as extra dimensions, multiverses, the problem of the time, the renormalization, or the so small interaction with the matter or particles that we just know. Nevertheless, before thinking about the theoretical problems, for which we have not found a *Complete Quantum Gravity Theory*, perhaps, QM or GR are not complete theories

therefore we cannot make them compatible in an Everything Theory. The main question would be *Is Gravity Quantum?*, if the answer is negative, we do not need to continue solving the theoretical problems that have the different candidate theories and we must stop looking for a theory of the unification between GR and QM.
In the last years, several physicist have tried to answer if gravity is a quantum interaction with different proposals for experiments and observations, some proposals are not feasible with the technology today, there is a proposal to detect the graviton measuring the fluctuations of the gravitational waves, however just at 2016 the first gravitational wave was detected by Laser Interferometer Gravitational-Wave Observatory (LIGO), now we do not have the precision for measuring the fluctuations of these gravitational waves, to detect these waves was an incredible work of scientists, thus this idea to detect the graviton should wait some years more.

Other ideas are given by analogies of the quantum effects but now in a curved space-time, there is a proposal experiment that involve the gravity-based entanglement of particle, this proposals is a tabletop experiment that use laser beams and microscopic diamond. The crystals should be in a vacuum to avoid collisions with other atoms, then they should interact between them through only gravity. The diamonds would drop at the same time, if the gravity is a quantum interaction, the gravitational pull each crystal exerts on the other could entangle them together, by shining lasers into each diamond's heart after the drop. If particles in the crystals' centers spin one way, they would fluoresce, however they would not if they spin the other way. With this we could conclude if the gravity is a quantum interaction or not. See [1] for more information about this topic.

Other example is the gravitational Casimir effect[2], analogous to the Casimir effect in QM is the attraction or repulsion seen between two mirrors placed close together in vacuum by virtual photons, now it is suggested superconductors might reflect gravitons more strongly than normal matter. The resulting force could be 10 times stronger than due to the standard Casimir effect with virtual phonon. Nevertheless, the experiment cannot see some gravitational Casimir effect. This null result does not necessarily rule out the existence of gravitons, thus quantum nature of gravity. It could be because gravitons do not interact with superconductors as strongly as prior work estimated.

Using the Weak Equivalence Principle (WEP) that says, the inertial mass of an object is the same as the gravitational mass, but it is not clear that the idea still holds at the quantum level. In paper[3] they add the principle of quantum superposition, since the different energy levels have different masses, then the total mass gets smeared across a range of values, too. This prediction allowed the pair to propose tests that would tease out the quantum behavior of gravitational acceleration. for an object in free fall in a superposition, the entanglement would develop between the internal states of the particle and their position, the particle would actually smear across space as it falls, which would violate the equivalence principle. In fact, some quantum gravity theories predict that equivalence principle will be violated, the tests proposed by[3] could help if these approaches are corrects. They did also other paper[4] on quantum interference of photons in curved space-time, here it had experimental results on this topic.

In this thesis, we do not want to propose a new Everything Theory, rather we want to give a new different way to measure the gravitational effect due to the curvature of space-time on quantum system, specially a scalar particle. Previously, we made mention to some papers on proposal experiments or ideas that their realization will be so complex in these days, nevertheless others where it has just made but the results are not definitive to say if the gravity is or not a quantum interaction but it is a closer path to answer if gravity has quantum nature.

Using the *Einstein Equivalence Principle* (EEP), that says us. At every space-time point in an arbitrary gravitational field it is possible to choose a locally inertial (or freely falling) coordinate system such that, within a sufficiently small region of this point, the laws of nature take the same form as in unaccelerated cartesian coordinate systems in the absence of gravitation[5]. Sometimes it exists a distinction between 'gravitational laws of physics' and 'non-gravitational laws of physics', EEF is defined to apply only to the latter, while the *Strong Equivalence Principle* (SEP) includes all of the laws of physics, i.e., gravitational and otherwise. Another way to enunciate EEP is[6]. The experiments in a sufficiently small freely falling laboratory, over a sufficiently short time, give results that are indistinguishable from those of the same experiments in an inertial frame in empty space.

Since the properties of a non-inertial system are the same as an inertial system when there is a certain gravitational field, we use this principle to develop this work, studying some different examples of QM on an inertial frame immersed in a gravitational field, nevertheless to measure this effects in a laboratory, we will locate a quantum system on a non-inertial frame, hoping to get the same results both in the theoretical part and in the experimental part, also we expect to obtain results on quantization as in QM, this is the reason why we have chosen *On the Quantization of Inertia* as the title of this thesis.

We may hope that a regime exists for quantum aspects of gravity, in which the gravitational field is retained as a classical background, while the matter field are quantized in usual way. A simple dimensional analysis one obtain a relation between of mass M that produces the gravitational field, and the mass m of the scalar particle, which is immersed in the gravitational field, when either quantum and gravitational effects are compared

$$M \sim \frac{e^2}{4\pi\epsilon_0 G}\left(\frac{1}{m}\right) = \frac{3.45x10^{-18}}{m}kg^2,$$

where $m[kg]$, e is electron's charge, ϵ_0 is the permeability at vacuum, G is the universal gravitational constant, all of them in international system of units (SI), from this expression we can obtain for the electron mass m_e, the mass $M \sim 3.8 \times 10^{12}kg$, that makes the gravitational field comparable to quantum effects, on the other hand, the mass of Earth is $\sim 5 \times 10^{24}kg$, i.e., we should measure in Earth the quantum gravitational effects on an electron. It should be noted that if we have a scalar particle with mass $m \sim 10^{-22}eV/c^2$ to see these quantum gravitational effects is necessary to have a mass $M \sim 10^{10}M_{\odot}$, that produces the gravitational field, note that this mass is comparable with the mass of some galaxies or of some Supermassive Black Holes in core of galaxies, this scalar particle is proposed in models of dark matter[7], thus we can say that the galaxies could have a quantum behavior.

Adopting Einstein's general relativity theory as a description of gravity, it is possible to take a quantum field theory in curved background space-time[8], which is based this thesis. In the first chapters from 2 to 5 we will give theoretical foundations that we will use subsequently, reviewing briefly some concepts (without extending in the calculations), that we will need on *Classical Field Theory*, formalism and some applications on *Quantum Mechanics*, later we will see some results on *Quantum Field Theory* for scalar field, the last we give a summary on *General Relativity*. In the last chapters, we combine results of previous chapters where we obtain a description on behavior of scalar field, that is immersed on gravitational field, we find a general Schrödinger equation in Newtonian and Schwarzschild geometries, to solve this differential equation we use perturbation theory from QM, also we propose a general Hamiltonian operator for the Klein-Gordon and the Schrödinger equations in curved background space-time mixing the formalism of QM and GR through a Field Theory.

2 Classical Field Theory

It is necessary to refer to *Classical Field Theory* due to the dynamics of any macroscopic physics phenomenon can be described by this theory, the gravitational and electromagnetism field are fields that use this formalism.

In this case, the systems are formed by a infinity number of degrees of freedom, their motion equations are given by ordinary differential equations.
The Lagrangian and Hamiltonian formalism are adopted in different places of the physics because they can be extended to both *General Relativity* and *Quantum Mechanics*.

2.1 The Principle of Least Action

The Action is a fundamental concept that was introduced in *Classical Mechanics* by the Lagrangian formalism for the systems with a finite number of degrees of freedom. The Action S is defined by [9]

$$S = \int_{t_1}^{t_2} L(q^i(t), \dot{q}_i(t), t)dt \tag{2.1}$$

where $i = 1, 2, ..., N$ and $L(q^i(t), \dot{q}^i(t), t)$ is the Lagrangian function of the system, q_i are the generalized coordinates and we use $\dot{q}^i = \dfrac{dq^i}{dt}$, these generalized coordinates are the degrees of freedom the system.
The Action $S(q^i(t), \dot{q}^i(t), t)$ is a extremal function that compares the trajectories with the same initial and final configurations.

The Action or the Least Action Principle says that the movement of a dynamic system from a configuration $q^i(t_1)$ in a time t_1 to a configuration $q^i(t_2)$ in a time t_2 where the action is extremal

$$\delta S = 0 \tag{2.2}$$

this is an infinitesimal variation on the change of configuration and we can defined this variation by[10]

$$\delta q^i(t) = q'^i(t) - q^i(t) \tag{2.3}$$

the variation in terms of δq^i between q^i at the end and of the actual path and q^i and the end points of the varied path, including the change in end points times.

We can obtained the Euler-Lagrange equations with arbitrary variations $\delta\tilde{q}^i$ in the definition of action.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = 0 \tag{2.4}$$

The Action Principle provides the Euler-Lagrange equations, with these equations obtain the motion equation of the system and they give certain geometry to the solution space of dynamic system. This geometry, called symplectic, is relevant as classical much as quantum mechanics and it can extract both in the Lagrangian and Hamiltonian formalism.

The Euler-Lagrange equations are covariant, i.e., they have the same form under transformations.

The fundamental physics interactions are susceptible to the Lagrangian description.

2.2 Lagrangian Density

The Lagrangian formalism can be generalized to the fields with the previous development, the important difference is that the field has an infinite number of freedom degrees, we have introduced the concept of the Lagrangian function as function of finite number of degrees of freedom .

Now, [9] we define a 4-dimensional space-time with x^μ, $\mu = 0, 1, 2, 3$, conventionally $x^0 = ct, x^1 = x, x^2 = y, x^3 = z$, where c is the speed of light, for simplicity, we consider a metric

$g^{\mu\nu} = diag(-1, 1, 1, 1)$ that is a Minkowski space or flat space although these results can be extended to an arbitrary transformation and arbitrary metric, as we will see later.
We consider a system with N scalar fields $\Phi^{(i)}$, $i = 1, ..., N$, each scalar field is defined in every point of the space-time $\Phi^{(i)} = \Phi^{(i)}(x^\mu)$, we introduce the concept of the Lagrangian density $\mathcal{L}$ that only depends of the fields and their first space-time derivative.

$$\mathcal{L} = \mathcal{L}(\Phi^{(i)}, \partial_\mu \Phi^{(i)}, t) \tag{2.5}$$

The relationship between the Lagrangian L and the Lagrangian density $\mathcal{L}$ is given by

$$L = \int_V \mathcal{L}(\Phi^{(i)}, \partial_\mu \Phi^{(i)}, t) d^3\vec{x} \tag{2.6}$$

where V is the volume, it is only the spatial part.

If we use the definition in eq.(2.1) with the Lagrangian form in eq.(2.6), we obtain the next expression.

$$S = \int_{t_1}^{t_2} \int_V \mathcal{L}(\Phi^{(i)}, \partial_\mu \Phi^{(i)}, t) d^3\vec{x} dt \tag{2.7}$$

In this case, the Action $S = S(\Phi^{(i)}, \partial_\mu \Phi^{(i)})$. If we apply the *Action Principle*, it is possible obtained the Euler-Lagrange equations for the fields (analogous with the previous section) with a arbitrary variation $\delta\Phi^{(i)}$

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi^{(i)})} - \frac{\partial \mathcal{L}}{\partial \Phi^{(i)}} = 0 \tag{2.8}$$

The eq.(2.8) gives the motion equations for the scalar fields, these equations have almost derivatives of the second order.
The Action is a local functional of the fields and their derivate, in a flat space must be invariant for the Poincaré group, nevertheless in a curved space it must be general covariant.[11]

2.3 Hamiltonian Formalism

We start to examine the case when we have a finite number of freedom degrees, then we will analyze when we have an infinity number of degrees of freedom.

The principal difference between the Hamiltonian formalism and the Lagrangian formalism is that the integral of the definition of Action for the Hamiltonian formalism is evaluated in a phase space and for the Lagrangian formalism is evaluated in configuration space. The configuration space uses $q(t), \dot{q}(t)$ as generalized coordinates, for the phase space we use $p(t), q(t)$ as independent coordinates and their time derivatives, where p is a canonical momentum.[10]
Also, we work for a system with n freedom degrees in a N-dimensional configuration space for the Lagrangian formalism and $2N$-dimensional phase space for the Hamiltonian formalism, moreover, the motion equation that we can find for the Lagrangian formalism are N differential equation of second order and for the Hamiltonian formalism we have $2N$ differential equations of first order.

We start to define a Hamiltonian function H of the system.

$$H(p_j, \dot{q}^j, t) = p_j \dot{q}^j - L(p_j, \dot{q}^j, t) \tag{2.9}$$

Using the sum convention (or Einstein convention), it can define the momentum p with relationship of the Lagrangian function.

$$p_j = \frac{\partial L}{\partial \dot{q}^j} \tag{2.10}$$

If we apply the *Action Principle*, but now we consider the Lagrangian function at definition of Hamiltonian eq.(2.9), it is possible obtained the motion equation in terms of $p_j, \dot{q}^j$. Hence the new motion equations are

$$
\begin{aligned}
\dot{p}_j &= -\frac{\partial H}{\partial q^j} \\
\dot{q}^j &= \frac{\partial H}{\partial p_j}
\end{aligned}
\tag{2.11}
$$

Another equation that relates the Lagrangian with Hamiltonian formalism is

$$
\frac{\partial L}{\partial t} = -\frac{dH}{dt} \tag{2.12}
$$

I mean when the Lagrangian function does not depend explicitly of the time, the Hamiltonian is conserved (or it is constant at all time).
The eq.(2.11) and eq.(2.12) are known as the canonical equations of Hamilton.

Nominally, the Hamiltonian for each constructed via the Lagrangian formalism, the formal procedure is:
With a chosen set of generalized coordinates q^i, the Lagrangian function $L(q^i(t), \dot{q}^i(t), t) = T - U$ is constructed, where T is the kinetic energy and U is the potential energy of the system.
The conjugate momenta p_j are defined as function of $q^i, \dot{q}^i, t$.
It is eliminated $\dot{q}$ from H so as so to express it solely as a function of (q, p, t).

When the both next conditions are satisfied, if the equations defining the generalized coordinates do not depend on time explicitly and if the forces are derivable from a conservative potential U (that is, work is independently of the path) then the Hamiltonian H is automatically the total energy E.

$$
H = T + U = E \tag{2.13}
$$

In this point, we have introduced the concept of Hamiltonian for a finite number of degrees of freedom, now we consider the case analogous when we have scalar field (systems with a infinity number of degrees of freedom), it is necessary defined a Hamiltonian density $\mathcal{H}$ as we saw on the previous section with the Lagrangian density, it can relate the Hamiltonian with the Hamiltonian density by

$$H = \int_V \mathcal{H}(\Phi^{(i)}, \pi_{(i)}, t) d^3\vec{x} \tag{2.14}$$

where we consider a system with N scalar fields $\Phi^{(i)}$, $i = 1, ..., N$, each scalar field is defined in every point of the space-time $\Phi^{(i)} = \Phi^{(i)}(x^\mu)$, and we take the Hamiltonian density $\mathcal{H}$ that only depends of the fields and the fields of their conjugate momenta $\pi_{(i)} = \pi_{(i)}(\Phi^{(i)}, \dot{\Phi}^{(i)})$, the analogous way we can define these conjugate momenta and Hamiltonian density respectively, as previously we did it, thus

$$\pi_{(i)} = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}^{(i)}} \tag{2.15}$$

$$\mathcal{H} = \pi_{(i)} \dot{\Phi}^{(i)} - \mathcal{L} \tag{2.16}$$

where $\dot{\Phi}^{(i)} = \partial_0 \Phi^{(i)}$ for a flat space, nevertheless as it was mentioned these concepts can be extended for the curved spaces (but with covariant derivatives)[11].

Every relationship and method for the Hamiltonian formalism with a finite number of degrees of freedom can be extended (similarly) for a Hamiltonian formulation with scalar fields.

3 Quantum Mechanics

At the end of the nineteenth century, it was believed that physics was a complete science in terms of principles until at the beginning of the twentieth century it had many physics fundamental problems that had not an answer, not just because we did not have a method or this method was so complex once known the theory (for example, the gravitational problem of three bodies) else due to they had fundamental problems that could not analyze with the existing theories or in the best of the cases, it was obtained erroneous results, even more meaningless in some cases, the physicists were forced to change the fundamental perception of the physical world.

In the later decades, it was realized hard work to establish a new physics theory to describe the microsystems (atoms, molecules, crystals, etc). This new theory is known *Quantum Mechanics* (QM). This new theory differs from *Classical Mechanics* and it can apply to any quantum system, regardless its size or structure. It was necessary to leave many old ideas and to change well establishing principles, for example, show that Newtonian Mechanics was not applicable to the study of the atom or that Maxwell electrodynamics cannot describe every elemental processes of interaction between atom and its radiation field.[12]

One of the first problems that solved QM was black body radiation, with which this new theory began to have a greater credibility, afterward it resolved other problems and it had more formality that led to the more important postulate which is the *Schrödinger Equation* (SE) that describes the motion of a quantum system.

In the next Chapters, we will refer to this Chapter to compare or to use some results. After *Section 3.2* we will see some important examples of Quantum Mechanics.

3.1 Quantum Mechanics Postulates

The mathematical formalism of Quantum Mechanics was introduced mostly by Paul Dirac [13], who published in 1930 his classical text *The Principles of Quantum Mechanics*, this formulation uses abstract vectors that are denoted by $|\psi\rangle$, called ket or kets, each vector represents the state of a system. The kets are elements of an infinity dimension space, known Hilbert space $\mathcal{H}$. Each ket has a corresponding unique bra vector $\langle\phi|$, which belongs to the dual space of Hilbert $\mathcal{H}^*$. The inner product between these vectors can be represented by $\langle\phi|\psi\rangle$, called *bra-ket*. In addition, Dirac used also operators that represent an observable quantities. Observables quantities are the quantities that we can measure (ej. coordinates, linear or angular momentum, energy).

Another important thing about the Quantum Mechanics formalism is the Square-Integrable Functions, in the case of function spaces, a *vector* element is given by a complex function and the scalar or inner product of two functions $\psi(\vec{r},t)$ and $\phi(\vec{r},t)$ is given by

$$(\psi,\phi) = \int \psi^*(\vec{r},t)\phi(\vec{r},t)d^3r \tag{3.1}$$

if we want the function space to possess a scalar product, we must select only those functions for which (ψ,ϕ) is finite.In particular, a function $\psi(\vec{r},t)$ is said to be square integrable if the scalar product of ψ with itself is finite

$$(\psi,\psi) = \int |\psi(\vec{r},t)|^2 d^3r < \infty \tag{3.2}$$

It is easy to verify that the space of square-integrable functions possesses the properties of a Hilbert space. For instance, any linear combination of square-integrable functions is also a square-integrable function and eq.(3.1) satisfies all the properties of the scalar product of a Hilbert space.

A good example of square-integrable functions is the wave function of quantum mechanics, according to Born's probabilistic interpretation of $\psi(\vec{r},t)$, the quantity $|\psi(\vec{r},t)|^2d^3r$ represents the probability of finding, at time t, the particle in a volume d^3r, centered around the point $\vec{r}$. The probability of finding the particle somewhere in space must then be equal to 1:

$$(\psi, \psi) = \int |\psi(\vec{r}, t)|^2 d^3r = 1 \tag{3.3}$$

hence the wave functions of quantum mechanics are square-integrable. Wave functions satisfying eq.(3.3) are said to be normalized or square-integrable. As wave mechanics deals with square-integrable functions, any wave function which is not square-integrable has no physical meaning in quantum mechanics.

In Dirac Notation, the meaning of a vector is, of course, independent of the coordinate system chosen to represent its components. Similarly, the state of a microscopic system has a meaning independent of the basis in which it is expanded. Dirac denoted the scalar (inner) product by the symbol $\langle|\rangle$, which he called a a bra-ket. For instance, the scalar product (ψ, ϕ) is denoted by the bra-ket $\langle\phi|\psi\rangle$.

There are other different mathematical tools especially linear algebra. The collection postulates, in which the formalism of Quantum Mechanics is based, it involves the idea about observables or vectors that represent states of the system[14].

- **Postulate 1.** The state of any physical system is specified, at each time t, by a state vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$; $|\psi(t)\rangle$ contains all the needed information about the system. Any superposition of state vectors is also a state vector.

- **Postulate 2.** To every physically measurable quantity A, called an observable or dynamical variable, there corresponds a linear Hermitian operator $\hat{A}$ whose eigenvectors form a complete basis.

- **Postulate 3.** The measurement of an observable A may be represented formally by the action of $\hat{A}$ on a state vector $|\psi(t)\rangle$. The only possible result of such a measurement is one of the eigenvalues an (which are real) of the operator $\hat{A}$. If the result of a measurement of A on a state $|\psi(t)\rangle$ is a_n the state of the system immediately after the measurement changes to $|\psi_n\rangle$

$$\hat{A}\,|\psi_n\rangle = a_n\,|\psi_n\rangle\,. \tag{3.4}$$

where $a_n = \langle\psi_n|\psi(t)\rangle$, a_n is a component of $|\psi(t)\rangle$ when projected onto the eigenvector $|\psi_n\rangle$. I mean, if we have a system in an eigenstate $|\psi_n\rangle$, the result of the measurement will be a_n.

In general on eq.(3.4), a_n is a complex number for an arbitrary operator, nevertheless for a Hermitian operator a_n is always a real number, even more the corresponding states to two different eigenvalues are orthogonal. The set of eigenvalues is called spectrum of operator $\hat{A}$.

- **Postulate 4.** When measuring an observable A of a system in a state $|\psi(t)\rangle$, the probability of obtaining one of the non-degenerate eigenvalues a_n is given by

$$P_n(a_n) = |\,\langle\psi_n|\psi\rangle\,|^2 = |c_n|^2 \tag{3.5}$$

where $|\psi_n\rangle$ is the eigenstate of $\hat{A}$ with eigenvalue a_n. If the eigenvalue a_n is m-degenerate, P_n becomes

$$P_n(a_n) = \sum_{j=1}^{m} |\left\langle\psi_n^j\middle|\psi\right\rangle|^2 = \sum_{j=1}^{m} |c_n^{(j)}|^2 \tag{3.6}$$

Even more, the expected value of an observable A on an arbitrary state $|\psi\rangle$ is defined by

$$\left\langle\hat{A}\right\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_n a_n|c_n|^2. \tag{3.7}$$

we have considered that $\psi(\vec{r},t)$ is a normalized function. I mean, $\langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$ (similarly for degenerate or non-degenerate case) and the eigenstates are orthonormal $\langle\psi_n|\psi_m\rangle = \delta_{nm}$.

- **Postulate 5.** The time evolution of the state vector $|\psi(t)\rangle$ of a system is governed by the time-dependent *Schrödinger equation*

$$i\hbar\frac{d\,|\psi(t)\rangle}{dt} = \hat{H}\,|\psi(t)\rangle\,, \tag{3.8}$$

where $\hat{H}$ is the Hamiltonian operator corresponding to the total energy of the system[14]. The Hamiltonian operator $\hat{H}$ is an observable, therefore it must be Hermitian, for a particle with mass m in a potential V is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V} \tag{3.9}$$

Using eq.(3.8) and (3.9) we can obtain depend time Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \hat{V}\psi = \hat{H}\psi \tag{3.10}$$

where $\psi = \psi(\vec{r},t) = \langle\vec{r}|\psi(t)\rangle$ is the state vector or wave function.
If we assume that $\hat{V}$ is time-independent, we can resolve the eq.(3.10) using variable separation, it is obtained

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{3.11}$$

This equation is known as time-independent Schrödinger equation, it can also be rewritten as an eigenvalue equation of Hamiltonian operator

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle\,, \tag{3.12}$$

where E are the eigenvalues of $\hat{H}$ that represent every possible energy values of system, i.e., E is the spectrum of energy.

3.2 Unidimensional Problems

In this Section, we consider three typical examples on Quantum Mechanics, it is shown the most important results without going into so technical details because this results can be seen in any book of Quantum Mechanics [12][14][15][16].

3.2.1 Harmonic Oscillator

The Harmonic Oscillator is one of the most important problems not only in quantum mechanics, it is important in any branch of physics since provides a useful model for a variety of vibrational phenomena that are encountered.
The Hamiltonian of a particle of mass m which oscillates with angular frequency ω under a one-dimensional simple harmonic potential is

$$\hat{H} = \frac{\hat{p}}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{3.13}$$

where $\hat{q}$ and $\hat{p}$ are the canonical position and momentum operator respectively. The problem is to find the energy eigenvalues and eigenstates of this Hamiltonian. This problem can be studied by means of two separate methods but we show only a way, called the ladder or algebraic method, here it is defined the creation and annihilation or ladder operators

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{q} + i\hat{p}), \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{q} - i\hat{p}), \tag{3.14}$$

where $\hat{a}$ is the annihilation operator and $\hat{a}^\dagger$ is the creator operator. Using the canonical commutation relation, $[\hat{q}, \hat{p}] = i\hbar$, we obtain

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{3.15}$$

We define the number operator or occupation number operator $\hat{n}$ that is Hermitian.

$$\hat{n} = \hat{a}^\dagger\hat{a} \tag{3.16}$$

Due to $\hat{H}$ is a linear function of $\hat{n}$, therefore $\hat{H}$ and $\hat{n}$ have the same set of eigenstates $|n\rangle$, called eigenstates of energy.

$$\hat{n}\,|n\rangle = n\,|n\rangle \tag{3.17}$$

We can write the Hamiltonian eq.(3.13) as

$$\hat{H} = \hbar\omega\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right) = \hbar\omega\left(\hat{n} + \frac{1}{2}\right) \tag{3.18}$$

with eq.(3.18) and (3.12) we obtain

$$\hat{H}\,|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega\,|n\rangle \tag{3.19}$$

Hence, the eigenvalues of energy are given by $(n = 0, 1, 2...)$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{3.20}$$

It is easy to proof that the eigenvalue equations of $\hat{a}^{\dagger}$ and $\hat{a}$ are given by

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{3.21}$$

$$\hat{a}^{\dagger}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{3.22}$$

Since the energy of a harmonic oscillator is not negative, we define that

$$\hat{a}\,|0\rangle = 0 \tag{3.23}$$

The eq.(3.22) shows that repeated applications of the operator $\hat{a}$ on $|n\rangle$ generate a sequence of eigenvectors $|n-1\rangle, |n-2\rangle, ...$ Since $n \geq 0$ and since $\hat{a}\,|0\rangle = 0$ this sequence has to terminate at $n = 0$; this is true if we start with an integer value of n. It is similar for eq.(3.21), here the repeated applications of the operator $\hat{a}^{\dagger}$ on $|n\rangle$ generate a sequence of eigenvectors $|n+1\rangle, |n+2\rangle, ...$ Since n is a positive integer, the energy spectrum of a harmonic oscillator is discrete. Thus the energy of ground state or the lowest energy eigenvalue of the oscillator is

not zero but is instead equal to $E_0 = \hbar\omega/2$ when $n = 0$.
It is possible to know any state, if we apply $\hat{a}^\dagger$ multiple times over ground state $|0\rangle$

$$|n\rangle = \left[\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\right]|0\rangle \tag{3.24}$$

Therefore, we must know the solution of ground state from eq.(3.23) and the definition from eq.(3.14), it is easy to show that the solution is

$$\psi_0(x) = \langle x|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{3.25}$$

Combining eq.(3.25) and (3.24) the solution for any eigenstate is

$$\psi_n(x) = \langle x|n\rangle = \left[\frac{1}{2^n n!}\left(\frac{\hbar}{m\omega}\right)^n\right]^{1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\frac{m\omega}{\hbar} - \frac{d}{dx}\right]^n \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{3.26}$$

Also it can expressed in terms of Hermite polynomials $H_n(y)$[17].

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}2^n n! x_0}} \exp\left(-\frac{x^2}{2x_0^2}\right) H_n\left(\frac{x}{x_0}\right) \tag{3.27}$$

where $x_0 = \sqrt{\hbar/(m\omega)}$ and Hermite polynomials have the form

$$H_n(y) = (-1)^n \exp\left(y^2\right)\frac{d^n}{dy^n}\exp\left(-y^2\right) \tag{3.28}$$

3.3 Central Potential (Spherical Coordinates)

We study the structure of the Schrödinger equation for a system of particles moving in a spherically symmetric potential[1] $V(\vec{r}) = V(r)$ it is known as the central potential when the potential depends of the distance r.
First, we treat the problem of two bodies or two particles with an interaction potential. The motion description is through the Schrödinger equation, here, the motion equation of the system of two particles with masses m_i $(i = 1, 2)$ is built from the sum of the Hamiltonian $\hat{H}_i$

[1]We use the vectorial notation $\vec{x} = \mathbf{x}$

of each particle plus potential (or Hamiltonian) of interaction, if this potential depends only the position of the particle, we can write the Hamiltonian operator of the system $\hat{H}$ as

$$\hat{H}(\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2, \mathbf{r}_1, \mathbf{r}_2) = \hat{H}_1(\hat{\mathbf{p}}_1, \mathbf{r}_1) + \hat{H}_2(\hat{\mathbf{p}}_2, \mathbf{r}_2) + V(\mathbf{r}_1, \mathbf{r}_2) \tag{3.29}$$

where the Hamiltonian operator of each particle can be written as

$$\hat{H}_i = \frac{\hat{\mathbf{p}}_i^2}{2m_i} + V_i(\mathbf{r}_i) = -\frac{\hbar^2}{2m_i}\nabla_i^2 + V_i(\mathbf{r}_i) \tag{3.30}$$

where $i = 1, 2$, and $\hat{\mathbf{p}}_i$ represents the momentum of i-th particle, analyzing only the stationary case from eq.(3.11) note that $\psi = \psi(\mathbf{r}_1, \mathbf{r}_2)$ is a function of six variables, three for each particle, in general the wave function has $3N$ variables in a system of N particles. There is a specific physical interest considering that the potential of interaction between the particles depends only of the relative distance $V(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_1 - \mathbf{r}_2)$, the structure of the potential suggests going from the variables $\mathbf{r}_i$ to the relative variable $\mathbf{r}$ and the center of mass $\mathbf{R}$

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 \\ \mathbf{R} &= \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \end{aligned} \tag{3.31}$$

from eq(3.31) is possible to obtain at new coordinates the eq.(3.11) is

$$E\Psi = \left[-\frac{\hbar^2}{2m}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(\mathbf{r})\right]\Psi \tag{3.32}$$

We can solve this differential equation with method of separated variables, it is possible to written $\Psi(\mathbf{R}, \mathbf{r}) = \Phi(\mathbf{R})\psi(\mathbf{r})$ and decomposing the energy $E = E_R + E_r$, where total mass $m = m_1 + m_2$ and reduced mass $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$, with the separated variables is possible to obtain the next pair of equations

$$E_R\Phi(\mathbf{R}) = -\frac{\hbar^2}{2m}\nabla_R^2\Phi(\mathbf{R}) \tag{3.33}$$

$$E_r\psi(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\nabla_r^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) \tag{3.34}$$

For $\Phi(\mathbf{R})$ is obtained the solution of free "particle" with mass m (this particles are mathematically called *quasiparticles*) which position is center of mass coordinates $\mathbf{R}$ with energy E_R. This motion for our objective is irrelevant and we can demand that the system of coordinates of center of mass is at rest ($E_R = 0$, $\Phi = const$).

On the other hand, the differential equation of $\psi(\mathbf{r})$ describes the motion (by Schrödinger equation) of a quasiparticle with reduced mass μ which is affected by a potential $V(\mathbf{r})$.

The separated variables both relative and center of mass coordinates where the potential depends only the relative coordinate $\mathbf{r}$ due to the Hamiltonian is invariant to arbitrary displacement of the origin of coordinates. Therefore, $\hat{H}$ commutes with the total momentum operator $\hat{\mathbf{P}}$ (associated to motion of center of mass), it is an integral of motion that is cancelled at center of mass system. The potential depends only of relative position of particles, as it passes in the Classical Mechanics.

Analogous with the position coordinates, we can obtain the relative and center of mass momentum ($\hat{\mathbf{p}}$ and $\hat{\mathbf{P}}$ respectively) and it is possible to show that the angular momentum is given by $\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2 = \hat{\mathbf{L}} + \hat{\mathbf{l}}$, where $\hat{\mathbf{L}}_i = \hat{\mathbf{r}}_i \times \hat{\mathbf{p}}_i$ with $i = 1, 2$ are the angular momentum for the i-th particle, $\hat{\mathbf{l}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ is the angular momentum of relative motion and $\hat{\mathbf{L}} = \hat{\mathbf{R}} \times \hat{\mathbf{P}}$ is the angular momentum of the center of mass. These variables obey with the quantum laws of independent particles, the commutation relations are $[\hat{r}_i, \hat{p}_j] = [\hat{R}_i, \hat{P}_j] = i\hbar\delta_{ij}$ and $[\hat{R}_i, \hat{p}_j] = [\hat{r}_i, \hat{P}_j] = 0$. This shows that the change of variables is a canonical transformation.

Since the spherical laplacian operator ∇_r^2 is given by

$$\nabla_r^2 = \frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{r^2 sin\theta}\partial_\theta(sin\theta\partial_\theta) + \frac{1}{r^2 sin^2\theta}\partial_\phi^2 \tag{3.35}$$

we can write the Hamiltonian operator as

$$\hat{H} = \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{\mathbf{L}}^2}{2\mu r^2} + V(r) \tag{3.36}$$

Where $\hat{\mathbf{p}}^2 = -\hbar^2\nabla^2$, it is possible write $\hat{\mathbf{p}}^2 = -\hat{p}_r^2 + \hat{\mathbf{L}}^2/r^2$.

In the case for central potentials in eq.(3.34) is easy to solve using the separated variables method[17], we can propose $\psi_{nlm} = R(r)Y_l^m(\theta, \phi)$ where Y_l^m is the spherical harmonic function which are eigenfuctions of $\hat{\mathbf{L}}^2$, i mean, $\hat{\mathbf{L}}^2 Y_l^m = \hbar^2(l+1)Y_l^m$, the radial function $R(r)$ given by the differential equation

$$\left[\frac{\hat{p}_r^2}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right] R(r) = ER(r) \tag{3.37}$$

we can write $E = E_r$, without loss of generality, $\hat{p}_r$ is the conjugate canonical momentum of $\hat{r}$, hence

$$\hat{p}_r^2 = -\frac{\hbar^2}{r^2}\partial_r(r^2\partial_r) = -\frac{\hbar^2}{r}\partial_r^2 r \tag{3.38}$$

Due to the form of $\hat{p}_r^2$ on eq.(3.37) is not a Schrödinger equation, however it can be given the this structure, if we introduce a new radial function $u(r) = rR(r)$, thus eq.(3.37) take the next form

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V\right] u(r) = Eu(r) \tag{3.39}$$

Now, this equation is already an unidimensional Schrödinger equation with an effective potential $V_{eff} = \dfrac{\hbar^2 l(l+1)}{2\mu r^2} + V$. I mean, for a potential central of two particles it is reduced to the unidimensional problem of relative radial motion for a quasiparticle on a potential V_{eff} at region $r \geq 0$.

Since $u(r) = rR(r)$, there a factor $1/r$, it cannot be defined at $r = 0$; and we must give a boundary condition at origin of coordinates, we can observe if $\hat{p}_r^2$ is hermitian (square-integrable function) it can be obtained

$$\int_0^\infty R_2^*(\hat{p}_r R_1)r^2 dr = -i\hbar r^2 R_2^* R_2 \mid_0^\infty + \int_0^\infty R_1(\hat{p}_r R_2^*)r^2 dr \tag{3.40}$$

where R_1 and R_2 are two arbitrary radial functions. Therefore, we see if $lim_{r\to 0}(rR_i) = 0$, $i = 1, 2$, then $\hat{p}_r$ is hermitian operator, if $lim_{r\to 0}(r^2 R_1 R_2^*) = 0$ this is true if we demand the condition $u(0) = 0$. For all of the non-relativistic problems, this boundary condition is sufficient for choosing the acceptable radial solution at the origin, it is equivalent to say that the radial function $R(r) = u(r)/r$ is finite at the origin or the potential V is finite in eq.(3.39) at $r < 0$[12].

3.3.1 Infinite Spherical Well Potential

We use a infinity well potential V but now in spherical symmetry where

$$V(r) = \begin{cases} 0 \quad if \quad 0 < r < a, \\ \infty \quad otherwise. \end{cases} \tag{3.41}$$

This potential can be graphic as Fig.3.1. We find the solution at Region where $0 < r < a$, for the Schrödinger equation with this potential for a particle with mass M and without spin.

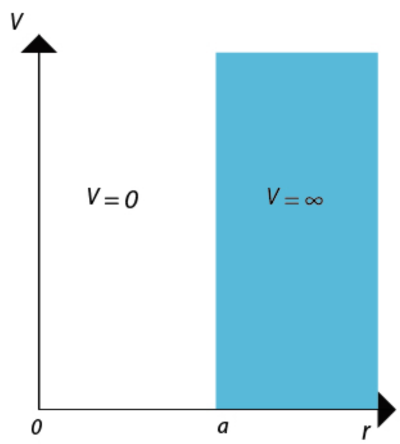

Fig. 3.1: Infinity Spherical Well Potential

It is possible to use the separated variable method to propose the wave function as $\psi_{nlm}(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi)$, where Y_{lm} are spherical harmonic, from eq.(3.37) we can find the radial solution that is given by this differential equation

$$-\frac{\hbar^2}{2Mr^2}\partial_r(r^2\partial_r R) + \frac{l(l+1)\hbar^2}{2Mr^2}R = ER. \tag{3.42}$$

The solution to this differential equation is given by

$$R_l(r) = Aj_l(kr) + Bn_l(kr) \tag{3.43}$$

where $j_l(x)$ are the spherical Bessel functions and $n_l(x)$ are Neumann functions, we define $k^2 = \frac{2ME}{\hbar^2}$, A and B are constants, with boundary conditions and the behavior of the spherical Bessel and Neumann functions, the value of $B = 0$. We must to have at $r = a$, $R(ka) = 0$, therefore $ka = q_{ln}$, where q_{ln} is n-th root of $j_l(x)$. Thus we can obtain the eigenvalue of energy E

$$E_{ln} = \frac{\hbar^2}{2M}\frac{q_{ln}^2}{a^2}. \tag{3.44}$$

Eigenfunction for this problem is given by

$$\langle nlm|r\theta\phi\rangle = \psi_{nlm}(r,\theta,\phi) = A_{ln} j_l\left(\frac{q_{ln}}{a}r\right) Y_{lm}(\theta,\phi), \tag{3.45}$$

where A_{ln} is the constant of normalization

$$A_{ln}^2 = \frac{2}{a^3[j_{l+1}(q_{ln})]^2}, \tag{3.46}$$

the first spherical Bessel functions[14] are

$$\begin{aligned} j_0(x) &= \frac{\sin(x)}{x} \\ j_1(x) &= \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \\ j_2(x) &= \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin(x) - \frac{3\cos(x)}{x^2} \end{aligned} \tag{3.47}$$

It is possible plot these functions to view the behavior of spherical Bessel functions.

3.3.2 Spherical Barrier Potential

Now, we consider the spherical square well potential V for a particle with mass M, this potential is attractive

$$V(r) = \begin{cases} -U_0 & if \quad r < a, \\ 0 & if \quad r > a, \end{cases} \tag{3.48}$$

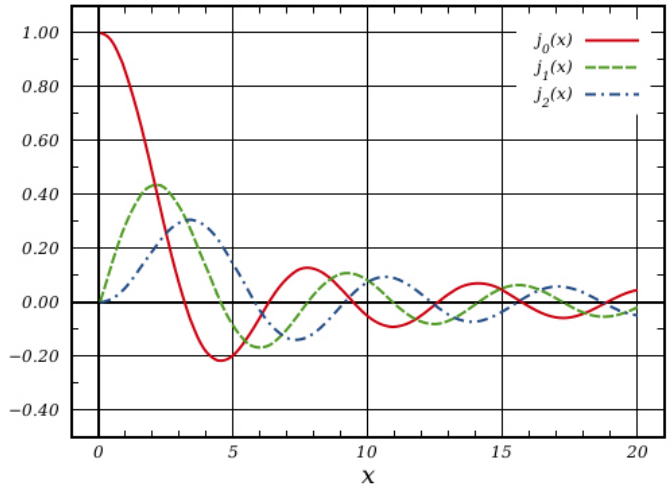

Fig. 3.2: Spherical Bessel Functions from $l = 0$ to $l = 2$.

where $U_0 > 0$ and constant. From Schrödinger equation, we can propose to solve with the separated variables method where $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$, where $Y_{lm}(\theta, \phi)$ are the spherical harmonic functions and $R(r)$ is radial function, which is the solution to radial differential equation where we can separate the problem in two regions, at $Region\ I$ where $0 < r < a$, we must to solve the radial differential equation

$$-\frac{\hbar^2}{2Mr^2}\partial_r(r^2\partial_r R) + \frac{l(l+1)\hbar^2}{2Mr^2}R = (E + U_0)\,R. \tag{3.49}$$

The solution to this differential equation is given as in eq.(3.43) taking the boundary conditions and defining $k_1 = \dfrac{\sqrt{2M(E+U_0)}}{\hbar}$. Hence

$$R_l(r) = Aj_l(k_1 r), \tag{3.50}$$

where A is the constant of normalization and $j_l(x)$ are the spherical Bessel functions.

Now, at $Region\ II$ where $r > a$, here, outside of barrier the particle moves freely and the radial part for its Schrödinger equation is

$$-\frac{\hbar^2}{2Mr^2}\partial_r(r^2\partial_r R) + \frac{l(l+1)\hbar^2}{2Mr^2}R = ER. \tag{3.51}$$

There are two possibilities when the energy has positive or negative value.

When $E < 0$, we have a discrete energy spectrum, this case corresponds to bound states, the solution to eq.(3.51) is similar as in Section 3.3.1, however with the imaginary argument k, defining $k = ik_2$, where $k_2 = \dfrac{\sqrt{-2ME}}{\hbar}$ is a real parameter. The solution to the radial differential equation (3.51) is given by

$$R_l(r) = Bj_l(ik_2r) \pm Bn_l(ik_2r), \tag{3.52}$$

where B is a constant of normalization and $n_l(x)$ are the spherical Neumann functions, whose behavior is shown in Fig.3.3

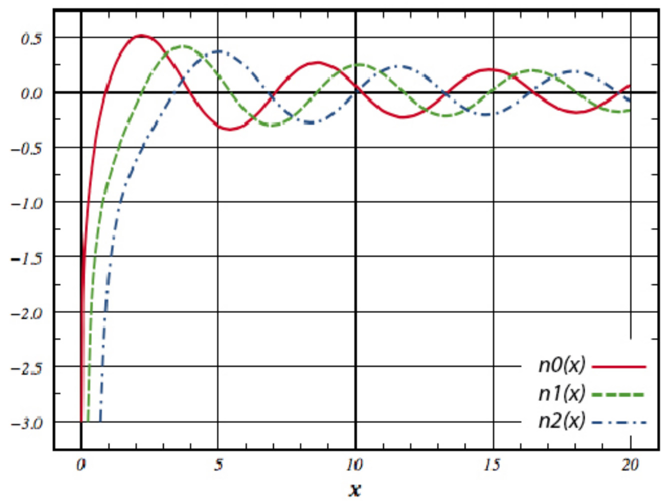

Fig. 3.3: Spherical Neumann Functions from $l = 0$ to $l = 2$.

It is possible to write the Bessel and Neumann functions in terms of the *Spherical Hankel Functions* of First Kind $h_l^{(1)}(x)$ and Second Kind $h_l^{(1)}(x)$[17][14] are defined as follow way

$$h_l^{(1)}(x) = \left(h_l^{(2)}(x)\right)^* = j_l(x) + in_l(x), \tag{3.53}$$

the first spherical Hankel functions of first kind from $l = 0$ to $l = 2$ are explicitly

$$\begin{aligned} h_0^{(1)}(x) &= -\, i\frac{e^{ix}}{x}, \\ h_1^{(1)}(x) &= -\left(\frac{1}{x} + \frac{i}{x^2}\right) e^{ix}, \\ h_2^{(1)}(x) &= \left(\frac{i}{x} - \frac{3}{x^2} - \frac{3i}{x^3}\right) e^{ix}. \end{aligned} \tag{3.54}$$

The asymptotic limit of these functions ($x \to \infty$), we can see the behavior

$$h_l^{(1)}(x) \to -i\frac{e^{i(x-l\pi/2)}}{x}, \tag{3.55}$$

Since the solution must be finite everywhere at large values of r. Only the spherical Hankel function of first kind $h_l^{(1)}(x)$ is finite when $x \to \infty$. Thus the radial solution of eq.(3.51) it can be rewritten as

$$R_l(r) = Bh_l^{(1)}(ik_2r) = Bj_l(ik_2r) + iBn_l(ik_2r), \tag{3.56}$$

with $k_2 = \dfrac{\sqrt{-2ME}}{\hbar}$. The boundary conditions and continuity condition in radial solutions and their derivative at $r = a$, we obtain

$$\frac{1}{h_l^{(1)}(ik_2r)}\frac{dh_l^{(1)}(ik_2r)}{dr}|_{r=a} = \frac{1}{j_l(ik_1r)}\frac{dj_l(ik_1r)}{dr}|_{r=a}. \tag{3.57}$$

For $l = 0$, it reduces to solve the follow transcendental equation

$$-k_2 = k_1 \cot(k_1a). \tag{3.58}$$

In the limit when $|E| << U_0$, we can return the solution for first root, when $l = 0$ as the same in Section 3.3.1, thus $k_1a \approx \pi/2$.
If the energy is positive, then we have a continuous spectrum (unbound or scattering states), where the solution is oscillatory in the asymptotic limit. The solution consists in a linear combination of $j_l(k'r)$ and $n_l(k'r)$, where $k' = \dfrac{\sqrt{2ME}}{\hbar}$. Due to the solution must be finite everywhere, the continuous condition of the solution at $r = a$ determines the coefficients of the linear combination. The particle can be moving freely to infinity with finite kinetic energy

$$E = \frac{\hbar^2}{2M}(k')^2 \tag{3.59}$$

The case when $E < 0$ in the $Region\ II$, we need to solve the transcendental equation, with $k_2 = \gamma_{ln}^*$ is the solution. Hence

$$E_{II} = \frac{\hbar^2}{2M}(\gamma_{ln}^*)^2 = \frac{\hbar^2}{2M}\left(\frac{\sigma_{ln}^*}{a}\right)^2 \tag{3.60}$$

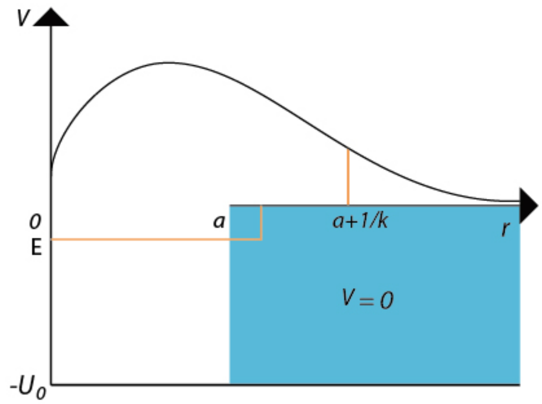

Fig. 3.4: Behavior of wave function in an attractive potential.

Defining a new parameters $\sigma^*_{ln} = a\gamma^*_{ln}$, and $\eta^* = \gamma^*_{ln}/q_{ln}$, if $\eta = 1$, we know just the solution for this problem in the previously section. Furthermore, in the *Region I* the solution to transcendental equation is $k_1 = \gamma_{ln}$. Thus the energy is given by

$$E_I = \frac{\hbar^2}{2M}(\gamma_{ln})^2 = \frac{\hbar^2}{2M}\left(\frac{\sigma_{ln}}{a}\right)^2 \tag{3.61}$$

Analogous to the eigenvalue in *Region II*

3.3.3 Isotropic Harmonic Oscillator

We treat the problem of a particle of mass M in a three-dimensional harmonic oscillator potential that is given by $V = \frac{1}{2}M\omega^2(x^2+y^2+z^2)$, nevertheless the solution of this problem can be seen as the solution of the one-dimensional harmonic oscillator if we propose in Schrödinger equation separated variables for wave function of the form $\psi(x,y,z) = X(x)Y(y)Z(z)$, where the each function $X(x), Y(y), Z(z)$ has the solution as in eq.(3.27) and it is obtained the energy of system is then $E_{n_x n_y n_z} = \hbar\omega(n_x+n_y+n_z+3/2)$. Note that it is a degenerated system, where the energy levels are $E_n = \hbar\omega(n+3/2)$, with $n = n_x + n_y + n_z$, where $n_x, n_y, n_z \geq 0$.

The degree of degeneracy g_n of E_n is therefore equal to the number of different sets that satisfy $n = n_x + n_y + n_z$. It is possible to show that the degree degeneracy g_n is

$$g_n = \frac{(n+1)(n+2)}{2} \tag{3.62}$$

The principal objective for this section is to consider the $V(\mathbf{r})$ like a central potential, i mean, depends only on the distance $r = |\mathbf{r}|$ of the particle from the origin (V(r) is consequently invariant under an arbitrary rotation), this harmonic oscillator is said isotropic which potential can be seen as $V = \frac{1}{2}M\omega^2 r^2$. We do not treat the case anisotropic that is when the potential is given by $V = \frac{1}{2}M(\omega_x^2 x^2 + \omega_Y^2 y^2 + \omega_z^2 z^2)$, where $\omega_x, \omega_y, \omega_z$ are different constants.
We give more attention to Three-dimensional Isotropic Harmonic Oscillator problem, using spherical coordinates (r, θ, ϕ) for a particle with mass M with this potential

$$V(r) = \frac{1}{2}M\omega^2 r^2 \tag{3.63}$$

If we use the Schrödinger equation, proposing separated variables for wave function $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$ where Y_l^m is the spherical harmonic function[17], $R(r)$ is the radial function which is described by the differential equation from eq.(3.39)

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2Mr^2} + \frac{1}{2}M\omega^2 r^2\right]U_{nl}(r) = EU_{nl}(r) \tag{3.64}$$

where $R_{nl}(r) = U_{nl}(r)/r$. The solution for his differential equation is given by

$$R_{kl}(r) = r^l e^{-\gamma r^2} L_k^{(l+1/2)}(2\gamma r^2) \tag{3.65}$$

with $\gamma = \frac{m\omega}{2\hbar}$ and $L_q^p(x)$ is the generalized associated Laguerre polynomial[17].
Therefore the eigenfunction is given by

$$\langle r\theta\phi|klm\rangle = \psi_{klm}(r,\theta,\phi) = N_{kl} r^l e^{-\gamma r^2} L_k^{(l+1/2)}(2\gamma r^2) Y_l^m(\theta,\phi) \tag{3.66}$$

where N_{kl} is the normalized constant and its value is

$$N_{kl} = \sqrt{\sqrt{\frac{2\gamma^3}{\pi}} \frac{2^{k+2l+3} k! \gamma^l}{(2k+2l+1)!!}} \tag{3.67}$$

In addition, it is possible to obtain at once the quantization condition

$$E_{kl} = \hbar\omega(2k + l + \frac{3}{2}) \tag{3.68}$$

but we can rewrite this energy expression as

$$E_n = \hbar\omega(n + \frac{3}{2}) \tag{3.69}$$

where $n = 2k + l$, with $k = 0, 1, 2, ...$

The ground state, whose energy is $E_0 = \frac{3}{2}\hbar\omega$, is not degenerate; the first excited state, $E_1 = \frac{5}{2}\hbar\omega$ is threefold degenerate. Thus, it is possible to show that the degeneracy relation for nth level is given by

$$g_n = \frac{(n+1)(n+2)}{2}$$

This expression is in agreement with eq.(3.62) obtained for an isotropic oscillator in Cartesian coordinates.

3.3.4 Hydrogen Atom

We will give the most important results about Hydrogen Atom problem without explicitly showing the calculations. This is a fundamental atomic physics problem, more general, hydrogenoid atom. To solve this problem, it is about studying the relative motion of an electron around a nucleus with arbitrary positive charge Ze (Z is the atomic number or number of protons in the nucleus). For simplicity, we will ignore their spins.

The potential is given by $V = -\frac{Ze^2}{r}$ with Z positive charges and one negative charge (electron). This potential is known *the Coulomb potential*, however we can define a new constant $Q^2 = Ze^2$, which we call *quadratic charge*, therefore we can rewrite the potential as

$$V = -\frac{Q^2}{r} \tag{3.70}$$

Since the Coulomb potential is a central potential then we can propose the solution for the eigenfunction by separated variables in spherical coordinates (r, θ, ϕ) due to the spherical symmetry $\psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$ in stationary case from Schrödinger equation, nevertheless, for the time-depend Schrödinger equation it is given by $\psi(r, \theta, \phi, t) = R(r)Y_l^m(\theta, \phi)e^{-iEt/\hbar}$, where Y_l^m are the spherical harmonics and $R(r)$ is the radial function given by differential equation eq.(3.39)

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Q^2}{r}\right] U(r) = EU(r) \tag{3.71}$$

where $U(r) = rR(r)$ and μ is the reduced mass. To solve this radial equation, we are going to consider first its asymptotic solutions and then attempt a power series solution.
To obtain physically acceptable solutions from potential series, it is possible to infer the energy E_n, where n is known as the principal quantum number $(n = 1, 2, 3...)$

$$E_n = -\frac{\mu Q^4}{2\hbar^2 n^2} = -\frac{ZQ^2}{2a_0 n^2} \tag{3.72}$$

since (from Bohr theory of the hydrogen atom) the Bohr radius is given by

$$a_0 = \frac{\hbar^2}{\mu e^2} \tag{3.73}$$

The length wave λ is given by $\lambda = 1/(na_0)$. The ground state, when $n = 1$ and $l = 0$, has the energy (for $Z = 1$) $E_1 = -e^2/(2a_0) \simeq -13.6eV$. Thus, for $Z > 1$ and an excited state $n > 1$, we can obtain

$$E_n = -\frac{\mu Q^4}{2\hbar^2 n^2} = -\frac{Z^2 E_1}{n^2} \tag{3.74}$$

The solution for radial wave function of hydrogen atom from eq.(3.71) is given by

$$R_{nl}(r) = N_{nl}\left(\frac{2r}{na_0}\right)^l \exp\left(-\frac{r}{na_0}\right) L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right) \tag{3.75}$$

where $L_p^q(x)$ the associated Laguerre polynomials[17] and N_{nl} is the normalized constant given by

$$N_{nl} = -\left(\frac{2}{na_0}\right)^{3/2}\sqrt{\frac{(n-l-1)}{2n[(n+l)!]^3}} \tag{3.76}$$

Hence, we can write the wave function

$$\langle r\theta\phi|nlm\rangle = \psi_{nlm}(r,\theta,\phi) = N_{nl}\left(\frac{2r}{na_0}\right)^l \exp\left(-\frac{r}{na_0}\right) L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right) Y_l^m(\theta,\phi) \tag{3.77}$$

The energy depends only the principal quantum number n. Only at ground state when $n = 1$ it is not degenerated, for $n > 1$ there are different associated functions to the same energy. The degeneration order is determined by each value of l and there are $2l + 1$ values of m. Since the total number of wave functions are independent linear for n given, the degeneration degree g_n is

$$g_n = \sum_{l=0}^{n-1}(2l+1) = n^2 \tag{3.78}$$

Note that the degeneration of level n of the hydrogen atom is the order n^2. This degeneration has two origins. Since there is not a preferential spacial direction, it is introduced by number m, called magnetic quantum number, also it is the projection of $\hat{\mathbf{L}}$ over z-axis (when it is introduced an external field at a fixed direction, the degeneration is broken). The azimuthal number l represents the magnitude of $\hat{\mathbf{L}}$, that determines its orbital angular momentum and describes the orbit form (if we introduce any additional potential, central, the form of orbit charges and it disappears the degeneration).

The radial wave functions of the hydrogen atom behave as follows:

- They behave like r^l.
- they decrease exponentially at large r, since L_{n+l}^{2l+1} is dominated by the highest power r^{n-l-1}.
- Each function $R_{nl}(r)$ has $n - l - 1$ radial nodes, since L_{n+l}^{2l+1} is a polynomial of degree $n - l - 1$

3.3.5 Kramers Formula

We show the *Kramers formula*[12] for an arbitrary central potential as integer power s of r, which is a recursive formula, considering $V(r) \sim r^s$ in Schrödinger equation. It is possible to prove with the virial generalized theorem the Kramers formula.

$$2E(s+1)\langle r^s \rangle - 2(s+1)\langle r^s V \rangle - \langle r^{s+1} V' \rangle + \frac{\hbar^2}{m} s \left(\frac{s^2-1}{4} - l(l+1) \right) \langle r^{s-2} \rangle = 0 \tag{3.79}$$

This is the most general Kramers formula from here it is possible to obtain a recursive formula for a specific case as a Coulomb Potential $V = -Q^2/r$

$$2E(s+1)\langle r^s \rangle + Q^2(2s+1)\langle r^{s-1} \rangle + \frac{\hbar^2}{m} s \left(\frac{s^2-1}{4} - l(l+1) \right) \langle r^{s-2} \rangle = 0 \tag{3.80}$$

Now, for an Isotropic Harmonic Oscillator Potential $V = m\omega^2 r^2/2$, we can obtain the Kramers formula

$$2E(s+1)\langle r^s \rangle + \frac{1}{2} m\omega^2 (2s+4)\langle r^{s-2} \rangle + \frac{\hbar^2}{m} s \left(\frac{s^2-1}{4} - l(l+1) \right) \langle r^{s-2} \rangle = 0 \tag{3.81}$$

3.4 Time-Independent Perturbation Theory

Most problems in quantum mechanics cannot be solved exactly. The exact solutions of the Schrödinger equation exist only for idealized cases. To solve general problems, it must resort to approximation methods. Though there are other time-independent methods as *The Variational Method* and *WKB Method*, in this section, we focus to study problems with stationary state and time-independent Hamiltonian with *the Time-Independent Perturbation Theory*[14][12].
Perturbation theory is based in the assumption that the problem, that we wish to solve, is slightly different from a problem with an exact solution. When the deviation between two problems is small, the perturbation theory helps to calculate the contribution associated with this deviation, which is added as a correction to the energy eigenvalue and the eigenfunction of the exactly solvable Hamiltonian. Also perturbation theory builds on the known exact

solutions to give an approximate solutions.

For studying approximation methods of stationary states, we can find the energy eigenvalues E_n and the eigenfunctions $|\psi_n\rangle$ of a time-independent Hamiltonian $\hat{H}$ that does not have exact solutions from eq.(3.12).

The perturbation theory is most suitable method when $\hat{H}$ is very close to a Hamiltonian $\hat{H}_0$ that has an exact solution. We can write $\hat{H}$ into two time-independent parts

$$\hat{H} = \hat{H}_0 + \hat{H}_p \tag{3.82}$$

$\hat{H}_p$ is called the perturbation while $\hat{H}_0$ is the Hamiltonian that it can be known the exact solutions, $\hat{H}_p$ is very small in comparison with $\hat{H}_0$, its effect on the energy eigenvalues and eigenfunctions will be small. The simple idea is to write $\hat{H}_p$ in terms of a dimensionless real parameter $\lambda << 1$, thus $\hat{H}_p = \lambda\hat{W}$ combining with eq.(3.12) and eq.(3.82), it is possible to obtain

$$(\hat{H}_0 + \lambda\hat{W})\,|\psi_n\rangle = E_n\,|\psi_n\rangle \tag{3.83}$$

There are two cases depending if the exact solution of $\hat{H}_0$ is degenerate or non-degenerate. Each of there two cases require its own approximation scheme.

3.4.1 Non-degenerate Perturbation Theory

When $\hat{H}_0$ has non-degenerate eigenvalues, which are correspond every energy eigenvalue $E_n^{(0)}$ to only one eigenstate $\left|\psi_n^{(0)}\right\rangle$. I mean

$$\hat{H}_0\left|\psi_n^{(0)}\right\rangle = E_n^{(0)}\left|\psi_n^{(0)}\right\rangle \tag{3.84}$$

The notation with superscript (0) in the exact eigenvalues $E_n^{(0)}$ and exact eigenfunctions $\left|\psi_n^{(0)}\right\rangle$ are known of Hamiltonian $\hat{H}_0$ for making distinction to the corresponding eigenvalues E_n of perturbed (or total) Hamiltonian. The principal idea of perturbation theory consists in assuming that the perturbed eigenvalues and eigenstates can both be expanded in power series in the parameter λ.

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...; \tag{3.85}$$

$$|\psi_n\rangle = \left|\psi_n^{(0)}\right\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \lambda^2 \left|\psi_n^{(2)}\right\rangle + ... \tag{3.86}$$

We might make to assumption that the expansions eq.(3.85) and (3.86) always exist, since the perturbation is sufficiently weak. However, this is not for all the cases. There are some cases with small perturbation but are not expandable in power series, sometimes the series are not convergent. An important detail is when $\lambda = 0$, we return to the unperturbed solutions $E_n = E_n^{(0)}$ and $|\psi_n\rangle = \left|\psi_n^{(0)}\right\rangle$. The notation $E_n^{(k)}$ and $\left|\psi_n^{(k)}\right\rangle$ represent the kth corrections to the eigenenergies and eigenvectors, respectively.
If we job with eq.(3.85), (3.86) and (3.83), we can determine the first three correction. Trivially, the zero-order correction are the known exact solutions given by eq.(3.84). The energy to second-order correction for perturbation is easy to show that.

$$E_n = E_n^{(0)} + \left\langle\psi_n^{(0)}\right| \hat{H}_p \left|\psi_n^{(0)}\right\rangle + \sum_{m \neq n} \frac{|\left\langle\psi_m^{(0)}\right| \hat{H}_p \left|\psi_n^{(0)}\right\rangle|^2}{E_n^{(0)} - E_m^{(0)}} + ... \tag{3.87}$$

The eigenvector to first-order correction

$$|\psi_n\rangle = \left|\psi_n^{(0)}\right\rangle + \sum_{m \neq n} \frac{\left\langle\psi_m^{(0)}\right| \hat{H}_p \left|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}} \left|\psi_m^{(0)}\right\rangle + ... \tag{3.88}$$

In general, we must obtain $E_n^{(1)} = \left\langle\psi_n^{(0)}\right| \hat{W} \left|\psi_n^{(0)}\right\rangle$ nevertheless for simplicity in the notation, we say that

$$E_n^{(1)} = \left\langle\psi_n^{(0)}\right| \hat{H}_p \left|\psi_n^{(0)}\right\rangle \tag{3.89}$$

The same way, for the other results of the eigenvalues and eigenvector, (Without losing generality, we say that $\hat{W} \rightarrow \hat{H}_p$)

$$\left|\psi_n^{(1)}\right\rangle = \sum_{m \neq n} \frac{\left\langle \psi_m^{(0)} \right| \hat{H}_p \left| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} \left|\psi_m^{(0)}\right\rangle \tag{3.90}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{| \left\langle \psi_m^{(0)} \right| \hat{H}_p \left| \psi_n^{(0)} \right\rangle |^2}{E_n^{(0)} - E_m^{(0)}} \tag{3.91}$$

From eq.(3.91), (3.90) and (3.89) in (3.86) and (3.86) is possible to say that

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + ...; \tag{3.92}$$

$$|\psi_n\rangle = \left|\psi_n^{(0)}\right\rangle + \left|\psi_n^{(1)}\right\rangle + \left|\psi_n^{(2)}\right\rangle + ... \tag{3.93}$$

When the first-order correction $E_n^{(1)} = 0$. We need to calculate the higher-order correction. Thus consecutively until some higher-order correction is different to zero.

3.4.2 Degenerate Perturbation Theory

Now, if we consider the level of energy $E_n^{(0)}$ with g-fold degenerate (i.e., there is a set of g different eigenstate $\left|\psi_{n_\alpha}^{(0)}\right\rangle$, where $\alpha = 1, 2, .., g$, for the same energy eigenvalue $E_n^{(0)}$)

$$\hat{H}_0 \left|\psi_{n_\alpha}^{(0)}\right\rangle = E_n^{(0)} \left|\psi_{n_\alpha}^{(0)}\right\rangle \tag{3.94}$$

where α is given by one or more quantum number; the energy eigenvalue is independent of α. Without details of calculus, we only show the most important results, starting to the zeroth-order approximation for eigenfunction $|\psi_n\rangle$, that can be written as a linear combination in terms of $\left|\psi_{n_\alpha}^{(0)}\right\rangle$

$$|\psi_n\rangle = \sum_{\alpha=1}^{g} a_\alpha \left|\psi_{n_\alpha}^{(0)}\right\rangle \tag{3.95}$$

Since $\left|\psi_{n_\alpha}^{(0)}\right\rangle$ is orthonormal with respect to the label α (i.e., $\left\langle\psi_{n_\beta}^{(0)}\middle|\psi_{n_\alpha}^{(0)}\right\rangle = \delta_{\beta\alpha}$) and it must be normalized the wave function with these and from eq.(3.94), it is possible to prove that the next equation of the eigenvalues

$$\sum_{\alpha=1}^{g}\left(\hat{H}_{p_{\alpha\beta}} - E_n^{(1)}\delta_{\alpha\beta}\right)a_\alpha = 0 \tag{3.96}$$

where $\alpha, \beta = 1, 2, ..., g$, with $\hat{H}_{p_{\alpha\beta}} = \left\langle\psi_{n_\alpha}^{(0)}\right|\hat{H}_p\left|\psi_{n_\beta}^{(0)}\right\rangle$ is the $g \times g$ perturbation matrix and $E_n^{(1)} = E_n - E_n^{(0)}$. This is a system of g homogeneous linear equations for the coefficients a_α.These coefficients are non-vanishing only when the determinant $|\hat{H}_{p_{\alpha\beta}} - E_n^{(1)}\delta_{\beta\alpha}| = 0$. This system has a gth degree equation $E_n^{(1)}$, in general it has g different real roots $E_{n_\alpha}^{(1)}$. These roots are the first-order correction to eigenvalues E_{n_α} of $\hat{H}$. Knowing these coefficients, it can be obtain the zero-order correction the eigenfunction from eq.(3.94).

3.4.3 Feynman-Hellman Method

This method is a generalization of the *Feynman-Hellman formula*[12] which establishes that if a hermitian operator $\hat{F}(\lambda)$ depends on a parameter λ, taking $|\psi(\lambda)\rangle$ and $f(\lambda)$ as its eigenvectors and the eigenvalues respectively

$$\langle\frac{\partial\hat{F}}{\partial\lambda}\rangle = \langle\psi(\lambda)|\frac{\partial\hat{F}}{\partial\lambda}|\psi(\lambda)\rangle = \frac{\partial f}{\partial\lambda} \tag{3.97}$$

Generalizing this expression, we assume that $|\psi_n(\lambda)\rangle, |\psi_m(\lambda)\rangle$ are two eigenvectors of $\hat{F}(\lambda)$, with eigenvalues f_n, f_m, respectively, the vectors are orthonormal. It is possible to show that

$$\langle\psi_m|\frac{\partial\hat{F}}{\partial\lambda}|\psi_n\rangle + \frac{1}{2}(f_n - f_m)\left(\frac{\partial\langle\psi_m|}{\partial\lambda}|\psi_n\rangle - \langle\psi_m|\frac{\partial|\psi_n\rangle}{\partial\lambda}\right) = \frac{\partial f_n}{\partial\lambda}\delta_{nm} \tag{3.98}$$

Using $n = m$, we return to Feynman-Hellman formula. In perturbation theory, we take $\hat{F}(\lambda) = \hat{H}_0 + \lambda\hat{W} = \hat{H}_0 + \hat{H}_p = \hat{H}$. Thus

$$\langle\psi_m|\hat{W}|\psi_n\rangle + \frac{1}{2}(E_n - E_m)\left(\frac{\partial\langle\psi_m|}{\partial\lambda}|\psi_n\rangle - \langle\psi_m|\frac{\partial|\psi_n\rangle}{\partial\lambda}\right) = \frac{\partial E_n}{\partial\lambda}\delta_{nm} \tag{3.99}$$

In particular, when $n = m$ we have

$$\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \hat{W} | \psi_n \rangle = \langle \hat{W} \rangle \tag{3.100}$$

From these equations, we can obtain the development on perturbation in a systematic way. Using the Feynman-Hellman formula from (3.97) with $\hat{F} = \hat{H}$ where $\hat{H}$ is the Hamiltonian eq.(3.36) for hydrogen atom with potential $V = -Q^2/r$, if we take $\lambda = Q^2$, we obtain

$$\langle \frac{1}{r} \rangle = \frac{1}{n^2 a_0} \tag{3.101}$$

where a_0 is the Bohr radius, furthermore taking $\lambda = l$, where l and n are quantum numbers, moreover, $n = n(l)$, thus

$$\langle \frac{1}{r^2} \rangle = \frac{2}{n^3 a_0^2 (2l+1)} \tag{3.102}$$

In addition, it is possible to show the next properties combining with Kramers' rule from eq.(3.80)

$$\langle r \rangle = \frac{1}{2} \Big[3n^2 - l(l+1) \Big] a_0 \tag{3.103}$$

$$\langle r^2 \rangle = \frac{1}{2} n^2 \Big[5n^2 + 1 - 3l(l+1) \Big] a_0^2 \tag{3.104}$$

$$\langle \frac{1}{r^3} \rangle = \frac{2}{a_0^3 n^3 l(l+1)(2l+1)} \tag{3.105}$$

$$\langle \frac{1}{r^4} \rangle = \frac{4[3n^2 - l(l+1)]}{a_0^4 n^5 l(l+1)(2l+1)[(2l+1)^2 - 4]} \tag{3.106}$$

Now, for $\hat{F} = \hat{H}$ with the Isotropic Harmonic Oscillator Hamiltonian $\hat{H}$ from eq.(3.36) with (3.63), using $\lambda = \omega$ it is easy to show with Feynman-Hellman formula

$$\langle r^2 \rangle = \frac{\hbar}{M\omega} (n + \frac{3}{2}) \tag{3.107}$$

Now, taking $\lambda = l$ and recalling that $n = 2k + l$, where n, k, l are quantum numbers, we obtain

$$\langle \frac{1}{r^2} \rangle = \frac{2M\omega}{\hbar(2l+1)} \tag{3.108}$$

We can continue using the Kramers' formula as the previous case, nevertheless it is easy to look at eq.(3.81), it cannot solve for odd-power of s of $\langle r^s \rangle$ with s integer negative or positive, since with this method we find less equations that unknown,using this method we can only assure that the system is only solved for s even (negative or positive integer).
Other property that we can use is that

$$\langle r^s \rangle = \langle nlm | \, r^s \, | nlm \rangle = \langle nl | \, r^s \, | nl \rangle \tag{3.109}$$

where $|nlm\rangle$ is the eigenvector of the Hamiltonian of Atom Hydrogen or Isotropic Harmonic Oscillator, respectively and s is an integer number.

4 Quantum Field Theory

To understand the fundamental laws governing elementary particles has to grapple with the principles of *Quantum Field Theory* (QFT) which is the best theory currently available to describe the world around us and, in a particular the *Quantum Electrodynamics* (QED), is the most accurately tested physical theory.

We do not know if a full theory of *Quantum Gravity* (QGT) will be some kind of quantum upgrade of *General Relativity* (GR).

The ideas making up quantum field theory have fundamental consequences. They explain why all electrons are identical due to each electron is an excitation of the same electron quantum field and therefore they all have the same properties. QFT constrains the symmetry of the representations of the permutation symmetry group of any class of identical particles, some classes obey the Fermi–Dirac statistics and others the Bose–Einstein statistics. Interactions in quantum field theory involve products of operators which are found to create and annihilate particles and so interactions correspond to processes in which particles are created or annihilated.

The Field is an object that takes the position in space-time and can be given the amplitude of something at that point in space-time, the amplitude can be a scalar, a vector, a complex number, a spinor or tensor.

In classical physics, gravity and electromagnetism are fields, that can be described their behavior by a set of equations. The field can oscillate in space and time, thus wave-like excitations of the field. This has been observed in electromagnetic and gravity waves. The advantage of quantum mechanics is to remove the distinction between wake-like and particle-like objects. Therefore even matter itself is an excitation of a quantum field and quantum fields become the fundamental objects which describe reality[18].

For this work, we study only a scalar field for simplicity nevertheless in recent years, the studio of scalar field has had a great interest since the Higgs field is a fundamental scalar field and there are some theories about dark matter as scalar field.

4.1 Canonical Quantization

Although there are several types of quantization, the canonical quantization is not the only. This process is analogous to quantum mechanics, an advantage of this process is that we have some results in QM that can apply, other advantage is that we can use the Lagrange-Hamilton formalism that it is very well suited to the analysis of symmetries, a crucial aspect of gauge theories. The important disadvantage with this mechanism is to consider to the time as a special coordinate respect to the spacial coordinates, due to General Relativity is a covariant theory, i mean, there is not a distinction of coordinates.

We now turn to classical mechanics which we want to review. We define the Poisson bracket $\{A, B\}_{PB}$ by

$$\{A, B\}_{PB} = \frac{\partial A}{\partial q^i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q^i} \tag{4.1}$$

Considering any function F which depends on the coordinates q^i and p_i, using the Hamilton's equations. Thus if the field is not itself a function of time, we have

$$\frac{dF}{dt} = \{F, H\}_{PB} \tag{4.2}$$

so that if $\{F, H\}_{PB} = 0$, then F is a constant of motion. This result is entirely classical. In QM, the rate of change of the expectation value of an operator $\hat{F}$ is given by

$$\frac{d\langle F\rangle}{dt} = \langle [F, H]\rangle \tag{4.3}$$

We are led to visualize the classical to quantum crossover as involving the replacement $\{F, H\}_{PB} \to (1/i\hbar)\langle [F, H]\rangle$, in fact for any Poisson bracket $\{A, B\}_{PB} \to (1/i\hbar)\langle [A, B]\rangle$.

We have introduced the 'coordinate-like' field $\phi(x^\mu)$ from Classical Mechanics and also 'momentum-like' field $\pi(x^\mu)$. To pass to the quantized version of the field theory, we follow in the discrete case and promote both the quantities ϕ, π to operator $\hat{\phi}, \hat{\pi}$ in the Heisenberg picture. As usual, the distinctive feature of quantum theory is the non-commutativity of certain basic quantities in the theory, for example, the fundamental commutator of the discrete case $[\hat{q}^r, \hat{p}_s] = i\hbar\delta^r_s$. Thus we expect that the operators will obey some commutation relation which is a continuum generalization. Thus the fundamental commutator of quantum field theory is taken to be[19][8]

$$\left[\hat{\phi}(t,\mathbf{x}), \hat{\phi}(t,\mathbf{x}')\right] = \left[\hat{\pi}(t,\mathbf{x}), \hat{\pi}(t,\mathbf{x}')\right] = 0 \tag{4.4}$$

$$\left[\hat{\phi}(t,\mathbf{x}), \hat{\pi}(t,\mathbf{x}')\right] = i\hbar\delta^{n-1}(\mathbf{x}-\mathbf{x}') \tag{4.5}$$

The field $\hat{\phi}, \hat{\pi}$ are Heisenberg picture operator, that obey the equations of motion

$$\dot{\hat{\phi}}(\mathbf{x},t) = \frac{1}{i\hbar}\left[\hat{\phi}, \hat{H}\right] \qquad \dot{\hat{\pi}}(\mathbf{x},t) = \frac{1}{i\hbar}\left[\hat{\pi}, \hat{H}\right] \tag{4.6}$$

We may note that this formalism encompasses both the wave and the particle aspects of matter and radiation. From the discrete nature of the energy spectrum and the associated operators $\hat{a}, \hat{a}^\dagger$ [1] which refer to individual quanta i.e. particles[19]. For the state when $n(k) = 0$ for all k, i.e. the state with no quanta in it, in our new interpretation, no particles in it. It is therefore the vacuum. However, this has an important implication for the particle interpretation: since the state is symmetric under interchange of the particle labels k_1 and k_2, it must describe identical bosons.

Suppose we form a state containing one quantum of the $\hat{\phi}$ field, with momentum k'

$$|k'\rangle = N\hat{a}^\dagger(k')\,|0\rangle \tag{4.7}$$

where N is normalization constant. The field modes and their respectively complex conjugates form a complete orthonormal basis with scalar product, so $\hat{\phi}$ may be expanded

$$\hat{\phi}(t,\mathbf{x}) = \sum_k \left[\hat{a}_k u_k(t,\mathbf{x}) + \hat{a}^\dagger_k u^*_k(t,\mathbf{x})\right] \tag{4.8}$$

[1]These are annihilation and creation operators analogous to Harmonic Oscillator problem, this problem can possible be generalized to more one particle.

where mode field is given by $u_k = [2\omega(2\pi)^{n-1}]^{1/2} e^{i\mathbf{k}.\mathbf{x}-i\omega t}$ The equal time commutation relations for $\hat{\phi}$ and $\hat{\pi}$ are the equivalent to

$$[\hat{a}_k, \hat{a}_{k'}] = \left[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\right] = 0 \tag{4.9}$$

$$\left[\hat{a}_k, \hat{a}_{k'}^\dagger\right] = \delta_{kk'} \tag{4.10}$$

and $u_{\mathbf{k}}$ are normalized functions. $(u_{\mathbf{k}}, u_{\mathbf{k'}}) = i\hbar\delta^{n-1}(\mathbf{k} - \mathbf{k}')$

4.2 Schrödinger equation from Lagrangian

We consider the non-relativistic Lagrangian, without the self-interaction, but in the presence of an external potential V which enters as $V\psi\psi^*$. The Lagrangian density for complex scalar field with the external potential is given by

$$\mathcal{L} = -\frac{i\hbar}{2}\left(\psi^*\dot{\psi} - \psi\dot{\psi}^*\right) + \frac{\hbar^2}{2m}\nabla\psi.\nabla\psi^* - V\psi\psi^* \tag{4.11}$$

where $\partial_0\psi = \dot{\psi}$. From the Euler-Lagrange equation (2.8), where the fields are ψ, ψ^*, yields the Schrödinger equation and the complex Schrödinger equation, we will not work with the complex Schrödinger equation. Thus

$$-i\hbar\frac{\partial}{\partial t}\psi - \frac{\hbar^2}{2m}\nabla^2\psi + V\psi = 0 \tag{4.12}$$

From eq.(2.15) it is possible to obtain the momenta

$$\pi_1 = \pi_2^* = \frac{i\hbar}{2}\psi \tag{4.13}$$

where π_2 is the associated momentum to ψ. From eq.(2.16) yields to the density Hamiltonian to the Schrödinger equation.

$$\mathcal{H} = \frac{\hbar^2}{2m}\nabla\psi.\nabla\psi^* + V\psi\psi^* \tag{4.14}$$

Applying $H = \int_V \mathcal{H} d^3\vec{x}$, it is possible to show that

$$H = \int_V \psi^* \left[-\frac{\hbar^2}{2m}\nabla^2 + V \right] \psi d^3\vec{x} = \langle\psi| \hat{H} |\psi\rangle = \langle\hat{H}\rangle \tag{4.15}$$

We can identify that return to the already known from QM at eq.(3.10), the momenta and fields obey the relations (4.4) and (4.5). Note that there is a significant difference to the Hamiltonian, the density Hamiltonian and the operator Hamiltonian. These objects are not the same, they have a different fundamental meaning.

4.3 Klein-Gordon Equation

The *Klein-Gordon* equation (KG) was the first step at relativistic quantum mechanics. Returning to QM from the Schrödinger equation of a free particle, we start with the dispersion relationship, which links the energy and momentum of the particle using the simple expression for kinetic energy, unlike from non-relativistic QM when momentum $\hat{\mathbf{p}}$ and energy $\hat{E}$ operator are $\hat{\mathbf{p}} = -i\hbar\nabla$ and $\hat{E} = i\hbar\frac{\partial}{\partial t}$. In other hand from relativistic particle we know that

$$E^2 = \mathbf{p}^2c^2 + (mc^2)^2 \tag{4.16}$$

Replacing on the Schrödinger equation we can obtain

$$\left(-\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \nabla^2 \right) \phi(\mathbf{x}, t) = \left(\frac{mc}{\hbar} \right)^2 \phi(\mathbf{x}, t) \tag{4.17}$$

We try to be consistent with the units for future possible calculations. Nevertheless, it uses natural units where $\hbar = c = 1$ this gives us the following form of the Klein–Gordon equation

$$\left(\partial^2 - m^2 \right) \phi(\mathbf{x}, t) = 0 \tag{4.18}$$

The KG equation fits in nicely with our relativistically covariant language, thereby there is not difference between space and time derivatives[2].

[2]Using the notation $\partial^2 = \partial_\mu\partial^\mu = \partial_\nu\eta^{\nu\mu}\partial_\mu$ where $\eta = diag(-, +, +, +)$

This equation has a problem due to probability current. The probability density ρ and probability current density[3] **J** obey a continuity equation, in covariant form is given by

$$\partial_\mu J^\mu = 0 \tag{4.19}$$

From non-relativistic QM we use the spatial part, with this and eq.(4.19), it is possible to show that covariant probability current for the KG equation is then given by

$$J^\mu = i\left[\phi^* \partial^\mu \phi - \left(\partial^\mu \phi^*\right)\phi\right] \tag{4.20}$$

Substituting in our wave function $\phi = Ne^{-\mathbf{p}\cdot\mathbf{x}}$ the time-like component of the probability current as $J^0 = \rho = 2|N|^2 E$. Since E can be positive or negative we cannot interpret ρ as a probability density, since there's no such thing as negative probability.

The Lagrangian density yields the KG equation with an external potential V, it is given by

$$\mathcal{L} = \partial^\mu \phi^* \partial_\mu \phi - V(\phi, \phi^*) \tag{4.21}$$

with this Lagrangian density is possible to obtain the KG equation applying to the Euler-Lagrange equation for ϕ^* field

$$\partial_\mu \partial^\mu \phi - \frac{dV}{d\phi^*} = 0 \tag{4.22}$$

This is known as a complex scalar field theory. Although we originally made it up from two sorts of field, we can imagine that it describes one sort of complex-valued field ϕ. The Lagrangian from eq.(4.21) is invariant with respect to rotations in the complex plane

$$\phi \to \phi e^{i\alpha}, \quad \phi^* \to \phi^* e^{-i\alpha}$$

which express a $U(1)$ symmetry[4][18].

[3] In non-relativistic QM, **J** is defined by $\mathbf{J} = -(i\hbar/2m)(\psi^* \nabla \psi - \psi \nabla \psi^*)$

[4] $U(1)$ is the one-dimensional group pf unitary transformations. Note that $SO(2)$ is isomorphic to $U(1)$.

5 General Relativity

In 1905, Albert Einstein published three article, on light quanta, on the foundations of the theory of *Special Relativity* (SR), and on Brownian motion. These publications changed the way to look at physics. After Special Relativity, Einstein looked for giving a realistic invariant formulation about gravity. To culminate *General Relativity Theory* (GR) later many trials and errors, it was presented in 1915. It is considered one of the most beautiful theory, which was derived from pure thought and physical intuition explaining, or at least describing, still today, more than 100 years later, every aspect of gravitational physics ever observed.

The principal idea of Einstein on GR was the (local) equivalence of gravitation and inertia, now is more known the *Einstein Equivalence Principle*. This theory does not describe the physical external forces like a force of nature, rather it is a manifestation of the *geometry and curvature of space-time* itself[20].

We will not see all the formalism on GR, we will give only the most important results on GR that we will use in the next chapters [11][8].

5.1 Principle of Minimal Coupling

From the Principle of General Covariance (analogous to the Action Principle from Section 2.1) that says, by the Einstein Equivalence Principle, a generally covariant equation will be valid in an arbitrary gravitational field provided that it is valid in Minkowski space in inertial coordinates. The fact that the covariant derivative ∇ maps tensor to tensors and reduces to the ordinary partial derivative in a locally inertial coordinate system suggests the following procedure or algorithm for obtaining equations that satisfy the Principle of General Covariance[11].

Replace the coordinates ξ^a by arbitrary coordinates x^μ, the Minkowski metric η_{ab} by the metric $g_{\mu\nu}$ that describes the gravitational field, a partial derivative $\partial_a = \partial_{\xi_a}$ by covariant derivative ∇_μ, the 4-D volume element $d^4\xi = dtd^3x$ by $\sqrt{-diag(g_{\mu\nu})}d^4x = \sqrt{-g}d^4x$.

Using the minimal coupling, we can rewrite the KG equation in flat space from eq.(4.21). It is possible to write the covariant action in general gravitational field for the KG equation in a external or potential or the self-interaction, or massive scalar field, where $\mathcal{V} = \mathcal{V}(\Phi, \Phi^*)$

$$S = \int d^4x\sqrt{-g}\left[-g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi^* - \mathcal{V}\right] \tag{5.1}$$

The equation of motion for Φ^* is derived from this is

$$\Box\Phi - \frac{d\mathcal{V}}{d\Phi^*} = 0 \tag{5.2}$$

This equation is the KG covariant equation. This is not (yet) a dynamical field, though, just the gravitational background field. With

$$\Box = g^{\mu\nu}\nabla_\mu\nabla_\nu = \frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu) \tag{5.3}$$

where $\Box$ is the Laplacian or D'Alembertian operator associated to the metric $g_{\mu\nu}$. For flat space eq.(5.2) returns to eq.(4.18), this is precisely what one would have obtained by applying the minimal coupling description.

5.2 Newtonian Limit

We want to find the relation of these potentials to the Newtonian potential, and the relation between the geodesic equation and the Newtonian equation of motion for a particle moving in a gravitational field, we have the general relativistic equation of motion to reduce a linear equation from the Newtonian mechanics,

$$\phi = -\frac{GM}{r} \tag{5.4}$$

where ϕ is the gravitational potential, G is the Newtonian constant, M is the total mass of the relativistic source. The Newtonian gravity is known to be valid when the gravitational fields are too weak to produce velocities near the speed of light $|\phi|/c^2 << 1$, $|v|/c << 1$. The Newtonian gravity, of course, has no gravitational waves, so the ordering is just what we need if we want to reproduce Newtonian gravity in general relativity.
The metric (5.5) called Newtonian gives the correct Newtonian laws of motion[11][20]

$$ds^2 = -\left(1 + \frac{2\phi}{c^2}\right) dt^2 + \left(1 - \frac{2\phi}{c^2}\right) dx_i dx^i \tag{5.5}$$

This equation completes from the Einstein equations that Newtonian gravity is a limit case for GR. Most astronomical systems are well-described by Newtonian gravity as a first approximation. But there are many systems for which it is important to compute the corrections beyond Newtonian theory. These are called post-Newtonian effects, which in the Solar System include the famous fundamental tests of general relativity, such as the precession of the perihelion of Mercury and the bending of light by the Sun.
For any source of the full Einstein equations, we demand within a limited region of space (a localized source), if we go so far from it, its gravitational field, becomes weak enough that linearized theory applies in that region. We say that such a space-time is asymptotically flat at large distances from the source.

5.3 Schwarzschild Geometry

The *Schwarzschild geometry* is the geometry of the vacuum of the space-time outside a spherical star. It is given by the Schwarzschild metric

$$ds^2 = -\left(1 - \frac{2GM}{rc^2}\right) c^2 dt^2 + \left(1 - \frac{2MG}{rc^2}\right)^{-1} dr^2 + r^2 d\Omega^2 \tag{5.6}$$

where $d\Omega^2 = d\theta^2 + sen^2\theta d\phi^2$. Its importance is not just that it is the gravitational field of a star: we shall see that it is also the geometry of the spherical black hole. In natural units $2M = 2GM/c^2$, the mass M is the parameter that determines the geometry.

If we think on a star more compact than the Sun, but with the same mass, the scape velocity would be greater. Therefore it is possible to have a star that the scape velocity were greater that velocity of light, then the star would be dark, or invisible. For a spherical star, we can obtain the relation of critical size of star that would be invisible.

$$r_{sch} = \frac{2GM}{c^2} \tag{5.7}$$

this relation is known as the Schwarzschild radius r_{sch}.

To understand the casual structure of the Schwarzschild geometry, the radial null curve satisfy

$$\frac{dt}{dr} = \pm \left(1 - \frac{2GM}{rc^2}\right)^{-1} \tag{5.8}$$

In a (t, r)-digram, dt/dr represents the slope of the lightcones at a given value of r, in the limit $r \to r_{sch}$, we have $dt/dr \to \pm\infty$, the coordinate velocity goes to zero at $r = r_{sch}$, but this time for null rather than time-like geodesics.

For more suitable description at the region around r_{sch}. We can use new radial coordinate r^*, known as the Eddington–Finkelstein radial coordinate or tortoise coordinate

$$r^* = r + r_{sch} \ln\left(\frac{r}{r_{sch}} - 1\right) \tag{5.9}$$

$$ct = \pm r^* + cte \tag{5.10}$$

From eq.(5.8) describing the radial lightcones.

Lines of constant $t - r^*$ describes outgoing lightrays and lines of constant $t + r^*$ describes ingoing lightrays. Then the metric (5.6) with this new coordinates is

$$ds^2 = \left(1 - \frac{r_{sch}}{r}\right)\left(-c^2dt^2 + dr^2\right) + r^2 d\Omega^2 \tag{5.11}$$

In 1960, it was published new good coordinates are known as Kruskal–Szekeres coordinates given by (for $r > r_{sch}$)

$$\tau = \sqrt{\frac{r}{r_{sc}} - 1}\, \exp\left(\frac{r}{2r_{sc}}\right) \sinh\left(\frac{ct}{2r_{sc}}\right) \tag{5.12}$$

$$R = \sqrt{\frac{r}{r_{sc}} - 1}\, \exp\left(\frac{r}{2r_{sc}}\right) \cosh\left(\frac{ct}{2r_{sc}}\right) \tag{5.13}$$

For $r < r_{sch}$

$$\tau = \sqrt{1 - \frac{r}{r_{sc}}} \exp\left(\frac{r}{2r_{sc}}\right) \cosh\left(\frac{ct}{2r_{sc}}\right) \tag{5.14}$$

$$R = \sqrt{1 - \frac{r}{r_{sc}}} \exp\left(\frac{r}{2r_{sc}}\right) \sinh\left(\frac{ct}{2r_{sc}}\right) \tag{5.15}$$

This transformation is singular at $r = r_{sch}$, but that is necessary in order to eliminate the coordinate singularity there. With these coordinates we can prove the metric (5.6)

$$ds^2 = \frac{4r_{sc}^3}{r} \exp\left(-\frac{r}{r_{sc}}\right)(-d\tau^2 + dR^2) + r^2 d\Omega^2 \tag{5.16}$$

6 General Hamiltonian Operator

We study a Hamiltonian Operator in General Relativity from the Lagrangian density that yields the KG covariant equation afterwards we analyze the limit when we obtain the Schrödinger equation. QFT uses usually the Hamiltonian density as Hamiltonian operator and the fields as operators, nevertheless no always, they are not the same objects. An important example is shown from Section 4.2 when we have studied the case of Lagrangian density for the Schrödinger equation in flat space, where it was analyzed the difference between the Hamiltonian, the Hamiltonian density and the Hamiltonian operator, it can be feasible to believe for other the Lagrangian density or equivalent the Hamiltonian exists this difference. Despite in General Relativity, we can assume that there is an evolution parameter, which in a limit to flat space it is possible to compare this evolution parameter with what we know as 'time', this problem is important for to have a physical unify theory, this problem is called *Problem of Time*[21], since in QM and QFT the 'time' is a privileged parameter, while GR says that should not exist a privileged direction and the space and the time are only one.

6.1 General Hamiltonian Operator for KG

The action that yields us to the covariant KG equation is given by eq.(5.1), we can take the Lagrangian density[22] as

$$\mathcal{L} = \sqrt{-g}\left(-g^{\mu\nu}\nabla_{\mu}\Phi\nabla_{\nu}\Phi^{*} - \mathcal{V}\right) \tag{6.1}$$

since $\mathcal{V} = \mathcal{V}(\Phi, \Phi^*)$, it is possible to write $\mathcal{V} = V\Phi\Phi^*$, if we make a distinction between spatial parameters and we assume that there is an evolution parameter, which will be labeled for $\mu = 0$, thus we can separate eq.(6.1) in spatial and evolution part

$$\mathcal{L} = \sqrt{-g}\left(-g^{00}\nabla_0\Phi\nabla_0\Phi^* - g^{0j}\nabla_0\Phi\nabla_j\Phi^* - g^{i0}\nabla_i\Phi\nabla_0\Phi^* - g^{ij}\nabla_i\Phi\nabla_j\Phi^* - V\Phi\Phi^*\right) \quad (6.2)$$

where the index $\mu, \nu = 0, ..., n$ and $i, j = 1, ..., n$. We use a similar formalism from Section 4.1 where it was used the Canonical Quantization, from eq.(2.15) it is obtained

$$\pi_1 = \sqrt{-g}\left(-g^{00}\nabla_0\Phi - g^{i0}\nabla_i\Phi\right) \quad (6.3)$$

$$\pi_2 = \pi_1^* = \sqrt{-g}\left(-g^{00}\nabla_0\Phi^* - g^{0i}\nabla_i\Phi^*\right) \quad (6.4)$$

where π_1, π_2 are the conjugate momenta, now from eq.(2.16) we can obtain the Hamiltonian density

$$\mathcal{H} = \sqrt{-g}\left(-g^{00}\dot{\Phi}\dot{\Phi}^* + g^{ij}\nabla_i\Phi\nabla_j\Phi^* + V\Phi\Phi^*\right) \quad (6.5)$$

we use indistinct form the notation $\dot{\Phi} = \nabla_0\Phi$, $\nabla^0\Phi = g^{0i}\nabla_i\Phi$, if we take $n-1$ spatial parameters and one evolution parameter, from eq.(2.14) and working with spacial part though the Gauss Theorem, the Hamiltonian is written by

$$H = \int dx^{n-1}\sqrt{-g}\left[-g^{00}\dot{\Phi}\dot{\Phi}^* + \frac{1}{2}g^{ij}\left(-\Phi\nabla_i\nabla_j\Phi^* - \Phi^*\nabla_j\nabla_i\Phi\right) + V\Phi\Phi^*\right] \quad (6.6)$$

Now, working the part of evolution parameter, it is possible to obtain that the Hamiltonian

$$H = 2Re\int dx^{n-1}\sqrt{-g}\Phi^*\left[-\frac{1}{2}g^{00}\left(\frac{1}{2}\nabla_0^2(ln(\Phi\Phi^*)) + \nabla_0(ln(\Phi\Phi^*))\nabla_0 - \nabla_0^2\right)\right.$$
$$\left. -\frac{1}{2}g^{ij}\nabla_i\nabla_j + V\right]\Phi \quad (6.7)$$

If we remember scalar product and expectation value of $\hat{H}_{KG}$, since the scalar field is complex $H = \langle\hat{H}_{KG}\rangle + \langle\hat{H}_{KG}\rangle^* = 2Re\langle\hat{H}_{KG}\rangle$ and we think $dx^{n-1}\sqrt{-g}$ as the proper differential of volume then the Hamiltonian operator for the KG equation $\hat{H}_{KG}$

$$\hat{H}_{KG} = -g^{00}\left(\frac{1}{2}\nabla_0^2(ln(\Phi\Phi^*)) + \nabla_0(ln(\Phi\Phi^*))\nabla_0 - \nabla_0^2\right) - g^{ij}\nabla_i\nabla_j + V \quad (6.8)$$

From the KG equation, note that $\hat{H}_{KG}$ can also write

$$\hat{H}_{KG}\Phi = g^{00}\left(\frac{1}{2}\nabla_0^2(ln(\Phi\Phi^*)) + \nabla_0(ln(\Phi\Phi^*))\nabla_0\right)\Phi \tag{6.9}$$

As in Section 4.1 for Φ, Φ^*, π_1, π we can impose the canonical commutation relations

$$\left[\Phi(x^0, \mathbf{x}), \Phi(x^0, \mathbf{x}')\right] = \left[\pi(x^0, \mathbf{x}), \pi(x^0, \mathbf{x}')\right] = 0 \tag{6.10}$$

$$\left[\Phi(x^0, \mathbf{x}), \pi(x^0, \mathbf{x}')\right] = \frac{i\hbar}{\sqrt{-g}}\delta^{n-1}(\mathbf{x} - \mathbf{x}') \tag{6.11}$$

We have noted that the Hamiltonian (6.7), the Hamiltonian density (6.5) and the Hamiltonian operator (6.8) are different objects.

6.2 General Hamiltonian Operator for Schrödinger

Now, we consider a scalar field as $\Phi = \Psi e^{-i\omega t}$, where for simplicity it is said that $x^0 = t$ is the evolution parameter and ω is a frequency parameter, if we apply at this transformation to the scalar field from eq.(6.7) it is possible to obtain by analogous way the General Operator Hamiltonian for Schrödinger or the Hamiltonian Operator for the Schrödinger equation in curved space $\hat{H}_S$

$$\begin{aligned}\hat{H}_S = &- g^{00}\left(\frac{1}{2}\nabla_0^2(ln(\Psi\Psi^*)) + \nabla_0(ln(\Psi\Psi^*))\nabla_0 - \nabla_0^2 + 2i\omega\nabla_0 + \omega^2\right) \\ &- g^{ij}\nabla_i\nabla_j + V\end{aligned} \tag{6.12}$$

If we make the approximations to first order and in flat space with $\omega = mc^2/\hbar$, it is obtained the known the Hamiltonian operator for the Schrödinger equation in eq.(3.11).

It is important to be very noticeable that there are difference between the Hamiltonian density and the Hamiltonian operator, we have obtained a general Hamiltonian from the KG to the Schrödinger equation, we look at in curved space there are additional terms that in flat space we do not have, it is important to research what is the effect to curved space to the

Schrödinger equation or, in other words, to what we already know Quantum Mechanics of scalar field.

The problem here is the known Problem of Time, we have privileged the evolution parameter due to in QM and QFT in specific for the canonical quantization or in the Schrödinger equation, the evolution parameter plays a significantly role as the time, that we do not what is, nevertheless we can measure it and it is a common thing for us in flat space.

7

Klein-Gordon in the Schwarzschild Geometry

In this Section, we treat to analyze the quantum behavior close to a Black Hole, here there is an intense gravitational field, for simplicity this analysis will be on scalar field, to describe this behavior in this geometry we will study the KG covariant equation in the Schwarzschild background that is given by the Schwarzschild metric from eq.(5.6). Unlike what was shown in the previous section, we will study only the case of a free scalar particle with mass m, neither it will consider the self-interaction parameter, affected by the curvature of space-time, we will see that the equations are so complex to solve.

Considering the covariant KG equation (5.2) in the Schwarzschild geometry given by eq.(5.6), thus, it is possible to obtain the equation of motion from KG

$$-\left(1-\frac{2GM}{rc^2}\right)^{-1}\partial_0^2\Phi+\nabla^2\Phi-\frac{2GM}{r^2c^2}\partial_r(r\partial_r)-\frac{d\mathcal{V}}{d\Phi^*}=0 \tag{7.1}$$

where ∇^2 is the spherical laplacian, however we do not use this expression, it is more convenient to use the Eddington-Finkelstein (or tortoise) coordinates, it given by eq.(5.11) in the KG covariant equation (5.2), we can obtain

$$\left(1-\frac{2GM}{rc^2}\right)^{-1}(-\partial_0^2+\partial_{r_*}^2)\Phi+\Delta\Phi-\frac{d\mathcal{V}}{d\Phi^*}=0 \tag{7.2}$$

where $\triangle$ is the 2D laplacian for spherical solid angle, it is given by

$$\triangle=\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta)+\frac{1}{r^2\sin^2\theta}\partial_\phi^2 \tag{7.3}$$

Since we have taken a free scalar field then $\frac{d\mathcal{V}}{d\Phi^*} = \frac{m^2c^2}{\hbar^2}\Phi$. Considering the transformation $\Phi(t,\vec{x}) = \Psi(t,\vec{x})\exp(-i\omega t)$ as previous cases in the past section due to we can give an interpretation like QM but in a curved space closes to Black Hole. Although we can make the approximation $\ddot{\Psi} \approx 0$ due to the variation on the time is slow, also we have that $\omega = \frac{mc^2}{\hbar}$. Therefore the motion equation is

$$i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\partial^2_{r_*}\Psi - \frac{\hbar^2}{2m}\Delta\Psi - \frac{GMm}{r}\Psi + \frac{GM\hbar^2}{mc^2r}\Delta\Psi \tag{7.4}$$

Using separated variable method for this differential equation, it is possible to write $\Psi(t,r,\theta,\phi) = R(r)Y_{lj}(\theta,\phi)\exp\left(-i\frac{\omega_{nl}}{\hbar}t\right)$.

From the properties of spherical harmonics Y_{lj}[17] we know that $\triangle Y_{lj} = -\frac{l(l+1)}{r^2}Y_{lj}$. Consequently it is easy to shown that the radial motion equation is as follows

$$\omega_{nl}R = -\frac{\hbar^2}{2m}\partial^2_{r_*}R + \frac{\hbar^2 l(l+1)}{2mr^2}R - \frac{GMm}{r}R - \frac{GM\hbar^2 l(l+1)}{mc^2r^3}R \tag{7.5}$$

This equation is like-Schrödinger radial equation, therefore we can identify terms like-potential V and effective potential V_{eff}, hence

$$V(r) = -\frac{GMm}{r} - \frac{GM\hbar^2 l(l+1)}{mc^2r^3} \tag{7.6}$$

$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{GMm}{r} - \frac{GM\hbar^2 l(l+1)}{mc^2r^3} \tag{7.7}$$

Furthermore, note that the effective potential and potential depend explicitly of r, while in radial equation (7.5) the radial momentum is for r_*. If we wish to know how is the motion of particle through the potential because of the fact that is an equation like-Schrödinger, then the potential and effective potential must depend to r_* and not of r, hence we can use the relations

$$r_* = r + r_{sch}\ln\left(\frac{r_*}{r_{sch}} - 1\right) \qquad\qquad \frac{r}{r_{sch}} = 1 + W\left(\frac{r_*}{r_{sch}} - 1\right) \tag{7.8}$$

where W is the Lambert W function[23].

With this, we can make a plot in fig 7.1 for the potential and effective potential, being these

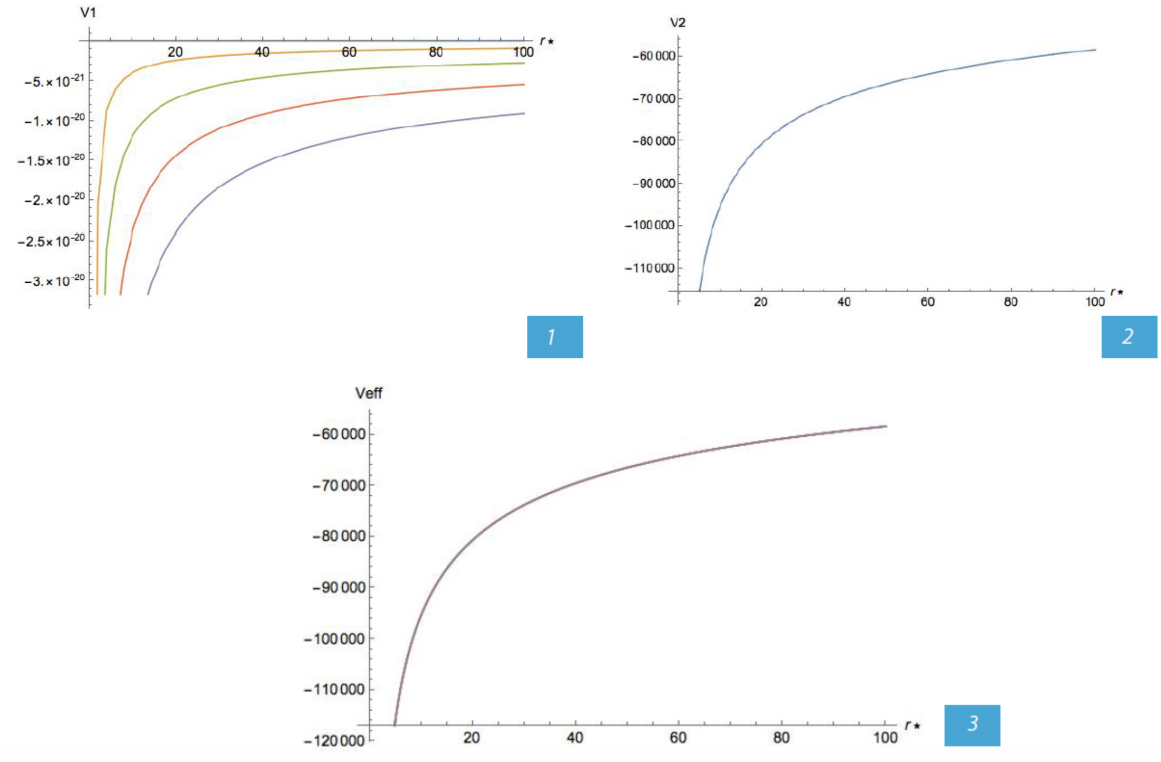

Fig. 7.1: *(1)* Plot V_1 vs r_*, where $V_1 = -\dfrac{GMm}{r}$; *(2)* Plot V_2 vs r_*, where $V_2 = -\dfrac{GM\hbar^2 l(l+1)}{mc^2r^3}$; *(3)* Plot V_{eff} vs r_*, where V_{eff} is defined in eq.(7.6). The scale of every quantity in these plots is in Schwarzschild radius, i.e., $r_* = r_*[r_{sch}]$, $V_1 = V_1[V_1/r_{sch}]$, $V_2 = V_2[V_2/r_{sch}]$ and $V_{eff} = V_{eff}[V_{eff}/r_{sch}]$.

the motion that the particle could follow For $r_{sch} < r < \infty$ goes to zero quite rapidly as $r \to \infty$ or $r \to r_{sch}$, it is equivalent to tortoise coordinates to say that $r \to +\infty \Leftrightarrow r_* \to +\infty$ and $r \to r_{sch} \Leftrightarrow r_* \to -\infty$, this is the reason because of the tortoise coordinates has this name. This means that at infinity (in r) and near the horizon, the solutions of this equation can be chosen to have the standard right-moving (outgoing) / left-moving (ingoing) form

$$\Psi(t, r_*) \sim e^{\pm i\omega(t-r_*)} = e^{\pm i\omega u} \quad or \quad \Psi(t, r_*) \sim e^{\pm i\omega(t+r_*)} = e^{\pm i\omega v} \tag{7.9}$$

However, this does not mean that a mode having the above form near infinity, say, evolved from a mode that had also had such a form near the horizon. Rather, the almost infinite exponential gravitational redshift between the near-horizon and asymptotic regions leads to an exponential relation between the parameter u, say, labelling an outgoing wave at infinity,

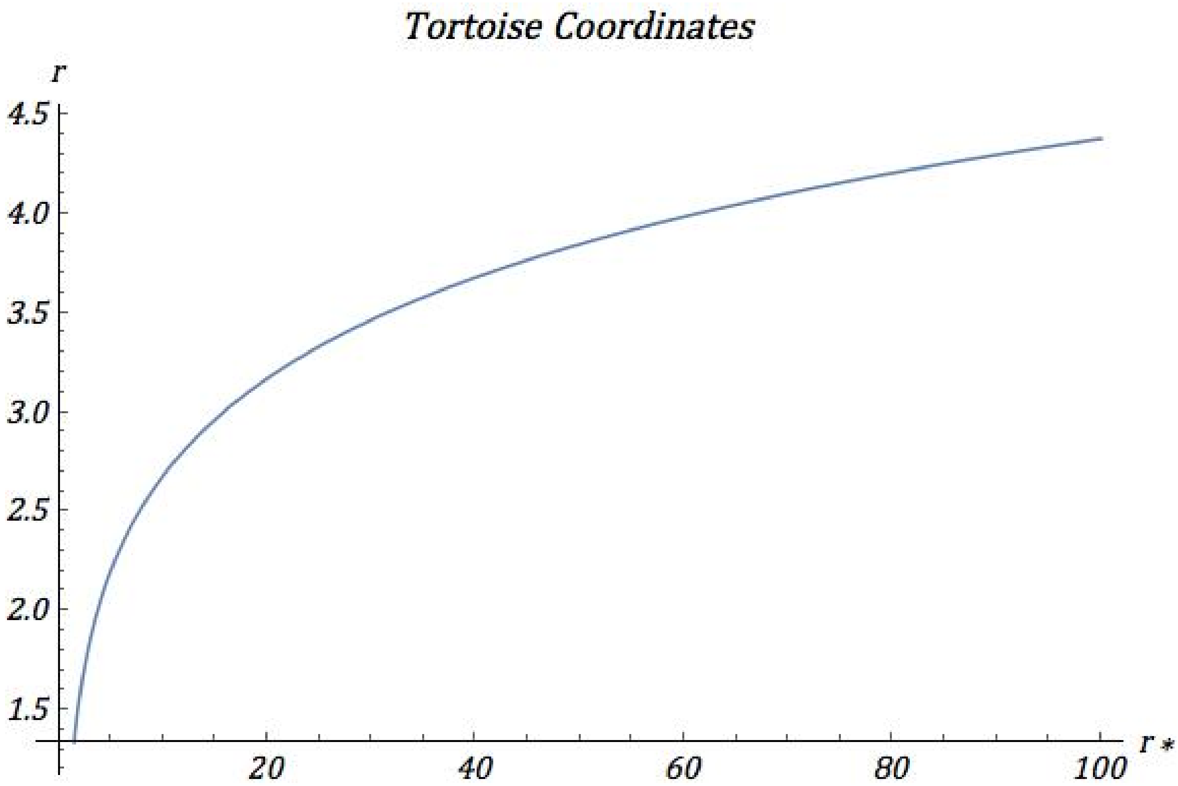

Fig. 7.2: We can view the behavior of Tortoise Coordinate from eq.(7.8) with W-Lambert function, where $r[r_{sch}]$ and $r_*[r_{sch}]$

and the corresponding parameter near the horizon.

For the Schwarzschild metric it is encoded in the precisely analogous between the coordinates u, v and the Kruskal-Szekeres coordinates τ , R to be introduced previously from eq.(5.14). These observations are at the heart of the called the *Hawking Effect*, i.e. the quantum radiation of the black holes.[11]

If we wish to study the dynamic of quantum system of a scalar field inside a Black Hole, it is possible if we use the Kruskal-Szekeres coordinates due to with these coordinates we can see at region where $r < r_{sch}$, this new geometry on the KG covariant equation, it will be possible to analyze the quantum dynamic on a Black Hole, with these coordinates from eq.(5.16) rewriting the metric

$$ds^2 = \frac{4r_{sch}^3}{r}\exp\left(-\frac{r}{r_{sch}}\right)(-d\tau^2 + dR^2) + r^2 d\Omega^2$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$, the Kruskal-Szekeres coordinates are given by (τ, R, θ, ϕ), introducing this metric on the KG covariant equation from eq.(5.2) and taking a free scalar field with mass m in natural units where $\hbar = c = 1$, we can show that

$$-\partial_\tau(r^2\partial_\tau\Phi) + \partial_R(r^2\partial_R\Phi) + 4rr_{sch}^3\exp\left(-\frac{r}{r_{sch}}\right)[\triangle\Phi - m^2\Phi] = 0 \tag{7.10}$$

for obtaining an equation like-Schrödinger as it was done in the previous cases, if we could find this equation, it would be possible to identify the terms that play the role of the potential, but we rewrite only this expression like

$$-\partial_\tau^2\Phi + \partial_R^2\Phi + \frac{4r_{sch}^3\exp\left(-\frac{r}{r_{sch}}\right)}{r}\left[\frac{1}{rr_{sch}}\left[\tau\partial_\tau\Phi + R\partial_R\Phi\right] - \frac{l(l+1)}{r}\Phi - m^2\Phi\right] = 0 \tag{7.11}$$

At first instance, we can propose a separated variables for solving this equation to the spatial part and evolution parameter part $\Psi = f(\tau, R)Y_{lj}(\theta, \phi)$, nevertheless, we have several problems, it is necessary to find a solution in terms of the Kruskal-Szekeres coordinates, in eqs (7.10) and (7.11) but $r = r(R, \tau)$ and $t = t(R, \tau)$, moreover the relations are given by

$$R^2 - \tau^2 = \left(\frac{r}{r_{sc}} - 1\right)\exp\left(\frac{r}{r_{sc}}\right) \tag{7.12}$$

$$\frac{r}{r_{sc}} = 1 + W\left(\frac{R^2 - \tau^2}{e}\right) \tag{7.13}$$

We find ourselves facing the problem of time[21], since we do not know what is the parameter of evolution and what is the spacial parameter, if we want to write the Schrödinger equation, we need a temporal partial or a partial derivative of evolution parameter, nevertheless if we do not know what would be this parameter, we cannot write this equation, when we are in curved space-time, there is not a privileged direction, the 'time' is only a parameter like any spatial parameter. We could to solve this equation with some numerical method, however this is not the object of this thesis, although the solution of $f(\tau, R)$ could be described the dynamic of quantum behavior of a scalar field inside a black hole. The problem of time is an open problem on physics, there are several ways or proposals to solve but there is still no convincing solution *ad hoc* to every interpretation or place where this problem appears, perhaps when this problem is resolved, we will be closer to having an unified theory in physics.

8

Klein-Gordon in the Newtonian Geometry

We did study different and well-known cases of QM, now it is analyzed the gravitational effect due to curvature to the space-time on a quantum system which, for simplicity, will be a scalar field, that is described by the KG equation since it is a covariant equation. The geometry or metric for this analysis will be Newtonian eq.(5.5), in this limit we can consider a small perturbation to the known solutions of QM, these perturbations could be observed on Earth. For every case that will be studied in this chapter, it is taken the transformation for scalar field as $\Phi(t,\vec{x}) = \Psi(t,\vec{x})e^{-i\omega t}$, where the evolution parameter $x^0 = t$ since we try to compare in some limit this parameter with the evolution parameter in flat space, also $\omega = mc^2/\hbar$ where m is the mass of scalar field, c is speed of light in the vacuum, we can interpret the function Ψ as wave function, analogous to QM interpretation. We know from the KG equation (5.2), it can make $\mathcal{V}(\Phi,\Phi^*) = V\Phi\Phi^*$, in general, it is possible to have for a complex scalar field $V = \dfrac{m^2c^2}{\hbar^2} + \dfrac{n\lambda}{2} + V_0$, here λ is the auto-interaction parameter, however this term is so small respect to others, that we take $n = 0$, for a simple dimensional analysis for obtaining an equation like- Schrödinger with an external potential V_0 which becomes to $\dfrac{2m}{\hbar^2}V_0$, therefore we use

$$V = \frac{m^2c^2}{\hbar^2} + \frac{2m}{\hbar^2}V_0 \tag{8.1}$$

where V_0 is any potential. With these arguments, we can obtain from eq.(5.2) in the Newtonian geometry, taking the transformation of the scalar field, it is possible to have

$$\frac{\hbar^2}{2m}\Box\Psi + \left(1+\frac{2U}{c^2}\right)^{-1}\left(i\hbar\frac{\partial\Psi}{\partial t} + \frac{mc^2}{2}\Psi\right) - \frac{\hbar^2}{2m}V\Psi = 0 \tag{8.2}$$

where $U = -GM/r$ is the gravitational potential, approaching for $\partial_0^2\Phi \approx 0$ since the evolution of this function is so small, also $U/c^2 < 1$, and we can ignore terms of major or equal order than $\left(\frac{2U}{c^2}\right)^2$. From eq.(8.2) with the approximations, we obtain

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi + \left(V_0 + \frac{2U}{c^2}V_0 - \frac{2\hbar^2 U}{mc^2}\nabla^2\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{8.3}$$

This equation is the motion equation that we will use for comparing different solutions of QM in flat space with the new curvature, in this case Newtonian geometry. Used the *Perturbation Theory* from Section 3.4 for different problems that we have seen in Chapter 3, and we will compare with the perturbation due to the curvature of space-time.

8.1 Free Particle

If we consider a free particle with mass m (mass of scalar field) under the influence of a gravitational field, in eq.(8.3) using an external potential $V_0 = 0$ but having the gravitational potential $U = -GM/r$, it can be obtained

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi - \frac{2\hbar^2 U}{mc^2}\nabla^2\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{8.4}$$

this is an equation like-Schrödinger, nevertheless if we take only Schrödinger equation with the gravitational potential, we would not have the term $-\frac{2\hbar^2 U}{mc^2}\nabla^2$, this correction is given because we have taken the KG equation and not only the formalism of QM, although the treatment on these equations will be in the QM formalism. Using the Perturbation Theory, we can write a principal Hamiltonian operator $\hat{H}_0$ and a perturbed Hamiltonian operator $\hat{H}_p$, where

$$\hat{H}_0\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi - \frac{GMm}{r}\Psi \tag{8.5}$$

$$\hat{H}_p\Psi = -\frac{2\hbar^2 U}{mc^2}\nabla^2\Psi = \frac{4U}{c^2}\left(\frac{\hat{P}^2}{2m}\right)\Psi = \frac{4U}{c^2}(E_n^{(0)} - mU)\Psi \tag{8.6}$$

Then the total Hamiltonian operator $\hat{H}\Psi = (\hat{H}_0 + \hat{H}_p)\Psi = E_n\Psi$. Analyzing the principal Hamiltonian, note that is the hydrogen atom problem, whose solution are well-known from Section 3.3.4, where quadratic charge Q^2 is now GMm, while the hydrogen atom problem $Q^2 = \frac{e^2}{4\pi\epsilon_0}$ (in SI). It can calculate the order of magnitude of the mass M that produces the curvature of space-time, it can be done this analysis if we compare the potential (or to compare Q^2 for both cases)

$$M \sim \frac{e^2}{4\pi\epsilon_0 G}\left(\frac{1}{m}\right) = \frac{3.45x10^{-18}}{m}kg^2, \tag{8.7}$$

This analysis is for different masses of a scalar field $m[kg]$, where we can obtain

$m(kg) =$	$M(kg) =$
m_e	$3.8x10^{12}$
1	$3.4x10^{-18}$
10	$3.4x10^{-19}$
$m_p \sim 10^{-27}$	$3.4x10^{9}$
$1.5x10^{-48}$	$M_\odot$

where m_e and m_p are the mass of electron or of proton respectively, $M_\odot$ ($\sim 2 \times 10^{30}kg$) is the solar mass this is a dimensional comparison between m and M when could have a quantum behavior, if we make the same analysis for a ultralight particle with mass $m \sim 10^{-22}eV/c^2$, which is considered in Scalar Field Dark Matter (SFDM)[7], for this it can obtain a mass $M \sim 10^{40}kg \sim 10^{10}M_\odot$, I mean, this is the mass that has a galaxy, we can say that the galaxy has a quantum behavior, if there is a scalar field with mass $m \sim 10^{-22}eV/c^2$.

Although we do not compare the same problem that is a free particle with spherical symmetry in QM and when it is in a curved space, our comparison is only dimensional for this reason, we have compared the hydrogen atom problem in QM in flat space with free particle in QM in curved space. The next problems that we will study, they will be compared from the same problem both in QM with and without curvature of space-time.

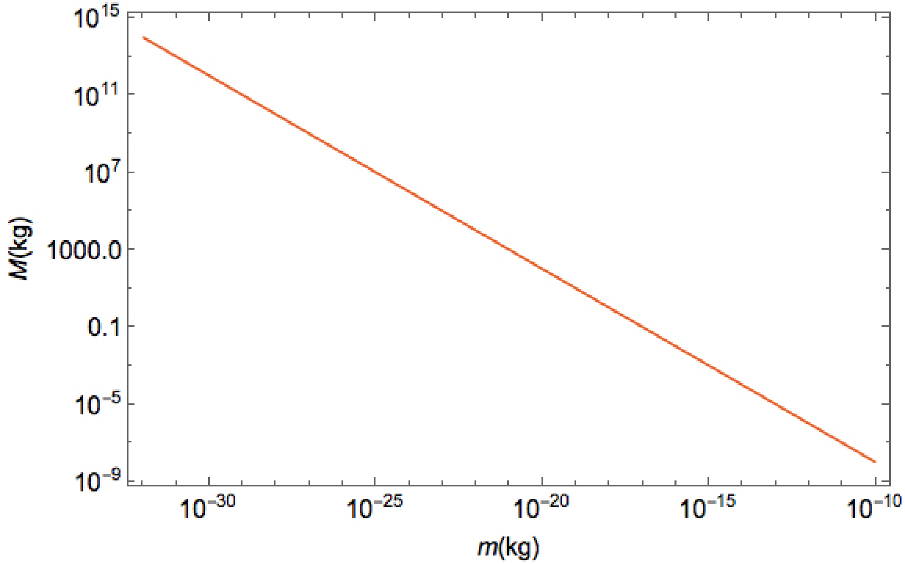

Fig. 8.1: Relation between mass that produces the gravitational field M and mass of scalar particle m, when the gravitational effects are comparable with quantum effects.

For the first order correction of energy from eq.(3.89) using the perturbed Hamiltonian from eq.(8.6)

$$\begin{aligned} E_n &\approx E_n^{(0)}\left(1 - \frac{4GM}{\rho_0 c^2 n^2} + \ldots\right) \\ &= E_n^{(0)}\left(1 + \frac{8E_n^{(0)}}{mc^2} + \ldots\right) \end{aligned} \tag{8.8}$$

where $E_n^{(0)}$ is the well-known energy for hydrogen atom from eq.(3.72) but now with quadratic charge $Q^2 = GMm$. Thus

$$E_n^{(0)} = -\frac{(GM)^2 m^3}{2\hbar^2 n^2} = -\frac{GMm}{2\rho_0 n^2} \tag{8.9}$$

8.2 Isotropic Harmonic Oscillator

In this section, we study a potential of an Isotropic Harmonic Oscillator in eq.(8.3), this analysis can be done in two ways, when the principal potential is the gravitational eq.(5.4) $U = -GM/r$ and we have a perturbation like-isotropic harmonic oscillator $V_0 = \dfrac{1}{2}m\omega_0^2 r^2$, the other way is taking as principal Hamiltonian as an isotropic harmonic oscillator, and the perturbation will be the gravitational potential. From eq.(8.3) with $V_0 = \frac{1}{2}m\omega_0^2 r^2$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi + \left[\frac{1}{2}m\omega_0^2 r^2 + \frac{2U}{c^2}\left(\frac{1}{2}m\omega_0^2 r^2\right) - \frac{2\hbar^2 U}{mc^2}\nabla^2\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{8.10}$$

8.2.1 Harmonic Oscillator inside a Gravitational Field

We think in an isotropic harmonic oscillator immersed in a gravitational field, I mean, $V_0 << U$, for solving this problem we can take the principal Hamiltonian operator $\hat{H}_0$ and perturbed Hamiltonian $\hat{H}_p$ in the following way

$$\hat{H}_0\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi - \frac{GMm}{r}\Psi \tag{8.11}$$

$$\hat{H}_p = \frac{1}{2}m\omega_0^2 r^2 - \frac{GMm\omega_0^2 r}{c^2} + \frac{4GME_n^{(0)}}{rc^2} \tag{8.12}$$

for eq.(8.11) are well-known the solutions of eigenvalues from eq.(3.72), its recurrence rule for powers of r from eqs.(3.101)-(3.106), it is possible to shown that the correction for first order of energy is

$$\begin{aligned} E_n =& E_n^{(0)}[1 - \frac{8E_n^{(0)}}{mc^2} - \frac{\omega_0^2\rho_0^2}{c^2}(3n^2 - l(l+1))] \\ &+ \frac{1}{4}m\omega_0^2\rho_0^2[n^2(5n^2 + 1 - 3l(l+1))] \end{aligned} \tag{8.13}$$

where $E_n^{(0)}$ is given by eq.(8.9), note that if $\omega_0 = 0$, we return to case of a free particle on a gravitational field of previous case. The solution of the wave function in spherical symmetry $\Psi = \Psi(t, r, \theta, \phi)$ after to apply separated variables for order zero $\Psi = R_{nl}(r)Y_{lj}(\theta, \phi)\exp\left(-\frac{iE_n}{\hbar}t\right)$ where Y_{lj} are the spherical harmonics[17] and the radial function $R_{nl}(r)$ is given by eq.(3.75).

8.2.2 Gravitational Field inside Harmonic Oscillator

In this section, we can consider the gravitational field like-perturbation on an isotropic harmonic oscillator with spherical symmetry, we use the solutions from Section 3.3.3, now the principal Hamiltonian operator $\hat{H}_0$ and the perturbed Hamiltonian $\hat{H}_p$ are given by

$$\hat{H}_0\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + \frac{1}{2}m\omega_0^2 r^2\Psi \tag{8.14}$$

$$\hat{H}_p = -\frac{GMm}{r} - \frac{GM}{c^2}m\omega_0^2 r + \frac{4GME_n^{(0)}}{rc^2} \tag{8.15}$$

The principal Hamiltonian is the Hamiltonian of an isotropic harmonic oscillator with spherical symmetry, the solution of eigenfunction is well-known by eq.(3.66) this solution is obtained after to do separated variables method, similar as the previous case $\Psi(t,r,\theta,\phi) = R_{nl}(r)Y_{lj}(\theta,\phi)\exp(-iE_n t)$ where $R_{nl}(r)$ is the radial function for an isotropic harmonic oscillator from eq.(3.65). For having the approximation to first order of eigenvalues (or energy), we should know to expected value of r and $1/r$, i.e., $\langle r\rangle$ and $\langle\frac{1}{r}\rangle$ since the correction to first order of energy is proportional to this terms due to eq.(3.89), nevertheless if we try to use Kramers' formula of a harmonic oscillator from eq.(3.81)

$$2E(s+1)\langle r^s\rangle + \frac{1}{2}m\omega^2(2s+4)\langle r^{s-2}\rangle + \frac{\hbar^2}{m}s\left(\frac{s^2-1}{4} - l(l+1)\right)\langle r^{s-2}\rangle = 0$$

It is only possible to obtain solutions to the even-power of expected values of r while for the odd-power, it is not possible by this method because of we have more unknown variables than equations, also if we use Hellman-Feynman formula from Section 3.4.3, it is only possible to obtain the same solutions as we have seen in this section. The reason because of we can use these methods for every power of expected values of r for hydrogen atom solution but only for even-power for isotropic harmonic oscillator is due to the radial solution for the hydrogen atom problem eq.(3.75) is equivalent to the radial solution of an isotropic harmonic oscillator eq.(3.65), if it is done a change of variable of quadratic form, i.e., for $\langle r^{2s}\rangle$ in the harmonic oscillator is equivalent to obtain $\langle r^s\rangle$ in the hydrogen atom, since s is an integer number, if we can have even-power in a harmonic oscillator would be equivalent to obtain a semi-integer power in a hydrogen atom, that with these methods it is not possible. In the paper [24], it studied this problem with a general solution for this problem, we will only take the solution for $\langle \frac{1}{r} \rangle$, the term of $\langle r \rangle$ we solve rewriting the principal and perturbed Hamiltonian as $\hat{H}_0^*$ and $\hat{H}_p^*$ respectively

$$\begin{aligned}
\hat{H}_0^* \Psi &= -\frac{\hbar^2}{2m} \nabla^2 \Psi + \frac{1}{2} m \omega_0^2 \left[\left(r - \frac{GM}{c^2} \right)^2 - \left(\frac{GM}{c^2} \right)^2 \right] \Psi \\
&\approx -\frac{\hbar^2}{2m} \nabla^2 \Psi + \frac{1}{2} m \omega_0^2 r^2 \Psi - \frac{1}{2} m \omega_0^2 \left(\frac{GM}{c^2} \right)^2 \Psi
\end{aligned} \tag{8.16}$$

we have approximated $r - \frac{GM}{c^2} \approx r$, since $\frac{GM}{c^2} << r$. Note that $\frac{GM}{c^2} = \frac{1}{2} r_{sch}$, where r_{sch} is the Schwarzschild radius from eq.(5.7). For the new perturbed Hamiltonian $\hat{H}_p^*$

$$\hat{H}_p^* = -\frac{GMm}{r} + \frac{4GME_n^{(0)}}{rc^2} \tag{8.17}$$

Thus, the correction of first order for the energy is given by

$$E_n = \hbar\omega \left(n + \frac{3}{2} \right) - \frac{1}{2} m \omega_0^2 \left(\frac{GM}{c^2} \right)^2 - GMm \left[1 - \frac{4E_n^{(0)}}{mc^2} \right] \langle \frac{1}{r} \rangle \tag{8.18}$$

where $E_n^{(0)} = \hbar\omega(n + \frac{3}{2})$ is well-known from eq.(3.68), the solution for $\langle \frac{1}{r} \rangle$ is given from [24] where

$$\begin{aligned}
\langle \frac{1}{r} \rangle = & \sqrt{\frac{m\omega_0}{\hbar}} \Gamma(l+1) [\frac{1}{2}(n-l-1)]! \times \\
& \sum_t \frac{(-1)^t}{[1/2(n-l-1)-t]! \Gamma(1/2(2l+1)+t+1)} \binom{-1/2}{t}^2
\end{aligned} \tag{8.19}$$

if we take only the first term of this solution, we obtain the energy value

$$\begin{aligned}
E_n = & \hbar\omega \left(n + \frac{3}{2} \right) - \frac{1}{2} m \omega_0^2 \left(\frac{GM}{c^2} \right)^2 \\
& - GMm \sqrt{\frac{m\omega_0}{\hbar}} \left[1 - \frac{4E_n^{(0)}}{mc^2} \right] \Gamma(l+1) [\frac{1}{2}(n-l-1)]!
\end{aligned} \tag{8.20}$$

Note that if we take $G = 0$, we returns to solution for an isotropic harmonic oscillator with symmetry spherical without gravitational field, well-known in QM, it is peculiar that Schwarzschild radius was obtained of natural form.

The two cases that were analyzed in this Section, they are extreme cases, when the gravitational field is so more intense than the harmonic oscillator and vice versa when the harmonic oscillator is so more intensive than gravitational field. The case when the two potentials are comparable, it is a problem so much complex, perhaps in a future analysis it could be treated.

8.3 Infinite Spherical Well Potential

This case was studied previously in Section 3.3.1, however now we start from the KG covariant equation in Newtonian geometry eq.(8.3) to compare the cases when there is a gravitational field and when there is not as in QM. The infinite spherical well potential $V_0(r)$ has two regions, we are only interested in studying the region where $0 < r < a$, here the motion equation is given by

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi - \frac{2\hbar^2 U}{mc^2}\nabla^2\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{8.21}$$

For a potential V_0

$$V_0(r) = \begin{cases} 0 \quad if \quad 0 < r < a, \\ \infty \quad otherwise. \end{cases} \tag{8.22}$$

We can choose a principal Hamiltonian operator $\hat{H}_0$ from motion equation, where

$$\hat{H}_0\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi = E^{(0)}\Psi. \tag{8.23}$$

The zero-order correction of energy $E^{(0)}_{ln} = \frac{\hbar^2}{2m}\frac{q^2_{ln}}{a^2}$ from eq.(3.44). We can define the perturbed Hamiltonian $\hat{H}_p$ from the KG equation

$$\hat{H}_p = -\frac{GMm}{r}\left(1 + \frac{4E^{(0)}}{mc^2}\right). \tag{8.24}$$

The first-order correction of the energy $E^{(1)}$ can be calculated from eq.(3.89), with the first-order correction of eigenfunction from eq.(3.45) $\langle nlk|r\theta\phi\rangle = \Psi^{(0)}_{nlk}(r,\theta,\phi)$. Therefore

$$E^{(1)}_{ln} = -GMm\left(1 + \frac{4E^{(0)}}{mc^2}\right)\langle\frac{1}{r}\rangle, \tag{8.25}$$

in general

$$\langle\frac{1}{r}\rangle = A^2_{ln}\int_0^a \left|j_l\left(\frac{q_{ln}}{a}r\right)\right|^2 r dr, \tag{8.26}$$

there is not a general relation to solve this equation in the well-known literature, thus we calculate the integral when $l = 0$, where $j_0(x) = \sin(x)/x$, its n-th root is $q_{0n} = n\pi$, the constant of normalization $A_{0n} = \sqrt{2/a}$. Due to the degeneration is $2l+1$, for this case there is a state, for the first root. Hence

$$\langle\frac{1}{r}\rangle \approx \frac{2a}{\pi^2}(1.218), \tag{8.27}$$

this solution and the next solution is solved numerically since there is not possible to have an analytic solution.

Now, for $l = 1$ the first excited state, which has 3 degenerated states, then we need the first three roots of $j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$, its roots are $q_{11} \approx 4.49340$, $q_{12} \approx 7.72525$ and $q_{13} \approx 10.90412$. Therefore for $n = 1$

$$\langle\frac{1}{r}\rangle \approx A^2_{11}\left(\frac{a}{q_{11}}\right)^2(0.4124), \tag{8.28}$$

for $n = 2$

$$\langle\frac{1}{r}\rangle \approx A^2_{12}\left(\frac{a}{q_{12}}\right)^2(0.4590), \tag{8.29}$$

and for $n = 3$

$$\langle\frac{1}{r}\rangle \approx A^2_{13}\left(\frac{a}{q_{13}}\right)^2(0.4778). \tag{8.30}$$

We can continue this process for the next exited states, as in the previously problems that we have studied if we make $G = 0$, we return to solutions for QM without gravitational field.

8.4 Spherical Barrier Potential

For this section, we use spherical symmetry, this case is a square well potential with spherical symmetry as in Section 3.3.2, the problem of square well potential with some symmetry (spherical, cartesian or cylindrical) is important for some experiments with quantum systems. Similar as the previous sections, we analyze the case of QM for square well potential with curvature of space-time. We use the Newtonian metric from eq.(5.5), with an analogous method for the KG covariant equation for a scalar field Φ with a transformation $\Phi = \Psi e^{-i\omega t}$, where $\omega = mc^2/\hbar$, it is possible to obtain an analogous motion equation from the KG covariant equation with the approximations that we have previously discussed, the motion equation is given by eq.(8.3)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + mU\Psi + V_0\left(1+\frac{2U}{c^2}\right)\Psi - \frac{4U}{c^2}\frac{\hbar^2}{2m}\nabla^2\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{8.31}$$

where $U = -GM/r$ is the gravitational potential, the laplacian operator ∇^2 is in spherical coordinates given by $\nabla^2 = \frac{1}{r}\partial_r^2(r) + \frac{1}{r^2 sin\theta}\partial_\theta(sin\theta\partial_\theta) + \frac{1}{r^2 sin^2\theta}\partial_\phi^2$, the potential V_0 is given by

$$V_0(r) = \begin{cases} -U_0 & if \quad r < a, \\ 0 & if \quad r > a, \end{cases} \tag{8.32}$$

Thus, from eq.(8.31) we can identify a principal Hamiltonian operator $\hat{H}_0$

$$\hat{H}_0\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V_0\Psi = E^{(0)}\Psi. \tag{8.33}$$

The perturbed Hamiltonian $\hat{H}_p$ can be defined from eq.(8.31)

$$\hat{H}_p = -\frac{GMm}{r}\left(1+\frac{4E^{(0)}}{mc^2} - \frac{2V_0}{mc^2}\right) \tag{8.34}$$

In general, we can find the fist-order correction of energy from eq.(3.89) with the perturbed Hamiltonian operator eq.(8.4)

$$E^{(1)} = -GMm\left(1+\frac{4E^{(0)}}{mc^2} - \frac{2V_0}{mc^2}\right)\langle\frac{1}{r}\rangle. \tag{8.35}$$

The case when $E < 0$ shows the quantum nature of the system due to the spectrum of energy is discrete as we have viewed in Section 3.3.2.

It can define two regions, $Region\ I$ for $(r < a)$ and $Region\ II$ for $(r > a)$. For these regions are well-known the solutions. For $Region\ I$ the first-order correction of energy $E_I^{(1)}$ is given by

$$E_I^{(1)} = -GMm\left(1 + \frac{4E^{(0)}}{mc^2} + \frac{2U_0}{mc^2}\right)\langle\frac{1}{r}\rangle_I. \tag{8.36}$$

Since the zero-order correction eigenfunction $\Psi_{lnj}(r,\theta,\phi) = R_{ln}(r)Y_{lj}(\theta,\phi)$ where $Y_{lj}(\theta,\phi)$ is the spherical harmonic function and $R_{ln}(r) = A_{ln}j_l(\gamma_{ln}r)$ is the radial solution, $j_l(x)$ are the spherical Bessel functions and $k_1 = \gamma_{ln}$ is the n-th solution of the transcendental equation showed in Section 3.3.2. Thus

$$\langle\frac{1}{r}\rangle_I = A_{ln}^2\int_0^a \left|j_l\left(\frac{\sigma_{ln}}{a}r\right)\right|^2 rdr, \tag{8.37}$$

where $\sigma_{ln} = a\gamma_{ln}$, using the parameter $\eta = \sigma_{ln}/q_{ln}$ that compares the n-th solution of the transcendental equation with the n-th root, the case when $\eta = 1$ we return to case of Section 8.3, where we know just some results. However the solution of this integral should be calculated through a numerical method in the particular case.

In $Region\ II$ the first-order order correction is similar for in the $Region\ I$

$$E_{II}^{(1)} = -GMm\left(1 + \frac{4E^{(0)}}{mc^2}\right)\langle\frac{1}{r}\rangle_{II}. \tag{8.38}$$

The eigenfunction $\Psi_{lnj}(r,\theta,\phi) = R_{ln}(r)Y_{lj}(\theta,\phi)$, nevertheless the radial function has a new form $R_{ln}(r) = Bh_l^{(1)}(i\gamma_{ln}^*r) = Bj_l(i\gamma_{ln}^*r) + iBn_l(i\gamma_{ln}^*r)$, where B is a constant of normalization, $h_l^{(1)}(x)$ are the spherical Hankel functions of first kind, $n_l(x)$ is spherical Neumann function and $k_2 = \gamma_{ln}^*$ is the solution of the transcendental equation given in Section 3.3.2. Therefore

$$\begin{aligned}\langle\frac{1}{r}\rangle_{II} =& B^2\int_a^\infty \left|h_l^{(1)}\left(i\gamma_{ln}^*\right)\right|^2 rdr\\ =& B^2\int_a^\infty \left(|j_l(i\gamma_{ln}^*r)|^2 - |n_l(i\gamma_{ln}^*r)|^2\right) rdr,\end{aligned} \tag{8.39}$$

This is a general solution on this perturbation, if we want to solve this integral, we need every parameter for a specific case and the solution will not be analytic, nevertheless to solve this integral we can use a numerical method.

9 Conclusions

To study the range where there are quantum gravitational effects without a definitive Everything Theory, which helps to understand these phenomena, it is difficult. We have not proposed a new theory, it was not the objective of the thesis, we try to be closer gravitational quantum effects in the laboratory with this new proposal. In this work, we have studied some different examples that are well-known in QM, nevertheless we have introduced the curvature of space-time (or gravitational effect) starting from the most general equation for bosons in QFT in curved space-time, we have not only add extra terms in the Schrödinger equation, rather we find a general Schrödinger equation from the KG covariant equation, to solve the differential equation, we identify the principal and perturbed Hamiltonian operator in each case, and compare with the well-known results in QM for each example. Every example, that we have studied, was worked on an inertial frame, this is so important to highlight it, due to the principal idea to this work is to obtain the same results when we will measure the gravitational effects on a quantum system in a lab, this quantum system (with scalar particles) will be on a non-inertial frame, we expect by the Einstein Equivalence Principle that between experimental and theoretical results are indistinguishable.

We have treated to view what is the limit where we could measure quantum gravitational effects with a simple dimensional analysis of a gravitational potential and a quantum potential (atom hydrogen), here if we consider a mass of scalar particle m as mass of electron, we obtain that the gravitational mass M that affects to electron mass by quantum gravitational effects is $\sim 10^{12}kg$. If we think on the easiest non-inertial frame, we could say, a spinning system, thus we would not have a real mass M, but it would have a effective mass given by angular frequency ω, where $\omega^2 = GM/r^3$, using a detector to $r = 1m$, we can obtain $\omega \approx 8.16rad/s = 1.29rev/s$ for $M \sim 10^{12}kg$, $\omega \approx 0.25rad/s = 0.039rev/s$ for $M \sim 10^9kg$, however if we would have a mass $M \sim M_{\odot}$, we would need to have an angular frequency $\omega \sim 10^9 rev/s$, this acceleration would have relativistic effects. With this analysis is possible to conclude that we can measure this results in a laboratory *On the Quantization of Inertia*.

When we will have a Complete Quantum Gravity Theory, we will understand better the limits where quantum and gravity coexist and to understand new the effects due to GR and QM, to predict the behavior of quantum gravitational objects, perhaps to know what is exactly Dark Matter, Dark Energy and Early Universe, but while Everything Theory comes, it would be good to try closer to study of quantum gravitational systems on Earth.
There is not yet a definitive proof on the quantum nature of gravity and this proposal is not definitive to say if gravity is a quantum interaction or not. No matter what is the true nature of gravity, I think that answer will be amazing.

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