Position Dependent Mass Quantum Particle

Ashwaq Eyad Kadhim Al-Aakol

Submitted to the
Institute of Graduate Studies and Research
in partial fulfillment of the requirements for the Degree of

Master of Science
in
Physics

Eastern Mediterranean University
August 2013
Gazimağusa, North Cyprus

Approval of the Institute of Graduate Studies and Research

Prof. Dr. Elvan Yilmaz
Director

I certify that this thesis satisfies the requirements as a thesis for the degree of Master of Science in Physics.

Prof. Dr. Mustafa Halilsoy
Chair, Department of Physics

We certify that we have read this thesis and that in our opinion it is fully adequate in scope and quality as a thesis of the degree of Master of Science in Physics.

Asst. Prof. Dr. S. Habib Mazharimousavi
Supervisor

Examining Committee

1. Prof. Dr. Ozay Gurtug
2. Prof. Dr. Mustafa Halilsoy
3. Asst. Prof. Dr. S. Habib Mazharimousavi

ABSTRACT

In this thesis we study a quantum particle with *position dependent mass* (PDM). We start from the general form of the kinetic energy operator in which the physical requirements are considered and then we show that the general form of the kinetic energy operator does not keep the Schrodinger equation invariant under the global Galilean transformation. To make out the problem we introduce instantaneous Galilean invariance and following this concept we show that in some specific case of the general form of the kinetic operator the Schrodinger equation remains invariant under the Galilean transformation. Furthermore we study a specific mass for a particle in an infinite square well potential. We show that the particle prefers to stay in a region with larger mass.

Keywords: Position dependent mass, Quantum particle, Galilean invariance, Instantaneous Galilean invariance, Particle in infinite well.

ÖZ

Bu tezde kütlesi pozisyona bağimlı bir kuantum partikülü incelenmektedir.Genel bir kinentik enerji operatörü ve dolayısıyle Schrödinger denklemi Galilei dönüşümü altında değişmektedir. Buna karşın anlık Galilei değişmezliğini Schrödinger denklmindeki kinetik enerjiye koyuyoruz. Sonsuz bir karesel kuyu potansiyelinde özel bir değişken kütle ele alınmakta ve partiküllerin ağır kütlesel noktaya çekildiği gözlemlenmektedir.

Anahtar Kelimeler: Pozisyona Bağımlı kütle, Kuantum Zerresi, Galilei değişmezliği, Anlik Galilei değişmezliği, Sonsuz çukurda Zerre.

To My Family

ACKNOWLEDGMENTS

I would like to express my gratitude to my supervisor Asst. Prof. Dr. S. Habib Mazharimousavi for the useful comments, remarks, patience and engagement through the learning process of this master thesis. A very special thanks to Prof. Dr. Omar Mustafa and Prof. Dr. Mustafa Halilsoy for reading the thesis and giving valuable comments to make my thesis much better. Furthermore I would like to thank my friends in Physics Department for their support on the way. Last, but by no means least, I would like to thank my family, who have supported me throughout entire process, by keeping me harmonious. I will be grateful forever for your kindness.

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Chapter 1

INTRODUCTION

Position dependent mass (PDM) quantum particle was first considered in the study of semiconductors and inhomogeneous crystals [7, 1]. From the beginning the problem was how to introduce a kinetic energy operator for a quantum particle with position dependent mass. For a one-dimensional quantum particle with constant mass one easily uses the form of the kinetic energy in classical mechanics to write

$$\hat{T} = \frac{\hat{p}^2}{2m_0} \tag{1.1}$$

where $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ is the momentum operator. However, for a PDM particle the kinetic energy operator can not be written as

$$\frac{\hat{p}^2}{2m(x)} \tag{1.2}$$

because of the non-zero commutator of the momentum operator $\hat{p}$ and position operator $\hat{x}$. Von-Roos [8] has introduced a general PDM kinetic energy operator

$$\hat{T} = \frac{1}{4}\left(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma} + m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha}\right) \tag{1.3}$$

where α, β and γ are arbitrary real constants which satisfy $\alpha+\beta+\gamma = -1$. So that when $m = m_0$ it reduces to (1.1). Furthermore, this PDM operator can be expanded in the following form

$$\hat{T} = \hat{p}\frac{1}{2m}\hat{p} + \Omega(x) \tag{1.4}$$

in which

$$\Omega(x) = \frac{1}{2}(\alpha+\gamma+\alpha\gamma)\frac{m'^2}{m^3} - \frac{1}{4}(\alpha+\gamma)\frac{m''}{m^2}. \tag{1.5}$$

Herein , primes stand for a derivatives with respect to x. In [2, 5] it has been shown that unless $\alpha = \gamma$, through some exact systems, the eigenvalues of the corresponding Hamiltonian results in a divergent energy. Nevertheless, in [3] it has been shown that although a global Galilean invariance for the Schrödinger equation with PDM is not possible by setting $\alpha = 0 = \gamma$ causes an instantaneous Galilean invariance IGI. Through all possible ordering, therefore, the only ordering which makes the eigenvalue problem of a PDM particle to be invariant under the Galilean transformation and finite energy spectrum is given when $\alpha = 0 = \gamma$ and therefore

$$\hat{T} = \hat{p}\frac{1}{2m}\hat{p}. \tag{1.6}$$

Chapter 2

Galilean Invariance

The general form of the Schrödinger equation for a PDM is given by

$$\hat{H}\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{2.1}$$

in which

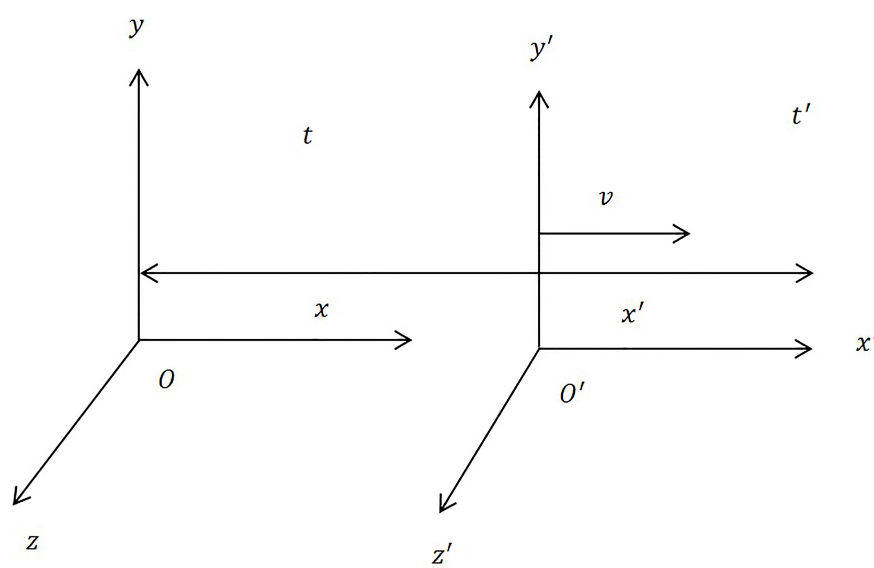

Figure 2.1: Galilean transformation from a fixed frame O to a moving frame with constant velocity O'

$$\hat{H} = \hat{p}\frac{1}{2m(x)}\hat{p} + W(x), \tag{2.2}$$

$W(x) = \Omega(x) + V(x)$, $V(x)$ is the interaction potential and $\psi(x,t)$ is the usual wave function. First of all we show that (2.1) is not invariance under the following Galilean transformation. The Galilean transformation is given by

$$x = x' + vt' \tag{2.3}$$

$$t = t' \tag{2.4}$$

where the two observer at $t' = t = 0$ share the same origin. Note that the prime in this part denotes the coordinates of the moving frame. Following the transformations (2.3) and (2.4) we find

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'} \tag{2.5}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - v\frac{\partial}{\partial x'}. \tag{2.6}$$

The Schrödinger equation (2.1), after all, reads

$$\left(\hat{p}'\frac{1}{2m(x')}\hat{p}' + W\left(x'\right)\right)\psi\left(x',t'\right) = -i\hbar v\frac{\partial\psi(x',t')}{\partial x'} + i\hbar\frac{\partial\psi(x',t')}{\partial t'}. \tag{2.7}$$

Next we try to eliminate the extra term in the right hand side by considering an extra phase for the wave function as usual i.e., $\psi(x',t') = \exp(i\Lambda(x',t'))\varphi(x',t')$. The latter equation, hence, yields

$$\left(-\hbar^2\partial_{x'}\frac{1}{2m(x')}\partial_{x'} + W\left(x'\right)\right)e^{(i\Lambda)}\varphi = -i\hbar v\frac{\partial e^{(i\Lambda)}\varphi}{\partial x'} + i\hbar\frac{\partial e^{(i\Lambda)}\varphi}{\partial t'} \tag{2.8}$$

which after expanding the terms

$$-\hbar^2\partial_{x'}\frac{1}{2m\left(x'\right)}\left(\partial_{x'}e^{(i\Lambda)}\varphi\right)+W\left(x'\right)e^{(i\Lambda)}\varphi=$$

$$-i\hbar v e^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar e^{(i\Lambda)}\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right) \quad (2.9)$$

and further

$$-\hbar^2\partial_{x'}\frac{1}{2m\left(x'\right)}\left[e^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)\right]+W\left(x'\right)e^{(i\Lambda)}\varphi=$$

$$-i\hbar v e^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar e^{(i\Lambda)}\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right) \quad (2.10)$$

or simply

$$-\hbar^2\partial_{x'}\left[\frac{e^{(i\Lambda)}}{2m\left(x'\right)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)\right]+W\left(x'\right)e^{(i\Lambda)}\varphi=$$

$$-i\hbar v e^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar e^{(i\Lambda)}\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right). \quad (2.11)$$

Some more expansions lead to

$$-\hbar^2\left[\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)\partial_{x'}\left(\frac{e^{(i\Lambda)}}{2m\left(x'\right)}\right)+\frac{e^{(i\Lambda)}}{2m\left(x'\right)}\partial_{x'}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)\right]$$

$$+W\left(x'\right)e^{(i\Lambda)}\varphi=-i\hbar v e^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar e^{(i\Lambda)}\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right) \quad (2.12)$$

and consequently

$$-\hbar^2\left[\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)e^{(i\Lambda)}\left(\frac{i\Lambda_{x'}}{2m(x')}-\frac{\partial_{x'}m(x')}{2m(x')^2}\right)+\frac{e^{(i\Lambda)}}{2m(x')}\left(i\Lambda_{x'x'}\varphi+i\Lambda_{x'}\partial_{x'}\varphi+\frac{\partial^2\varphi}{\partial x'^2}\right)\right]$$
$$+W(x')e^{(i\Lambda)}\varphi=-i\hbar ve^{(i\Lambda)}\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar e^{(i\Lambda)}\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right)\quad(2.13)$$

so that we cancel from both side the term $e^{(i\Lambda)}$ to find

$$-\hbar^2\left[\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)\left(\frac{i\Lambda_{x'}}{2m(x')}-\frac{\partial_{x'}m(x')}{2m(x')^2}\right)+\frac{1}{2m(x')}\left(i\Lambda_{x'x'}\varphi+i\Lambda_{x'}\partial_{x'}\varphi+\frac{\partial^2\varphi}{\partial x'^2}\right)\right]$$
$$+W(x')\varphi=-i\hbar v\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar\left(i\Lambda_{t'}\varphi+\frac{\partial\varphi}{\partial t'}\right).\quad(2.14)$$

If we subtract this expression from the standard form of the Schrödinger equation for PDM particle i.e.,

$$-\hbar^2\left[\frac{1}{2m(x')}\left(\frac{\partial^2\varphi}{\partial x'^2}\right)-\frac{\partial_{x'}m(x')}{2m(x')^2}\frac{\partial\varphi}{\partial x'}\right]+W(x')\varphi=i\hbar\frac{\partial\varphi}{\partial t'}\quad(2.15)$$

we find

$$-\hbar^2\left[\left(\frac{-\Lambda_{x'}^2\varphi}{2m(x')}-\frac{\partial_{x'}m(x')}{2m(x')^2}i\Lambda_{x'}\varphi\right)+\frac{i\Lambda_{x'}}{2m(x')}\frac{\partial\varphi}{\partial x'}+\frac{1}{2m(x')}\left(i\Lambda_{x'x'}\varphi+i\Lambda_{x'}\partial_{x'}\varphi\right)\right]$$
$$=-i\hbar v\left(i\Lambda_{x'}\varphi+\frac{\partial\varphi}{\partial x'}\right)+i\hbar\left(i\Lambda_{t'}\varphi\right)\quad(2.16)$$

For a general wave function φ, this is possible if and only if the coefficients of φ and $\partial_{x'}\varphi$ cancel each other separatly. These therefore yield

$$\text{i) }\frac{\hbar^2\Lambda_{x'}^2}{2m(x')}+\frac{\hbar^2\partial_{x'}m(x')}{2m(x')^2}i\Lambda_{x'}-\frac{i\hbar^2\Lambda_{x'x'}}{2m(x')}=\hbar v\Lambda_{x'}-\hbar\Lambda_{t'}\text{ for }\varphi\quad(2.17)$$

and

$$\text{ii)}\ \ \frac{\hbar\Lambda_{x'}}{m(x')} = v \quad \text{for } \partial_{x'}\varphi. \tag{2.18}$$

in which $\Lambda_{x'} = \frac{\partial\Lambda}{\partial x'}$ and $\Lambda_{t'} = \frac{\partial\Lambda}{\partial t'}$.

The condition ii) clearly suggests that $\Lambda_{x'}$ is independent of t' and therefore we have to write

$$\Lambda\left(x',t'\right) = \Lambda_1\left(x'\right) + \Lambda_2\left(t'\right) \tag{2.19}$$

in which Eq. (2.18) becomes

$$\text{ii)}\ \ \frac{\hbar}{m(x')}\frac{d\Lambda_1(x')}{dx'} = v \quad \text{for } \partial_{x'}\varphi \tag{2.20}$$

which admits

$$\Lambda_1\left(x'\right) = \frac{v}{\hbar}m\left(x'\right)dx'. \tag{2.21}$$

Considering this with the condition i) gives

$$\frac{\hbar^2}{2m(x')}\left(\frac{vm(x')}{\hbar}\right)^2 + i\frac{\hbar^2\partial_{x'}m(x')}{2m(x')^2}\frac{vm(x')}{\hbar} - \frac{i\hbar^2}{2m(x')}\partial_{x'}\left(\frac{vm(x')}{\hbar}\right) = \hbar v\frac{vm(x')}{\hbar} - \hbar\Lambda_{t'} \tag{2.22}$$

a after some simplification this reads

$$\frac{v^2 m(x')}{2} = \hbar \Lambda_{t'} \tag{2.23}$$

which upon (2.23) one finds

$$\frac{d}{dt'}\Lambda_2(t') = \frac{m(x')v^2}{2\hbar}. \tag{2.24}$$

The latter equation is meaningful only if $m(x')$ is a constant i.e., $m(x') = m_0$ and therefore

$$\Lambda_1(x') = \frac{v}{\hbar}m_0 x' \tag{2.25}$$

$$\Lambda_2(t') = \frac{m_0 v^2}{2\hbar}t' \tag{2.26}$$

which yield

$$\psi(x',t') = \exp\left(i\left(\frac{v}{\hbar}m_0 x' + \frac{m_0 v^2}{2\hbar}t'\right)\right)\varphi(x',t'). \tag{2.27}$$

Therefore,Schrödinger equation is invariant under the Galilean transformation only for constant mass quantum particles.

2.1 Instantaneous Galilean Invariance (IGI)

We have shown that the Schrödinger equation for a particle with position dependent mass is not invariant under Galilean transformation. In this section, we show that there are cases in which the Schrödinger equation for a particle with position dependent mass can be instantaneous Galilean invariant. Note that in the following calculation we consider $\hbar = 1$.

2.1.1 IGI for one-dimensional quantum particle with constant mass

For a one-dimensional classical particle with mass m the Galilean transformation applied at a time t_0 is given by

$$x'(t) = x(t) - u[t - t_0] \tag{2.28}$$

and

$$p'(t) = p(t) - mu \tag{2.29}$$

where u is the velocity of the moving frame. Following this, an instantaneous Galilean transformation (IGI) is applied at $t_0 = t$ to imply

$$x'(t) = x(t) \tag{2.30}$$

and

$$p'(t) = p(t) - mu. \tag{2.31}$$

Now, after knowing the form of IGI in classical mechanics we define a unitary transformation operator $\hat{U}(u)$ which represents the instantaneous Galilean transformation in one dimensional quantum theory for a particle with constant mass m. In analogy with the classical partner we impose

$$\hat{U}(u)\hat{X}\hat{U}^{-1}(u) = \hat{X} \tag{2.32}$$

and

$$\hat{U}(u)\hat{P}\hat{U}^{-1}(u) = \hat{P} - mu\hat{I} \tag{2.33}$$

in which $\hat{X}$ and $\hat{P}$ are canonical position and momentum operators while $\hat{I}$ is the identity operator. These two relations give the form of $\hat{U}(u)$ uniquely. This can be seen if we consider

$$\hat{U}(u) = \exp\left(iu\hat{K}\right) \tag{2.34}$$

in which $\hat{K}$ is the infinitesimal generator of $\hat{U}(u)$. Having $\hat{U}(u)$ unitary imposes $\hat{K}$ to be Hermitian i.e., $\hat{K} = \hat{K}^{\dagger}$ and therefore

$$\hat{U}^{-1}(u) = \exp\left(-iu\hat{K}\right). \tag{2.35}$$

The first relation Eq. (2.32) yields

$$\exp\left(iu\hat{K}\right)\hat{X}\exp\left(-iu\hat{K}\right) = \hat{X} \tag{2.36}$$

which upon using the well known Lie formula

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] + \frac{1}{2!}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \frac{1}{3!}\left[\hat{A},\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\right] + \ldots \tag{2.37}$$

implies

$$\hat{X}+\left[iu\hat{K},\hat{X}\right]+\frac{1}{2!}\left[iu\hat{K},\left[iu\hat{K},\hat{X}\right]\right]+\frac{1}{3!}\left[iu\hat{K},\left[iu\hat{K},\left[iu\hat{K},\hat{X}\right]\right]\right]+...=\hat{X}. \tag{2.38}$$

Clearly it dictates $\left[iu\hat{K},\hat{X}\right]=0$ or consequently $\left[\hat{K},\hat{X},\right]=0$ (iu is just a constant) and in turn implies that $\hat{K}$ is only a function of the position operator $\hat{X}$,i.e.,

$$\hat{K}=\hat{F}\left(\hat{X}\right). \tag{2.39}$$

Now we use the Lie formula (2.37) for the second condition Eq. (2.33) to obtain

$$\hat{P}+\left[iu\hat{K},\hat{P}\right]+\frac{1}{2!}\left[iu\hat{K},\left[iu\hat{K},\hat{P}\right]\right]+\frac{1}{3!}\left[iu\hat{K},\left[iu\hat{K},\left[iu\hat{K},\hat{P}\right]\right]\right]+...=\hat{P}-mu\hat{I}. \tag{2.40}$$

Due to the following relations

$$\left[\hat{X},\hat{P}\right]=i\hat{I} \tag{2.41}$$

and

$$\left[\hat{K},\hat{P}\right]=\left[\hat{F}\left(\hat{X}\right),\hat{P}\right]=i\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}} \tag{2.42}$$

one finds from (2.40)

$$-u\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}+\frac{1}{2!}\left[iu\hat{K},-u\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}\right]+\frac{1}{3!}\left[iu\hat{K},\left[iu\hat{K},-u\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}\right]\right]+...=-mu\hat{I}. \tag{2.43}$$

obviously, this will be satisfied if and only if

$$\frac{dF\left(\hat{X}\right)}{d\hat{X}} = m\hat{I}. \tag{2.44}$$

Therefore, $\hat{F}\left(\hat{X}\right)$ is unique and reads as

$$\hat{F}\left(\hat{X}\right) = m\hat{X} + C\hat{I} \tag{2.45}$$

where C is an integration constant. This constant does not bring any further contribution because it will be canceled in all transformations in the form of (2.32) or (2.33) and therefore we set it to zero. Hence, $\hat{K} = \hat{F}\left(\hat{X}\right) = m\hat{X}$ and

$$\hat{U}(u) = \exp\left(ium\hat{X}\right). \tag{2.46}$$

Nevertheless, in the usual Galilean transformation, the velocity operator $\hat{V}$ is transformed as

$$\hat{U}(u)\hat{V}\hat{U}^{-1}(u) = \hat{V} - u\hat{I} \tag{2.47}$$

in which the velocity operator is defined as

$$\hat{V} = i\left[\hat{H},\hat{X}\right], \tag{2.48}$$

with the Hamiltonian $\hat{H}$. Here we impose the condition that the velocity operator transforms in the same way as the usual Galilean transformation (2.47). Therefore

$$\hat{V}+\left[iu\hat{K},\hat{V}\right]+\frac{1}{2!}\left[iu\hat{K},\left[iu\hat{K},\hat{V}\right]\right]+\frac{1}{3!}\left[iu\hat{K},\left[iu\hat{K},\left[iu\hat{K},\hat{V}\right]\right]\right]+...=\hat{V}-u\hat{I} \quad (2.49)$$

which implies

$$\left[iu\hat{K},\hat{V}\right]=cons.=-u\hat{I} \quad (2.50)$$

and consequently

$$\left[\hat{K},\hat{V}\right]=i\hat{I}. \quad (2.51)$$

So far we found $\left[\hat{X},\hat{P}\right]=i\hat{I}$, $\left[\hat{X},\hat{K}\right]=0$, $\left[\hat{K},\hat{V}\right]=i\hat{I}$ together with $\hat{K}=m\hat{X}$. Eq. (2.51) then becomes

$$\left[m\hat{X},\hat{V}\right]=i\hat{I} \quad (2.52)$$

or

$$\left[\hat{X},m\hat{V}\right]=i\hat{I} \quad (2.53)$$

which clearly implies that

$$m\hat{V}=\hat{P}-\hat{A}\left(\hat{X}\right) \quad (2.54)$$

where $\hat{A}\left(\hat{X}\right)$ is just an arbitrary operator as a function of $\hat{X}$. Furthermore, one simply finds that

$$\begin{aligned} \left[\hat{K},\hat{H}-\frac{1}{2}m\hat{V}^2\right] &= \left[\hat{K},\hat{H}\right]-\left[\hat{K},\frac{1}{2}m\hat{V}^2\right]= \\ m\left[\hat{X},\hat{H}\right]-m\left[\hat{X},\frac{1}{2}m\hat{V}^2\right] &= mi\hat{V}-mi\hat{V}=0, \end{aligned} \tag{2.55}$$

which results is

$$\hat{H}-\frac{1}{2}m\hat{V}^2=\hat{W}\left(\hat{X}\right) \tag{2.56}$$

with $W\left(\hat{X}\right)$ as an arbitrary function of operator $\hat{X}$. Combining (2.54) and (2.56) we finalize the form of the Hamiltonian in one-dimensional quantum system which is an IGI i.e.,

$$\hat{H}=\frac{1}{2}m\hat{V}^2+\hat{W}\left(\hat{X}\right) \tag{2.57}$$

or more precisely

$$\hat{H}=\frac{1}{2m}\left(\hat{P}-\hat{A}\left(\hat{X}\right)\right)^2+\hat{W}\left(\hat{X}\right). \tag{2.58}$$

In the language of the field theory, $\hat{A}\left(\hat{X}\right)$ and $\hat{W}\left(\hat{X}\right)$ are scalar and vector coupling / interaction or potential respectively. We add that a phase transformation is always possible to remove $\hat{A}\left(\hat{X}\right)$ so one may set $\hat{A}\left(\hat{X}\right)=0$ to obtain a general form for the

Hamiltonian as

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \hat{W}\left(\hat{X}\right) \tag{2.59}$$

which is, in fact, a quantum mechanical Hamiltonian and is a one-dimensional IGI one-dimensional.

2.1.2 IGI for one-dimensional quantum particle with PDM

After finding the IGI form of the Hamiltonian of the quantum particle with constant mass we shall, in this section, find the possible form of the Hamiltonian for a position dependent mass quantum particle that is also an IGI. In this case we define another unitary transformation operator $\hat{U}(u) = \exp\left(iu\hat{K}\right)$ such that $\hat{K} = \hat{K}^\dagger$ and therefore $\hat{U}^{-1}(u) = \exp\left(-iu\hat{K}\right)$. The IGT are given by

$$\hat{U}(u)\hat{X}\hat{U}^{-1}(u) = \hat{X} \tag{2.60}$$

and

$$\hat{U}(u)\hat{P}\hat{U}^{-1}(u) = \hat{P} - \hat{M}\left(\hat{X}\right)u \tag{2.61}$$

where $\hat{M}\left(\hat{X}\right)$ is the PD-mass operator of the particle. As we have shown above (2.46) implies

$$\hat{K} = \hat{F}\left(\hat{X}\right)$$

but (2.61) yields

$$\hat{P}+\left[iu\hat{K},\hat{P}\right]+\frac{1}{2!}\left[iu\hat{K},\left[iu\hat{K},\hat{P}\right]\right]+\frac{1}{3!}\left[iu\hat{K},\left[iu\hat{K},\left[iu\hat{K},\hat{P}\right]\right]\right]+...=\hat{P}-\hat{M}\left(\hat{X}\right)u, \tag{2.62}$$

or consequently

$$\left[iu\hat{K},\hat{P}\right]=-\hat{M}\left(\hat{X}\right)u \tag{2.63}$$

which leads to

$$\left[\hat{P},\hat{K}\right]=-i\hat{M}\left(\hat{X}\right). \tag{2.64}$$

This equation, in turn, implies

$$\left[\hat{P},\hat{F}\left(\hat{X}\right)\right]=-i\hat{M}\left(\hat{X}\right) \tag{2.65}$$

or simply

$$\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}=\hat{M}\left(\hat{X}\right). \tag{2.66}$$

We recall that the velocity operator is defined as in Eq. (2.48) and the usual Galilean transformation (2.47) implies $\left[\hat{K},\hat{V}\right]=i\hat{I}$. Therefore a combination of (2.51) and (2.48) leads to

$$\left[\hat{K},\left[\hat{H},\hat{X}\right]\right]=\hat{I} \tag{2.67}$$

or equivalently

$$\left[\hat{F}\left(\hat{X}\right),\left[\hat{H},\hat{X}\right]\right]=\hat{I}. \tag{2.68}$$

Next, we use the Jacobi identity

$$\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0 \tag{2.69}$$

to write

$$\left[\hat{F}\left(\hat{X}\right),\left[\hat{H},\hat{X}\right]\right]+\left[\hat{H},\left[\hat{X},\hat{F}\left(\hat{X}\right)\right]\right]+\left[\hat{X},\left[\hat{F}\left(\hat{X}\right),\hat{H}\right]\right]=0. \tag{2.70}$$

Having $\left[\hat{X},\hat{F}\left(\hat{X}\right)\right]=0$, Eq.(2.70) reads

$$\left[\hat{F}\left(\hat{X}\right),\left[\hat{H},\hat{X}\right]\right]=-\left[\hat{X},\left[\hat{F}\left(\hat{X}\right),\hat{H}\right]\right] \tag{2.71}$$

which upon (2.68) one finds

$$\left[\hat{X},\left[\hat{F}\left(\hat{X}\right),\hat{H}\right]\right]=-\hat{I}. \tag{2.72}$$

This commutation simply means that

$$\left[\hat{F}\left(\hat{X}\right),\hat{H}\right]=i\left(\hat{P}-\hat{A}\left(\hat{X}\right)\right) \tag{2.73}$$

where $\hat{A}\left(\hat{X}\right)$ is an arbitrary operator and is a function of $\hat{X}$. As in the constant mass case, $\hat{A}\left(\hat{X}\right)$ is called vector potential which can be always eliminated by a simple phase transformation. As a result, the Hamiltonian of a PDM particle in one-dimensional quantum theory must satisfy

$$\left[\hat{F}\left(\hat{X}\right),\hat{H}\right]=i\hat{P}. \tag{2.74}$$

We note that

$$\hat{F}\left(\hat{X}\right)=\hat{K}=\int\hat{M}\left(\hat{X}\right)d\hat{X}. \tag{2.75}$$

From (2.74) one may conclude that if $\hat{H}=\hat{H}_0$ satisfies it, and other Hamiltonian $\hat{H}_1$ which satisfy $\hat{H}_1-\hat{H}_0=\hat{W}\left(\hat{X}\right)$ also satisfies the same condition. We call $\hat{W}\left(\hat{X}\right)$ to be the scalar potential if $\hat{H}_0$ does not include the scalar potential.

Finding a solution $\hat{H}$ for (2.74) is our next aim.

Let's start from the most general form of the Hamiltonian of a free particle with PDM which is given by (1.3), i.e.,

$$\hat{H}_0=\frac{1}{4}\left(\hat{M}^{\alpha}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\gamma}+\hat{M}^{\gamma}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\alpha}\right). \tag{2.76}$$

The condition (2.74) then, reads

$$\left[\hat{F}\left(\hat{X}\right),\frac{1}{4}\left(\hat{M}^{\alpha}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\gamma}+\hat{M}^{\gamma}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\alpha}\right)\right]=i\hat{P}. \tag{2.77}$$

Having (1.4) and (1.5) proved, the latter equation becomes

$$\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}+\hat{\Omega}\left(\hat{X}\right)\right]=i\hat{P} \tag{2.78}$$

which is simplified as

$$\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}\right]=i\hat{P} \tag{2.79}$$

due to considering $\left[\hat{F}\left(\hat{X}\right),\Omega\left(\hat{X}\right)\right]=0$. What we have on the left hand side can be expanded as

$$\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}\right]=\hat{P}\left[\hat{F}\left(\hat{X}\right),\frac{1}{2\hat{M}}\hat{P}\right]+\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\right]\hat{P} \tag{2.80}$$

and further

$$\begin{aligned}&\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}\right]\\&=\hat{P}\left(\frac{1}{2\hat{M}}\left[\hat{F}\left(\hat{X}\right),\hat{P}\right]+\left[\hat{F}\left(\hat{X}\right),\frac{1}{2\hat{M}}\right]\hat{P}\right)+\left(\hat{P}\left[\hat{F}\left(\hat{X}\right),\frac{1}{2\hat{M}}\right]+\left[\hat{F}\left(\hat{X}\right),\hat{P}\right]\frac{1}{2\hat{M}}\right)\hat{P}\end{aligned} \tag{2.81}$$

which finally yields

$$\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}\right]=\hat{P}\left(\frac{1}{2\hat{M}}\left[\hat{F}\left(\hat{X}\right),\hat{P}\right]\right)+\left(\left[\hat{F}\left(\hat{X}\right),\hat{P}\right]\frac{1}{2\hat{M}}\right)\hat{P} \tag{2.82}$$

or

$$\left[\hat{F}\left(\hat{X}\right),\hat{P}\frac{1}{2\hat{M}}\hat{P}\right]=\hat{P}\left(\frac{i}{2\hat{M}}\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}\right)+\left(\frac{d\hat{F}\left(\hat{X}\right)}{d\hat{X}}\frac{i}{2\hat{M}}\right)\hat{P}=i\hat{P}. \tag{2.83}$$

This satisfies the condition given in (2.74). Hence no matter what is the value of α, β and γ the general form of the Von-Roos Hamiltonian satisfies the IGT and therefore it is IGI. Adding a potential which is only a function of position operator $\hat{X}$ does not change the setting and in general

$$\hat{H} = \frac{1}{4}\left(\hat{M}^{\alpha}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\gamma} + \hat{M}^{\gamma}\hat{P}\hat{M}^{\beta}\hat{P}\hat{M}^{\alpha}\right) + \hat{V}\left(\hat{X}\right) = \hat{P}\frac{1}{2\hat{M}}\hat{P} + \hat{\Omega}\left(\hat{X}\right) + \hat{V}\left(\hat{X}\right) \quad (2.84)$$

is IGI. We note that

$$\hat{\Omega}\left(\hat{X}\right) = \frac{1}{2}\left(\alpha + \gamma + \alpha\gamma\right)\frac{\hat{M}'^2}{\hat{M}^3} - \frac{1}{4}\left(\alpha + \gamma\right)\frac{\hat{M}''}{\hat{M}^2} \quad (2.85)$$

where a prime stands for derivative with respect to $\hat{X}$.

Chapter 3

Continuity Conditions

In this short chapter we find the conditions which have to be counted for the wave function of a quantum particle with PDM. To do so, we look at the one-dimensional PDM Schrödinger equation for one dimensional particle whose mass is variable with position

$$\left(\hat{P}\frac{1}{2M}\hat{P}+\Omega(x)+V(x)\right)\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}. \tag{3.1}$$

We notice that $M(x)$, $\Omega(x)$ and $V(x)$ in position space are just functions of position x which is a variable rather than an operator but $\hat{P}=-i\hbar\frac{\partial}{\partial x}$ is still an operator. The first condition on $\psi(x,t)$ is to be at least differentiable up to first order with respect to time and second order with respect to position. This simply means that $\psi(x,t)$ must be continuous with respect to both x and t . In addition to these let's consider the time-independent Schrödinger equation

$$\left(-\hbar^2\frac{\partial}{\partial x}\frac{1}{2M}\frac{\partial}{\partial x}+\Omega(x)+V(x)\right)\varphi(x)=E\varphi(x) \tag{3.2}$$

where

$$\psi(x,t)=\exp(-iEt/\hbar)\,\varphi(x). \tag{3.3}$$

Suppose that $V(x)$ is finite in some interval in which $x = x_0$ belongs to that interval. Next, we integrate both side of (3.2) in a small neighberhood of $x = x_0$, i.e.,

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \left(-\hbar^2 \frac{\partial}{\partial x} \frac{1}{2M} \frac{\partial}{\partial x} + \Omega(x) + V(x)\right) \varphi(x)\, dx = \int_{x_0-\varepsilon}^{x_0+\varepsilon} E\varphi(x)\, dx. \tag{3.4}$$

Now we let $\varepsilon \to 0$ where $V(x)$ and $\varphi(x)$ are continuous and finite at $x = x_0$, one finds

$$\lim_{\varepsilon\to 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \left(-\hbar^2 \frac{\partial}{\partial x} \frac{1}{2M} \frac{\partial}{\partial x} + \Omega(x)\right) \varphi(x)\, dx = 0. \tag{3.5}$$

Since this is a general condition, the only way it can be satisfied is that both terms identically must vanish. To have the second term vanish we must assume $\Omega(x)$ is continuous at $x = x_0$. The explicit form of $\Omega(x)$ is given by

$$\Omega(x) = \frac{1}{2}(\alpha + \gamma + \alpha\gamma) \frac{m'^2}{m^3} - \frac{1}{4}(\alpha + \gamma) \frac{m''}{m^2} \tag{3.6}$$

which is continuous and implies m, m' and m'' are all continuous. This is not quite acceptable because of the physical situation where even at least one of them may not be satisfied. More precisely in semiconductor heterostructure there are cases where the mass is not continuous. Therefore, the only way we can solve this difficulty is by considering $\alpha+\gamma = 0$ and $\alpha+\gamma+\alpha\gamma = 0$. Solving this set of equations yields $\alpha = \gamma = 0$. As such, we are left up with

$$\lim_{\varepsilon\to 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} -\hbar^2 \frac{\partial}{\partial x} \frac{1}{2M} \frac{\partial \varphi(x)}{\partial x} dx = 0 \tag{3.7}$$

which simply suggests that

$$\lim_{\varepsilon\to 0}\frac{1}{M}\frac{\partial\varphi(x)}{\partial x}\bigg|_{x_0+\varepsilon}=\lim_{\varepsilon\to 0}\frac{1}{M}\frac{\partial\varphi(x)}{\partial x}\bigg|_{x_0-\varepsilon} \tag{3.8}$$

or in other words $\frac{1}{M}\frac{\partial\varphi(x)}{\partial x}$ must be continuous. Therefore, the constant mass continuity condition is just a special case of the more general one in (3.8).

To summarize, we can say that for a physical acceptable Schrödinger equation with position dependent mass, $\alpha=\gamma=0$ in the general form of the Hamiltonian and $\frac{1}{M}\frac{\partial\varphi(x)}{\partial x}$ must be continuous.

Chapter 4

PDM Particle in a one dimensional infinite well

In this chapter we concentrate on a one-dimensional position dependent mass particle trapped in an infinite potential well whose mass function is given by [4, 6]

$$M(x) = \frac{m_0}{\left(1+\frac{x}{a}\right)^2} \tag{4.1}$$

in which m_0 and a are constants. The potential well is given by

$$V(x) = \begin{cases} 0, & 0 < x < \ell \\ \\ \infty, & elsewhere \end{cases} \tag{4.2}$$

in which ℓ is the width of the well. As we have discussed above we choose $\alpha = \gamma = 0$ and write down the Schrodinger equation for $0 < x < \ell$ i.e.

$$\left(-\hbar^2 \frac{\partial}{\partial x} \frac{1}{2M} \frac{\partial}{\partial x}\right) \varphi(x) = E\varphi(x). \tag{4.3}$$

Setting $\frac{2Em_0}{\hbar^2} = k^2$ with $E > 0$ one finds

$$\left(\frac{\partial}{\partial x}\left(1+\frac{x}{a}\right)^2 \frac{\partial}{\partial x}\right) \varphi(x) + k^2 \varphi(x) = 0. \tag{4.4}$$

After expanding the equation it becomes

$$(a+x)^2 \varphi''(x) + 2(a+x)\varphi'(x) + k^2 a^2 \varphi(x) = 0 \tag{4.5}$$

which admits a general solution of the form

$$\varphi(x) = \frac{1}{\sqrt{\left(1+\frac{x}{a}\right)}} \left[C_1 \left(1+\frac{x}{a}\right)^{i\frac{\sqrt{4k^2a^2-1}}{2}} + C_2 \left(1+\frac{x}{a}\right)^{-i\frac{\sqrt{4k^2a^2-1}}{2}} \right]. \tag{4.6}$$

The boundary conditions on the walls impose that $\varphi(0) = \varphi(\ell) = 0$ which implies that

$$\varphi(0) = [C_1 + C_2] = 0 \tag{4.7}$$

or

$$C_1 = -C_2 \tag{4.8}$$

Equation (4.6) then reads

$$\varphi(x) = \frac{C_1}{\sqrt{\left(1+\frac{x}{a}\right)}} \left[\left(1+\frac{x}{a}\right)^{i\frac{\sqrt{4k^2a^2-1}}{2}} - \left(1+\frac{x}{a}\right)^{-i\frac{\sqrt{4k^2a^2-1}}{2}} \right] \tag{4.9}$$

or after considering

$$\varphi(x) = \frac{C_1}{\sqrt{\left(1+\frac{x}{a}\right)}} \left(\exp\left[i\frac{\sqrt{4k^2a^2-1}}{2} \ln\left(1+\frac{x}{a}\right) \right] - \exp\left[-i\frac{\sqrt{4k^2a^2-1}}{2} \ln\left(1+\frac{x}{a}\right) \right] \right) \tag{4.10}$$

it becomes

$$\varphi(x) = \frac{N}{\sqrt{\left(1+\frac{x}{a}\right)}}\left(\sin\left[\frac{\sqrt{4k^2a^2-1}}{2}\ln\left(1+\frac{x}{a}\right)\right]\right), \tag{4.11}$$

where $N = 2iC_1$ is the normalization constant. The second boundary condition imposes

$$\varphi(\ell) = \frac{N}{\sqrt{\left(1+\frac{\ell}{a}\right)}}\left(\sin\left[\frac{\sqrt{4k^2a^2-1}}{2}\ln\left(1+\frac{\ell}{a}\right)\right]\right) = 0 \tag{4.12}$$

which clearly implies

$$\frac{\sqrt{4k^2a^2-1}}{2}\ln\left(1+\frac{\ell}{a}\right) = n\pi \tag{4.13}$$

where $n = 1,2,3,....$This condition gives

$$\frac{\sqrt{4k^2a^2-1}}{2} = \frac{n\pi}{\ln\left(1+\frac{\ell}{a}\right)} \tag{4.14}$$

which leads to

$$\varphi(x) = \frac{N}{\sqrt{\left(1+\frac{x}{a}\right)}}\left(\sin\left[\frac{\ln\left(1+\frac{x}{a}\right)}{\ln\left(1+\frac{\ell}{a}\right)}n\pi\right]\right) \tag{4.15}$$

and

$$k^2 = \frac{n^2\pi^2}{a^2\ln^2\left(1+\frac{\ell}{a}\right)} + 1. \tag{4.16}$$

This also gines the energy spectrum i.e.,

$$E_n = \frac{\hbar^2}{2m_0}\left(1+\frac{n^2\pi^2}{a^2\ln^2\left(1+\frac{\ell}{a}\right)}\right). \tag{4.17}$$

One can also find the normalization constant N by applying

$$\int_0^{\ell} |\varphi(x)|^2 \, dx = 1, \tag{4.18}$$

which gives

$$N = \sqrt{\frac{2}{\ln\left(1+\frac{\ell}{a}\right)}}. \tag{4.19}$$

Finally the complete wave function reads

$$\varphi_n(x) = \sqrt{\frac{2}{\ln\left(1+\frac{\ell}{a}\right)}} \frac{\sin\left[\frac{\ln\left(1+\frac{x}{a}\right)}{\ln\left(1+\frac{\ell}{a}\right)} n\pi\right]}{\sqrt{\left(1+\frac{x}{a}\right)}}. \tag{4.20}$$

In Fig. 1 we plot $|\varphi_n(x)|^2$ in terms of x for the ground state with $n = 1$. The width of the well is chosen to be $\ell = 1$ and the value of a is variable. In Fig. 2 we display the mass function (4.1) versus x for the same values of a and $m_0 = 1$. From Fig. 1 it is observed that the particle chooses to be in the part of the well where its mass gets larger value. This can be seen from the form of the $|\varphi_n(x)|^2$ which is skewed to left with smaller a.

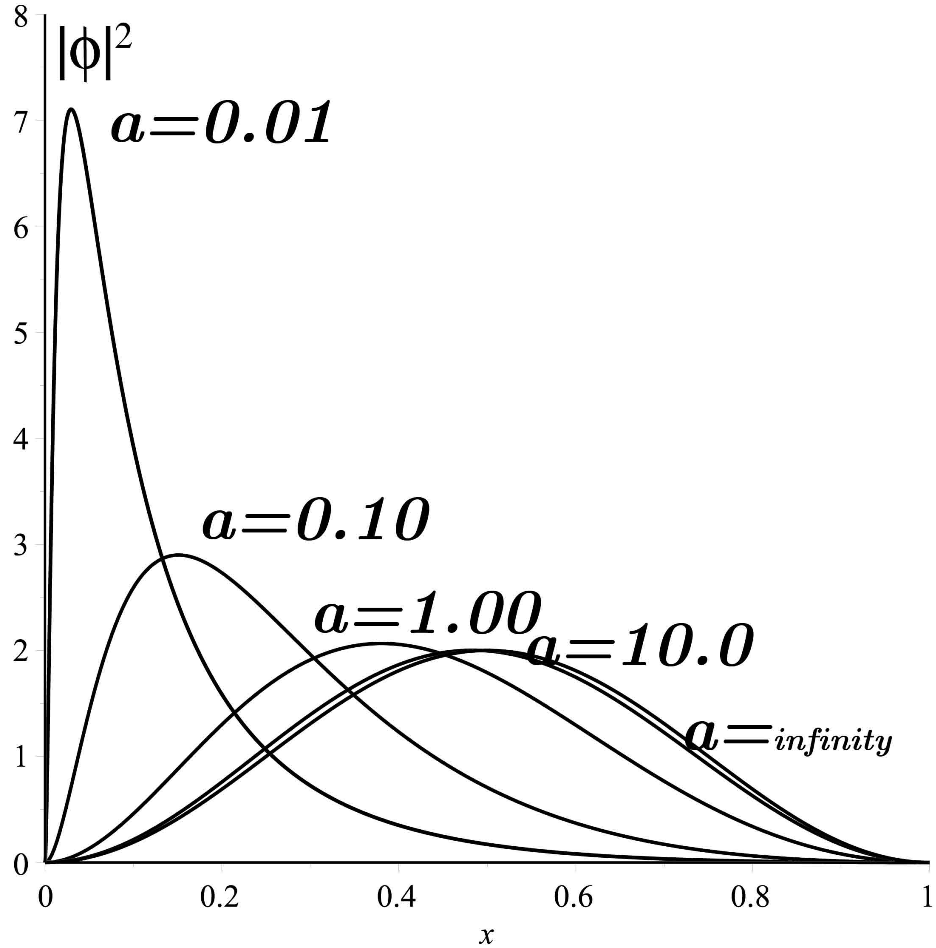

Figure 4.1: Probability density $|\varphi|^2$ in terms of x for different values of scale parameter a, $\ell = 1$ and $n = 1$ (ground state). It is seen that for small a the particle prefers to be localized near $x = 0$ where the mass takes larger value. Also when $a \to \infty$ the probability density coincides with the probability of a particle with constant mass

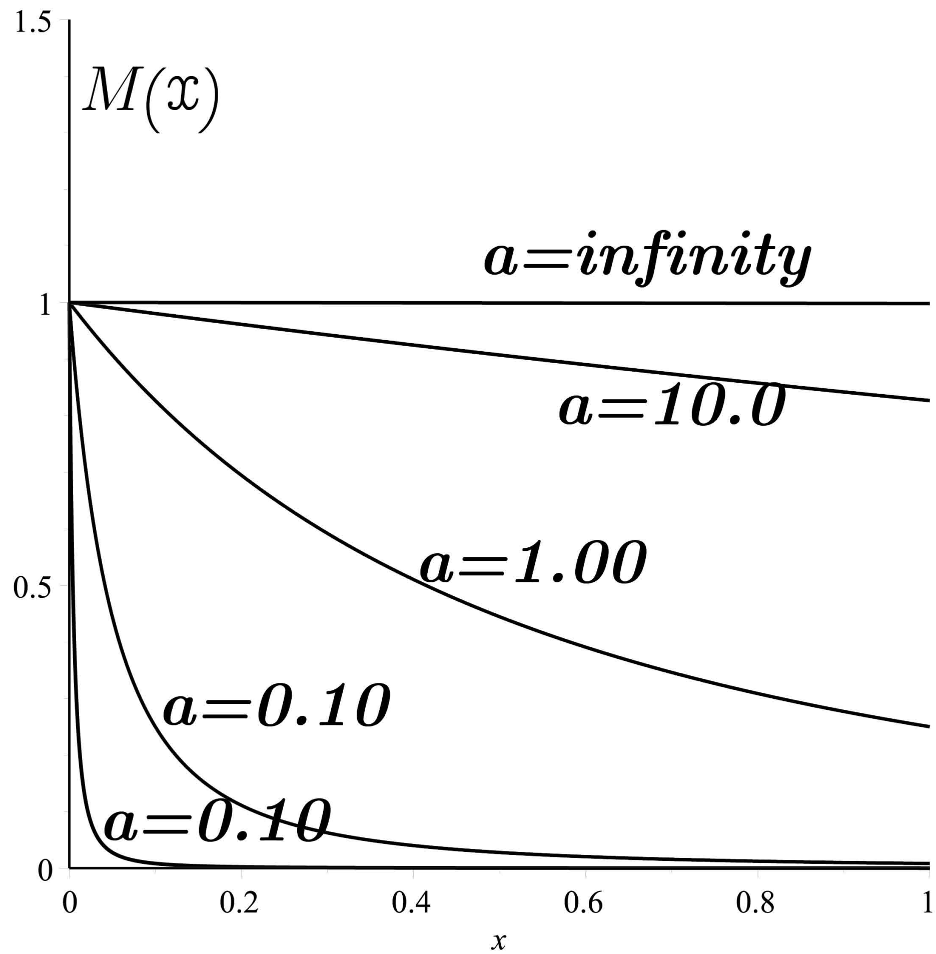

Figure 4.2: A plot of mass $M(x) = m_0/(1+\frac{x}{a})^2$ for $m_0 = 1$ and various values for the scale parameter a. As it is clear with large a the mass becomes constant while for small a the mass becomes very sensitive with respect to position and its maximum value takes place at $x = 0$

Chapter 5

CONCLUSION

In this thesis we have considered the one dimensional quantum particle with variable mass. The von-Roos form of the Hamiltonian for such particles with position dependent mass (PDM) has been given. Our main concern in this study is to consider the Galilean transformation of the Schrödinger equation of the particle with PDM. We have shown that the Schrödinger equation for PDM is not Galilean invariant but it is instantaneous Galilean invariant. We gave a definition for such kind of transformation and then we have shown that the PDM Schrödinger equation satisfies the requirement conditions. Following the Galilean transformation we have considered the conditions which the wave function and its first derivative must fulfill in the case of PDM.

An illustrative example which considers a PDM particle inside an infinite square well has been considered. In this example we have found the energy spectrum together with the energy eigenfunctions. Based on our results a position dependent mass quantum particle more likely is found with larger mass. This is very much clear from Fig.s 1 and 2.

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