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Al-Mustansiriyah University  
College of Science  
Department of Physics**



**SOME APPLICATIONS OF SCALE  
RELATIVITY THEORY IN QUANTUM  
PHYSICS**

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by

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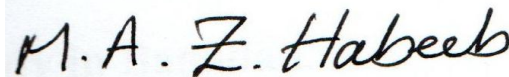
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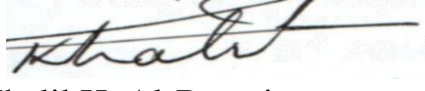
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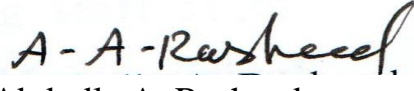
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# **Abstract**

The theory of scale relativity (ScR) is based on the extension of the principle of relativity of motion to include relativity of scale. Fractal space-time is the basis of this new theory as formulated by Nottale. Applications of this theory encompass diverse fields from microphysics, cosmology and complex systems. Previously, direct numerical simulations using this theory in quantum physics as performed by Hermann have resulted in the appearance of the correct quantum behavior without resorting to the Schrödinger equation. However these simulations were performed for only one limited case of a particle in an infinite one-dimensional square well. Hence, there is a need for more such applications using this theory to establish its validity in the quantum domain.

In the present work, and along the lines of Hermann, ScR theory is applied to other standard one-dimensional quantum mechanical problems. These problems are: a particle in a finite one-dimensional square well, a particle in a simple harmonic oscillator (SHO) potential and a particle in a one-dimensional double-well potential. Some mathematical problems that arise when obtaining the solution to these problems were overcome by utilizing a novel mathematical connection between ScR theory and the well-known Riccati equation. Then, computer programmes were written using the standard MATLAB 7 code to numerically simulate the behavior of the quantum particle in the above potentials utilizing the solutions of the fractal equations of motion obtained from ScR theory. Several attempts were made to fix some of the parameters in the numerical simulations to

obtain the best possible results in a practical computer CPU time within the limited local computer facilities.

Comparison of the present results for the particle probability density in the three potentials with the corresponding results obtained from conventional quantum mechanics by solving the Schrödinger equation, shows very good agreement. This agreement was improved further for some cases by utilizing the idea of thermalization of the initial particle state and by optimizing the parameters used in the numerical simulations such as the time step and number of coordinate divisions.

It is concluded from the present work that ScR theory can be used as a basis for describing the quantum behavior without reference to conventional quantum mechanics. Hence, it can also be concluded that the fractal nature of space-time, which is the basis of ScR theory, is the origin of the quantum behavior observed in these problems.

More applications to potentials in more than one-dimension, including asymmetric potentials, would give greater confidence along these lines. Also, the novel mathematical connection between ScR theory and the Riccati equation, that was previously used in quantum mechanics without reference to ScR theory, needs further investigation in future work.

# List of Symbols and Abbreviations

Symbol	Name
$C, C_1$	constants
$D$	fractal dimension
$D_T$	topological dimension
$\mathcal{D}$	diffusion coefficient
$E$	classical energy
$\mathbf{E}$	complex energy
$\mathbf{F}$	scale - force
$\mathcal{H}$	complex Hamiltonian
$\mathcal{L}$	length of function
$\mathbf{L}$	Lagrangian function
$N(0,1)$	normalized random variable
$\tilde{N}_1, \dots, \tilde{N}_{12}$	normalization constants
$P(x)$	quantum probability density
$\mathbf{P}$	complex momentum
$\mathcal{R}_{\mu\nu}$	scalar curvature
$\mathcal{R}^{\lambda}_{\rho\sigma\mu}$	Riemann tensor
$S$	proper time
$\mathbf{S}$	scale-action
$\mathcal{S}$	classical action
$T_{\mu\nu}$	energy-momentum tensor
$\mathcal{T}$	kinetic energy
$U$	imaginary part of velocity

<b>Symbol</b>	<b>Name</b>
$\mathcal{U}$	scalar potential
$V$	classical velocity
$\mathbf{V}$	complex velocity
$V_\mu$	4-vector velocity
$\tilde{V}$	4-component vector potential
$X$	subset of the Euclidean space
$Y(t)$	arbitrary function of t
$b_\pm$	forward and backward velocities
$c$	speed of light
$c_1, c_2, c_3, c_4$	constants of integration
$cc$	number of time steps
$d$	similarity dimension
$\partial/dt$	complex derivative
$f(x)$	number of occurrences in each box
$\hbar$	Dirac constant
$k$	force constant
$n$	quantum number
$p$	classical momentum
$ss$	number of starting points
$v_\pm$	forward and backward instantaneous velocities
$y(x)$	arbitrary function of $x$
$\psi$	wave function
$\phi$	golden mean
$\hat{\Omega}$	quantum mechanical operator



<b>Symbol</b>	<b>Name</b>
$\varepsilon$	resolution
$\varepsilon^{(0)}$	Cantor set
$\tilde{\varepsilon}$	magnetic moment
$\lambda_{dB}$	de Broglie scale
$\theta$	quantum phase
$\lambda_g$	cosmological constant
$\alpha$	volume of potential
$\sigma$	spatial distance
$\sigma\sigma$	standard deviation
$\rho\rho$	correlation coefficient
$\mu$	scale - mass
$\eta$	stochastic variable
$\Gamma$	scale - acceleration
$\Gamma_{\mu\nu}^{\rho}$	Christoffel symbol
$\Lambda$	length - time scale
$\xi$	fluctuation about the classical part of b
$\zeta$	fractal function
$\delta$	scale dimension
$\delta_{ij}$	Kronecker delta symbol
$\Gamma^i$	curvilinear coordinate
FODSW	Finite One-Dimensional Square Well Potential
HScR	Hermann's Scale - Relativity
IODSW	Infinite One-Dimensional Square Well Potential

<b>Symbol</b>	<b>Name</b>
NSA	Non-Standard Analysis
ScR	Scale Relativity
SHO	Simple Harmonic Oscillator
Std. Q. M.	Standard Quantum Mechanics

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# **Chapter One**

## **Introduction**

The beginning of the last century has witnessed the advent of two important events in physics, namely; the formulation of the theory of relativity by Einstein [1-7] and quantum mechanics by Schrödinger, Heisenberg, Dirac and others [8-13]. While the theory of relativity (special and general) is well-founded on physical (geometrical) basis [1-7], quantum mechanics is considered as an axiomatic theory based on purely mathematical rules. It was first introduced as a non-relativistic theory [8-15]. There is still a difficulty in understanding the connection between mathematical tools and the physical interpretation in quantum mechanics [16-18]. Also, the appearance of the constant  $\hbar$  (Dirac constant) in the Schrödinger equation is considered as one of the mysteries of quantum mechanics [16-18]. Another mystery is the wave nature of the solution to the Schrödinger and other relativistic quantum mechanical equations. This wave nature is axiomatically connected with the non-classical probabilistic behavior of quantum systems in analogy with the electromagnetic wave of classical electromagnetism and its connection with the probabilistic nature of photons in light fields with some differences [18-20].

Attempts to introduce Einstein's principle of special relativity into quantum mechanics has resulted in relativistic quantum mechanical wave equations for relativistic particles such as the Klein-Gordon equation and the Dirac equation [9-17].

More serious attempts to reconcile the principle of relativity with quantum mechanics have faced grave difficulties [15] even though some real progress has been made in this direction [16,18]. The reason for these difficulties is usually traced back to the different nature of the two fields stated at the beginning of this chapter, namely; the geometrical nature of relativity theory and axiomatic (non-geometrical) nature of quantum mechanics [8-12].

Attempts to geometrize quantum mechanics to ease its twining with relativity theory in a single more general theory were also made based on more than one direction [16,18]. A more serious attempt in this direction can be traced back to Feynman [21] who studied the geometrical structure of quantum paths and showed that the trajectory of a quantum particle is continuous and non-differentiable [22-24]. At that time the connection between non-differentiability and the concept of fractals and the modern field of fractal geometry (see Appendix A) was not well established. Later, Abbot and Wise [25] reconsidered the problem of the geometrical structure of quantum paths in terms of the concept of fractals

and they demonstrated that the trajectory of a quantum particle varies with the resolution. Hence, they showed that the fractal dimension  $D$  (see Appendix A) of this trajectory is 2 [26-28]. Going further in this direction, Ord [29] considered fractal space-time as a geometric analogue of relativistic quantum mechanics. He proposed two field equations for the description of what he called fractalons based on a random walk in space-time trajectories and subsequently related these equations to the free particle Klein-Gordon and Dirac equations [29].

Building on these geometrical concepts, and taking the fractal space-time concept more seriously into consideration, Nottale [30-32] introduced his theory of scale relativity (ScR) to reformulate quantum mechanics from first principles. The theory of ScR extends Einstein's principle of relativity of motion to scale transformations of resolutions. In other words, it is based on giving up the axiom of differentiability of the space-time continuum [30-39]. The new framework as formulated by Nottale generalizes the standard theory of relativity and includes it as a special case [31-35]. Three consequences arise from this withdrawal of differentiability of space - time [31-32,36,37], namely ;

- (i) The geometry of space-time must be fractal, i.e., explicitly resolution-dependent. This leads to non-classical behavior as a consequence.

- (ii) The geodesics of this non-differentiable space-time are themselves fractal and infinite in number.
- (iii) Time reversibility is broken at the infinitesimal level. This is again a behavior which has no analogue in classical systems.

According to Nottale [30-32], the ScR approach is expected to apply not only at small scales (quantum domain), but also at very large space-time scales (cosmological domain) although with different interpretation. Nottale also shows the applicability of his ScR theory to systems in the middle, namely; complex systems [31,40]. Therefore, there are three domains for the application of this theory which are microphysics[31,36,38],cosmology [31,36,39] and complex systems [31,40,44].

Most of the work done on ScR theory by Nottale [30-46] and others [47-52] in the quantum domain has focused on the formal side of the development of this theory and its application to put quantum mechanics on more sound physical basis, i.e., deriving most of it from ScR theory and fractal space-time. This sometimes obscures how the quantum probabilistic behavior arises as a result of the fractal nature of space-time. For this reason, there appears to be a need for a direct application of ScR theory to quantum problems so as to reveal this connection in a clear fashion. In this respect, Hermann [53] was the first to apply directly the fractal equations of motion obtained from ScR theory in

terms of a large number of explicit numerically simulated trajectories for the case of the quantum-mechanical problem of a free particle in an infinite one-dimensional box [8-12]. He constructed a probability density from these trajectories and recovered in this way the solution of the Schrödinger equation without explicitly using it. The results of this work as originally obtained by Hermann [53] are considered as pioneering in this respect since they show the importance of the direct application of ScR theory to quantum systems to reveal how quantum behavior arises from the fractality of space-time and the validity of this theory and also as laying the ground for the numerical methods needed in such applications.

### **Aim of the Present Work:**

Hermann [53] promised to do other similar applications to establish this validity in a more general sense. However, survey of literature did not indicate any such applications by him or other researchers in this field. Direct correspondence with him about this matter indicated the correctness of the results of this survey and emphasized the importance of pursuing further applications along the same lines [54].

It is believed that the results of such applications are important to prove the direct validity of ScR theory in more general cases and not in a single isolated case as done by Hermann [53]. Besides, such more applications are expected

to reveal novel concepts, such as the connection between ScR theory and the Riccati equation [55-58] as revealed in the present work which were not observed by Hermann [53], as will be discussed in details later.

Motivated by this, in the present thesis the quantum behavior of a particle in a finite one-dimensional square well potential, simple harmonics oscillator potential and double well potential is demonstrated by means of numerical simulations without using the Schrödinger equation or any conventional quantum axiom, along the lines of Hermann[53]. The results obtained in the present work are compared with the results obtained from conventional quantum mechanics. In this manner, the present work can be considered as an extension of Hermann's work [53] to the problems above.

The main conclusion of the present work is the validity of Hermann's method for more general examples taken from one-dimensional quantum mechanics. Besides, a novel connection between ScR theory and the Riccati equation is revealed, which need to be explored in future work along with other aspects.

To this end, this thesis is organized as follows. Chapter two presents a theoretical background to relativity theory and quantum mechanics as far as the present work is concerned, and discusses the need for extension of the

principle of relativity. Chapter three introduces the concept of fractal space-time, the general structure of ScR theory and gives a theoretical background for non-relativistic quantum mechanics in the new ScR approach. Chapter four includes a review of Hermann's work [53]. It also includes the application of Hermann's scale-relativistic approach (HScR) to the problem of a particle in a finite square well potential. Chapter five applies this HScR approach to a particle in a simple harmonic oscillator potential (SHO). The application of this approach to the problem of a particle in a double well potential is presented in chapter six. Chapter seven gives a discussion, conclusions and suggestions for possible extensions of the present work. Finally, some mathematical concepts related to fractal geometry, the Riccati equation, Cantorian fractal space-time and the computer programming performed in the present work are presented in appendices A, B, C and D respectively.

# **Chapter Two**

## **Relativity and Quantum Mechanics**

Our current understanding of the laws of physics can be broadly categorized into two main theories, namely; the theory of relativity and quantum mechanics. The theory of relativity includes the special and general theories of relativity as well as classical mechanics. Quantum mechanics traditionally includes its development into quantum field theories.

In this chapter an attempt is made to give some theoretical background to these theories as far as the theory of scale relativity, which is the subject of this thesis, is concerned. This may help in laying the grounds for the applications that are to be given in the following chapters.

### **(2-1) Relativity in Physics:**

Galilean relativity states that: "Motion is like nothing" [1-5]. Although at first sight it may seem trivial, the explicit expression of this imposes principal universal constraints on possible forms that physical laws take. In 1905, Einstein introduced the principle of general relativity which states that: "The laws of physics must be of such nature that they apply to systems of reference in any kind of motion"[1-2]. In this form, this statement implies strictly the relativity of motion. Special relativity leads to the constraint that no velocity can



exceed some universal velocity ( $c$ ) which is the velocity of light in vacuum ( $\approx 3 \times 10^8$  m/s).

Poincare in 1906 and Minkowski in 1909 [1,2,5] introduced the abstract four-dimensional space that is called space-time continuum or simply the four-space or (3+1)-space. Thus, in terms of this space-time, a homogeneous Lorentz transformation [1,2,3,5] ( $x_i = \sum_{j=1}^4 \alpha_{ij} x_j, i=1,2,3,4$ ) can be interpreted as a rotation of the system of coordinates in the four-space. The Minkowskian space-time is characterized by the invariant [1,2]:

$$ds^2 = c^2 dt^2 - (dx^2 + dy^2 + dz^2) \quad \text{----- (2.1)}$$

under any transformation from one inertial coordinate system to another. Eqn. (2.1) can be rewritten as:

$$ds^2 = c^2 dt^2 - d\sigma^2 \quad \text{----- (2.2)}$$

where  $d\sigma$  is the spatial distance between two space points in the physical space in which two events occur, while  $dt$  is the difference in time of occurrence of the two events.

General relativity is a theory based on fundamental physical principles, namely; the principles of general covariance and of equivalence. The principle of general covariance states that: "The general laws of nature are to be expressed by equations which hold good for all system of coordinates, that is, are covariant with respect to any substitutions whatever". While, the principle of equivalence states that: "At a given event point, all laws of nature have same form

as in the special relativity , when expressed in term of locally Lorentzian coordinates" [1,2,5]. From these principles, Einstein constructed the theory of general relativity, whose equations are constraints on the possible curvatures of space-time. Einstein's equations can be written in the form [1-6]:

$$\mathcal{R}_{\mu\nu} - \frac{1}{2} \mathcal{R} g_{\mu\nu} - \lambda_g g_{\mu\nu} = \mathcal{K} T_{\mu\nu} \quad \text{----- (2.3)}$$

where the  $g_{\mu\nu}$ 's are tensorial metric potentials which generalize the Newtonian gravitational scalar potential,  $\mathcal{R}_{\mu\nu}$  is the scalar curvature,  $\lambda_g$  is the cosmological constant,  $T_{\mu\nu}$  is the energy-momentum tensor,  $\mathcal{K} = \frac{8\pi\tilde{G}}{c^4}$  ,  $\tilde{G}$  is the gravitational constant( $\approx 6.6742 \times 10^{-11}$  N m<sup>2</sup> kg<sup>-2</sup>) and  $\mu, \nu=0,1,2,3$  .

Eqn. (2.3) is invariant under any continuous and differentiable transformation of coordinate systems. The general relativistic invariant is [1-6]:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu \quad \text{----- (2.4)}$$

where Einstein's summation convention on repeated upper and lower indices is implied . The covariant derivative  $D_\mu$  can be used to express how the curvature of space-time implies that the variation of physical entities (such as vectors and tensors) for infinitesimal coordinate variation depends also on space-time itself, as [1-3]:

$$D_\mu A^\nu = \partial_\mu A^\nu + \Gamma_{\rho\mu}^\nu A^\rho \quad \text{----- (2.5)}$$

which generalizes the partial derivatives ( $\partial_\mu$ ) where  $A^\nu$  is 4-vector .

In this expression, the effect of the curvature of space-time (i.e., of gravitation) is described by the Christoffel symbols  $\Gamma_{\mu\nu}^{\rho}$  that has the form [1-3]:

$$\Gamma_{\mu\nu}^{\rho} = \frac{1}{2} g^{\rho\lambda} (\partial_{\nu} g_{\lambda\mu} + \partial_{\mu} g_{\lambda\nu} - \partial_{\lambda} g_{\mu\nu}) \quad \text{-----} \quad (2.6)$$

which plays the role of the gravitational field .

The covariant derivatives do not commute, so that their commutator leads to the appearance of a four-indices tensor, which is called Rimmann tensor  $\mathcal{R}^{\lambda}_{\rho\nu\mu}$  defined as [1-3]:

$$(D_{\mu} D_{\nu} - D_{\nu} D_{\mu}) A_{\rho} = \mathcal{R}^{\lambda}_{\rho\nu\mu} A_{\lambda} \quad \text{-----} \quad (2.7)$$

By contraction of indices in the Riemann tensor, the symmetric second-rank Ricci tensor  $\mathcal{R}_{\mu\nu}$  can be formed [1,3,4,6]:

$$\mathcal{R}_{\mu\nu} = g^{\lambda\rho} \mathcal{R}_{\lambda\rho\mu\nu} \quad \text{-----} \quad (2.8)$$

or

$$\mathcal{R}_{\mu\nu} = \partial_{\rho} \Gamma_{\mu\nu}^{\rho} - \partial_{\nu} \Gamma_{\mu\rho}^{\nu} + \Gamma_{\mu\nu}^{\rho} \Gamma_{\rho\lambda}^{\lambda} - \Gamma_{\mu\lambda}^{\rho} \Gamma_{\nu\rho}^{\lambda} \quad \text{-----} \quad (2.9)$$

The quantity  $\mathcal{R} = g^{\mu\nu} \mathcal{R}_{\mu\nu}$  is called the scalar curvature [1,2] .

The equation of motion of a free particle is that of inertial motion [1,3]:

$$D V_{\mu} = 0 \quad \text{-----} \quad (2.10)$$

where  $V_{\mu}$  is the 4-velocity of the particle . This equation becomes the geodesics equation [1,3,5,6]:

$$d^2 x^{\mu} / ds^2 + \Gamma_{\nu\rho}^{\mu} (dx^{\nu} / ds)(dx^{\rho} / ds) = 0 \quad \text{-----} \quad (2.11)$$

## **(2.2) Quantum Mechanics:**

Classical physics deals with macroscopic phenomena. Most of the effects with which classical theory is concerned are either directly observable or can be made observable with relatively simple instruments. When physicists turn their attention to the study of atomic systems, they find the concepts and methods of classical macroscopic physics inapplicable directly to atomic phenomena. In the period from 1925 to 1930, an entirely new theoretical discipline, quantum mechanics, was developed by Schrödinger, Heisenberg, Dirac and others [8-15].

In Young's interference experiment [8-10], particles seem to behave in certain situations as if they were waves. This interference experiment suggested several new ideas [8,11]:

- 1- Probability enters into quantum mechanics in a fundamental and non-classical way. Considering light as a stream of photons reveals an associated wave the amplitude of which plays the role of a probability amplitude. The square of the amplitude (i.e, the wave intensity) gives a measure of the probability of finding a photon at a particular point.
- 2- In the case of a photon and, presumably for other particles as well, the probability amplitude propagates as a typical wave.
- 3- For photons, the wave amplitude contains all the information available about the photon probability distribution, thus, the wave function for a particle is sometimes called the state function of the particle.

The paradox of a particle which sometimes behaves like a wave or of a wave which sometime behave like a particle can thus be resolved by noting that the wave plays the role of probability amplitude in the probabilistic description of particles [8,11].

In non-relativistic quantum mechanics, there are axioms which are given briefly in the following [8-11,59]:

- 1- The complex wave function  $\psi$  associated with a physical system contains all relevant information about the behavior of the system and thus describes it completely. In other words, any meaningful question about the result of an experiment performed upon the system can be answered if the wave function is known. The quantity  $\psi^*\psi=|\psi|^2$  is to be interpreted as a probability density for a particle in the state  $\psi$ . In the measurement of the position of the particle, the probability  $P(\vec{r})d\vec{r}$  of finding it in a volume element  $d\vec{r} = dx dy dz$  at the point  $\vec{r}$  is proportional to  $|\psi(\vec{r})|^2 d\vec{r}$ .
- 2- If two solutions  $\psi_1$  and  $\psi_2$  of the system are known, they obey the principle of superposition, so that other solutions can be constructed of the form :

$$\psi = a_1 \psi_1 + a_2 \psi_2 \quad \text{-----}(2.12)$$

with arbitrary choice of the constants  $a_1$  and  $a_2$ . The function  $\psi$  will satisfy the same condition of continuity and integrability that are satisfied by  $\psi_1$  and  $\psi_2$ .

- 3- An operator  $\hat{\Omega}$  representing an observable quantity must, for every state  $\psi$ , yield an expectation :

$$\langle \hat{\Omega} \rangle = \int \psi^* \hat{\Omega} \psi d\vec{r} \equiv (\psi, \hat{\Omega} \psi) \quad \text{-----} (2.13)$$

which is real .  $\hat{\Omega}$  must satisfy the condition :

$$(\psi , \hat{\Omega} \psi) = (\psi , \hat{\Omega} \psi)^* = (\hat{\Omega} \psi , \psi) \quad \text{----- (2.14)}$$

for every function  $\psi$  to which it may be applied . A linear operator which obeys eqn. (2.14) is called a Hermitian operator. This rule is sufficient to insure that the eigenvalues of  $\hat{\Omega}$  are real, for if  $\psi$  is an eigenfunction of  $\hat{\Omega}$  belonging to the eigenvalue  $\omega_i$  , then :

$$(\psi , \hat{\Omega} \psi) = (\psi , \omega_i \psi) = \omega_i (\psi , \psi) \quad \text{----- (2.15)}$$

where  $\omega_i$  is real .

- 4- Any state function can be expanded as  $\psi = \sum_{n=1}^N a_n \psi_n$  in an orthonormal basis set  $\{\psi_n; n=1, 2, 3...N\}$ , and  $|a_n|^2$  gives the probability that the system is in the  $n^{\text{th}}$  eigenstate.
- 5- The time evolution of the system satisfies the Schrödinger equation :

$$\hat{H}\psi = i\hbar(\partial\psi / \partial t) \quad \text{----- (2.16)}$$

where the Hamiltonian  $\hat{H}$  is a linear Hermitian operator .

- 6- Immediately after a measurement, the system is in the state given by the first measurement. This is von Neumann's axiom [31,36]. This axiom is necessary to account for experiments: for example, after a spin measurement, the spin remains in the state given by the measurement; just after a measurement of position (at  $t+\delta t$ ,  $\delta t > 0$ ), a particle is in the position given by the measurement . Its absence may give a false impression of quantum mechanics as a theory where precise prediction can

never be done, while this depends on the pure or mixed character of the state of the system. It underlies the phenomenon of reduction of the wave packet [8-12].

The position and momentum wave functions may be derived one from the other by a reciprocal Fourier transform [8-12]. From this comes the Heisenberg inequality or uncertainty principle [31,36,38]:

$$\sigma_x \sigma_p \geq \hbar/2 \quad \text{-----}(2.17)$$

which implies the non-deterministic character of quantum trajectories. Also, the solution of the Schrödinger equation for a free particle leads to the introduction of the de Broglie length and time: the phase of the complex wave function is  $\theta = (px - Et)/\hbar$ , where  $p$  and  $E$  are the classical momentum and energy of the particle. The de Broglie periods,  $\hbar/p$  and  $\hbar/E$ , correspond to a phase variation of  $2\pi$ . The de Broglie length and time are [10,14,18]:

$$\lambda = \hbar/p; \tau = \hbar/E \quad \text{-----} (2.18)$$

Then, the quantum phase becomes [5,6,31]:

$$\theta = (x/\lambda - t/\tau) \quad \text{-----} (2.19)$$

From the above six axioms, it is clear that there are mysteries in quantum mechanics such as [31]:

- 1- The mysterious character of the quantum rules, such as that to a real momentum  $\vec{p}$ , there corresponds a complex operator  $(-i\hbar\partial/\partial\vec{r})$  acting on a complex probability amplitude.
- 2- There is a complex plane in quantum mechanics. It is not clear where this complex plane lies.

- 3- Quantum mechanics is an axiomatic theory rather than a theory of principle. The physical origin of the axioms of quantum mechanics is not clearly understood.

### **(2.3) The Need for a More General Principle of Relativity:**

According to relativity and quantum theories, any object can be described by coordinate systems which are  $(x, y, z, t)$  [1-6,8-12]. The resolution of space-time is the minimal unit that may be used when characterizing the length or time interval by a final number. The perfect description of any physical system must include the measurement errors or uncertainties. Then, the complete information about the position and time of the system is not only the space-time  $(x, y, z, t)$  but also the resolutions  $(\Delta x, \Delta y, \Delta z, \Delta t)$  [31,36,38]. This analysis is important in the quantum interpretation since the results of measurement become dependent on the resolution, as a consequence of Heisenberg's relation [30,31,36,38]. Here, the quantum behavior is a consequence of a fundamental and universal dependence of space-time itself on resolution which is revealed in any measurement, namely; that the quantum space-time has properties of a fractal (see appendix A). In this way, Heisenberg's relations tell that the results of measurements of momentum and energy are relative to the state of scale of the reference system [31,36].

The super system can now be defined as a system which contains the usual coordinates and spatio-temporal resolutions, i.e.,



$(t, x, y, z, \Delta t, \Delta x, \Delta y, \Delta z)$  [30,31,38]. Applying the laws of nature to any coordinate super system gives an extension of the principle of relativity [1-3]. This extension in the principles of relativity gives a new theory of relativity which is the scale relativity (ScR) theory as first introduced by Nottale [30-32] in 1993.

This theory states that: "the fundamental laws of nature apply whatever the state of scale of the coordinate system". The state of a reference system is characterized by the resolutions at which a system is observed. It can be defined only in a relative way. The main idea of the theory is to give up the arbitrary hypothesis of differentiability of space-time [30,31,36,38]. This theory reformulated quantum mechanics from first principles. Which are the covariance and geodesics equations, by considering the particle as geodesic in fractal space-time (see Sec. (3-1)). ScR theory applies in three domains which are microphysics, cosmology and complex systems [31,33,34,37,40,41] (see Sec. (3.2)) .

# **Chapter Three**

## **Fractal Space-Time, Scale Relativity and Quantum Mechanics**

### **(3.1) Fractal Space-Time:**

In relativity theory and quantum mechanics, an event is described by 4 coordinates which are  $(x, y, z, t)$  [1-6,8-12]. One puts apart properties like charge, spin, ect, but this fact does not mean that knowing only one  $(x, y, z, t)$  is sufficient to determine the evolution of a system but that the necessary physical quantities only depend on  $x, y, z$  and  $t$  [60,61]. Space-time gives the set of all possible  $(x, y, z, t)$  quadruplets and their transformations. In relativity theory, space-time is continuous, curved and differentiable [1-3]. This kind of space-time cannot account for the quantum properties of matter. While, in quantum mechanics, space-time is in principle flat, Minkowskian and differentiable [60,61]. Here, there is a contradiction with relativity theory. That has led to attempts to include another kind of space-time in quantum mechanics. The role played by resolutions of space-time led Nottale [30-32] to give up the (implicit) hypothesis of the differentiability of space-time, which implies its fractal (see Appendix A) and curved nature. This has important physical consequences; one can demonstrate the continuous but non-differentiable nature of space-time as a consequence. One can also demonstrate that a non-differentiable function is explicitly resolution

( $\varepsilon$ )-dependent, and that its length  $\mathcal{L}(x)$  tends to infinity where the resolution interval  $\varepsilon$  tends to zero , i.e.,  $\mathcal{L} = \mathcal{L}(\varepsilon)_{\varepsilon \rightarrow 0} \rightarrow \infty$  [30,32,34,46,57,58,59].

The assumption of continuous but non-differentiable space-time proposes the concept of fractal space-time [62-64] which explicitly depends on resolutions. It can be defined as "Space–Time-Zoom" with 5 dimensions  $(x, y, z, t, D)$  [62,63] where  $D$  is the fractal dimension (see Appendix A) which is a variable and plays the role of a 5<sup>th</sup> dimension . The roots of the concept of fractal space-time go back to Feynman [21] who found that the trajectory of a quantum path is continuous but non-differentiable. Then, Ord [29] introduced this concept as a geometric analogue of relativistic quantum mechanics.

In a fractal space-time, there is an infinite number of fractal geodesics [30,31] between any two points, so particles can be identified with one particular geodesic of the family. Also, fractal space–time implies a breaking of time reflection invariance [31,33,35]. These properties of fractal space-time come from non-differentiability. A theory based on these concepts is ScR theory which was introduced by Nottale [48,63,64]. El Naschie [65] has attempted to go still one step further to give up continuity also. This leads to the concept of Cantorian fractal space-time (see Appendix C).

### **(3.2) General Structure of ScR Theory:**

The theory of ScR is constructed by completing the standard laws of classical physics (motion in space / displacement in space-

time) by new scale laws in which the space-time resolutions are playing for scale-transformations the same role of velocities in motion transformation. There are several levels of scale laws according to the historical development of the theory of motion [30,31,32,34,36,38]:

### **(3.2.1) Galilean Scale Relativity:**

#### *1- Standard Fractal Laws*

A power-law scale dependence is frequently encountered in many natural systems. It is described geometrically in terms of fractals (see Appendix A) and also algebraically in terms of the renormalization group [30-32]. Such simple scale-invariant laws can be identified with the Galilean version of scale-relativistic laws [30,31].

Let  $\mathcal{L}$  be a non-differentiable coordinate. Because there is a link between non-differentiability and fractality,  $\mathcal{L}$  is an explicit function  $\mathcal{L}(\varepsilon)$  of the resolution interval  $\varepsilon$ . Firstly, assume that  $\mathcal{L}(\varepsilon)$  satisfies a simple scale differential equation, then, this leads to the first order differential equation [31,32,33]:

$$\frac{d \ln \mathcal{L}}{d \ln(\lambda / \varepsilon)} = \delta \quad \text{-----} \quad (3.1)$$

where  $\delta$  is a constant and  $\lambda$  is a fundamental scale . The solution of this equation is the fractal power-law dependence:

$$\mathcal{L} = \mathcal{L}_0 (\lambda / \varepsilon)^\delta \quad \text{-----} \quad (3.2)$$

where  $\delta$  is the scale dimension, i.e.,  $\delta = D - D_T$ , where  $D$  is the fractal dimension (see Appendix A) and  $D_T$  is the topological dimension . The Galilean structure of the group of scale transformations that

corresponds to this law can be verified in a straightforward manner from the fact that it transforms under a scale transformation  $\varepsilon \rightarrow \varepsilon'$  as [30-32,36,38]:

$$\ln \frac{\mathcal{L}(\varepsilon')}{\mathcal{L}_0} = \ln \frac{\mathcal{L}(\varepsilon)}{\mathcal{L}_0} + \delta(\varepsilon) \ln \frac{\varepsilon}{\varepsilon'} \quad \text{----- (3.3)}$$

and,

$$\delta(\varepsilon') = \delta(\varepsilon) .$$

This transformation has the structure of the Galileo group [1,30,31] exactly, confirmed by the law of composition of dilations  $\varepsilon \rightarrow \varepsilon' \rightarrow \varepsilon''$  which can be written as:

$$\ln \rho'' = \ln \rho + \ln \rho' \quad \text{----- (3.4)}$$

where  $\rho = \varepsilon'/\varepsilon$  ,  $\rho' = \varepsilon''/\varepsilon'$  and  $\rho'' = \varepsilon''/\varepsilon$  .

## ***2- Breaking of the Scale Symmetry:***

In general, when the scale variation of  $\mathcal{L}$  depends on  $\mathcal{L}$  only, the first order differential equation becomes [30,31,34,36]:

$$\frac{d\mathcal{L}}{d\ln(\varepsilon)} = \beta(\mathcal{L}) \quad \text{----- (3.5)}$$

where the function  $\beta(\mathcal{L})$  is apriori unknown; that is to take the simple case [31] . Using the Taylor expansion of the perturbative approach eqn. (3.5) can be rewritten as:

$$\frac{d\mathcal{L}}{d\ln\varepsilon} = a + b\mathcal{L} + \dots \quad \text{----- (3.6)}$$

where  $a$  and  $b$  are two real constants . The solution of eqn. (3.6) is [30,31,34,36]:

$$\mathcal{L}(x, \varepsilon) = \mathcal{L}_0(x) [1 + \zeta(x) (\lambda/\varepsilon)^{-b}] \quad \text{----- (3.7)}$$

where  $\lambda^{-b}\zeta(x)$  is an integration constant and  $\mathcal{L}_0 = -a/b$ . These notations allow one to choose  $\zeta(x)$  such that  $\langle \zeta^2(x) \rangle = 1$ . Provided  $a \neq 0$ , eqn. (3.7) clearly shows two domains. Assume, first  $b < 0$ :

a- When  $\varepsilon \gg \lambda$ , this leads to  $\zeta(x)(\lambda/\varepsilon)^{-b} \ll 1$ , and  $\mathcal{L}$  is independent of scale. Eqn. (3.7) gives a fractal (scale invariant) behavior at small scale and a transition from fractal to non-fractal behavior at scales larger than some transition scale  $\lambda$ . Only the particular case  $a = 0$  yields unbroken scale invariance,  $\mathcal{L} = \mathcal{L}_0 (\lambda/\varepsilon)^\delta$  where  $\delta = -b$ .

b- When  $\varepsilon \ll \lambda$ , this leads to  $\zeta(x)(\lambda/\varepsilon)^{-b} \gg 1$ , then  $\mathcal{L}$  is given by a scale invariant fractal-like power law with fractal dimension  $D = 1 - \delta$ ; so  $\mathcal{L}(x, \varepsilon) = \mathcal{L}_0 (\lambda/\varepsilon)^\delta$ .

While, in the case  $b > 0$ , the solutions are mirror symmetric of the case  $b < 0$  as shown in fig. (3.1). One obtains an asymptotic fractal power law (resolution-dependent) at either large or small scales and transition to scale-independence toward classical domain (intermediate scales) [36]. The scale dependence is at large scale and is broken to give scale independence below the transition  $\lambda$ . The case  $b < 0$  is characteristic of microphysics (quantum mechanics in which  $\lambda = \lambda_{dB} \equiv$  de Broglie length) [30,31,36], while the case  $b > 0$  is in the cosmological domain ( $\lambda = \lambda_g \equiv$  cosmological constant) [30,31,36].

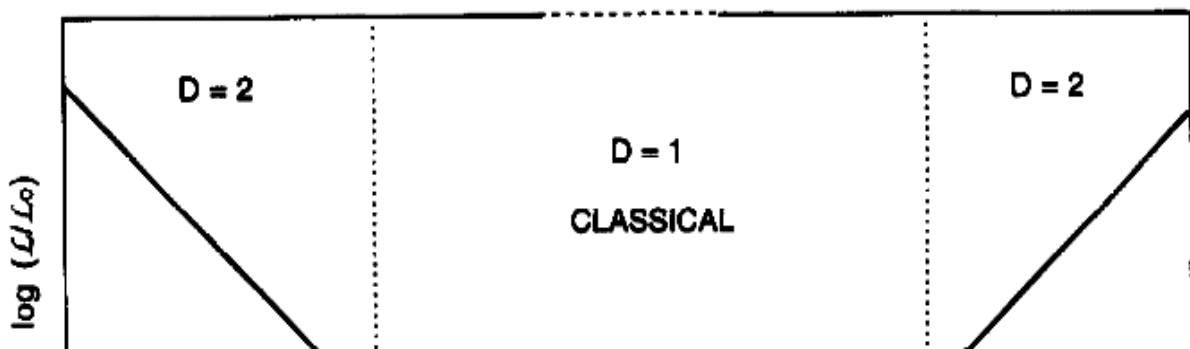


Fig.(3.1). Typical behavior of solution to the simplest linear scaled differential equation [36].

### ***3- Euler - Lagrange Scale Equations:***

Nottale [31,32,36] has considered as primary variables the position  $\mathcal{L}$  and the resolution  $\varepsilon$ . The scale dimension  $\delta$  remains constant only in a particular situation (in the case of scale invariance). It plays for scale laws the same role of time in motion laws. The new approach is including the motion and scale behavior in the same 5-dimensional (space-time-zoom) description. Then, the resolution can be defined as a derived quantity in terms of fractal space-time [10,14,15]:

$$\mathbf{V} = \ln(\lambda / \varepsilon) = \frac{d \ln \mathcal{L}}{d \delta} \quad \text{----- (3.8)}$$

where  $\mathbf{V}$  is the velocity scale . The motion and scale laws can be constructed from a Lagrangian approach. In terms of the Lagrange function  $\mathbf{L} (\ln \mathcal{L}, \mathbf{V}, \delta)$ , then scale-action  $\mathbf{S}$  can be constructed as [31,32,36]:

$$\mathbf{S} = \int_{\delta_1}^{\delta_2} \mathbf{L} (\ln \mathcal{L}, \mathbf{V}, \delta) d\delta \quad \text{----- (3.9)}$$

Then, the Euler-Lagrange equation is [31,32,36]:

$$\frac{d}{d\delta} \frac{\partial \mathbf{S}}{\partial \mathbf{V}} = \frac{\partial \mathbf{S}}{\partial \ln \mathcal{L}} \quad \text{----- (3.10)}$$

The simplest possible form for the Lagrange function is the equivalent for scales of what inertia is for motion, i.e.,  $\mathbf{L} \propto \mathbf{V}^2$  and  $\partial \mathbf{L} / \partial \ln \mathcal{L} = 0$

(no scale force) [31,32]. The Lagrange equation is in this case [31,32,36]:

$$\frac{d\mathbf{V}}{d\delta} = 0 \quad \Rightarrow \quad \mathbf{V} = \text{constant} \quad \text{----- (3.11)}$$

The constancy of  $\mathbf{V} = \ln(\lambda / \varepsilon)$  means that it is independent of scale-time.

### **(3.2.2) Special Scale-Relativity:**

The principle of ScR theory can be constructed from the general linear scale laws which have the structure of the Lorentz group [30,31]. The Lorentz group is obtained requiring linearity, and group law reflection invariance. Nottale [31,36] explains that in two



dimensions, only three axioms are needed (linearity, internal composition law and reflection invariance) . He replaced the Galilean laws of dilation (eqn. (3.4)) by the more general Lorentzian law:

$$\ln \rho'' = \frac{\ln \rho + \ln \rho'}{1 + \frac{\ln \rho \ln \rho'}{c^2}} \quad \text{-----} \quad (3.12)$$

In this equation, there appears a universal, purely numerical constant  $c = \ln \mathbf{K}$ , where  $\mathbf{K}$  plays the role of maximal possible dilation[30,31]. The effect of scale symmetry breaking arises at some scale  $\lambda_0$  to yield a new law in which the invariant is no longer a dilation  $\mathbf{K}$ ; but becomes length-time scale  $\mathbf{\Lambda}$ . This means that there appears a fundamental scale that plays the role of impassable resolution, under dilation [30,31,33,34].

Such a scale of length and time is an horizon for scale laws, in a way similar to the status of the velocity of light for motion laws. The new law of composition of the dilation and the scale-dimension becomes:

$$\ln(\varepsilon' / \lambda_0) = \frac{\ln(\varepsilon / \lambda_0) + \ln \rho}{1 + \frac{\ln \rho \ln(\varepsilon / \lambda_0)}{\ln^2(\mathbf{\Lambda} / \lambda_0)}} \quad \text{-----} \quad (3.13)$$

and

$$\delta(\varepsilon) = \frac{1}{\sqrt{1 - \frac{\ln^2(\varepsilon / \lambda_0)}{\ln^2(\mathbf{\Lambda} / \lambda_0)}}} \quad \text{-----} \quad (3.14)$$

A fractal curve linear coordinate system becomes now scale-dependent in a covariant way, namely;  $\mathcal{L} = \mathcal{L}_0 [1 + (\lambda_0 / \varepsilon)^{\delta(\varepsilon)}]$  .  $\delta$  in the

special scale relativity becomes explicitly varying with scale and it even diverges when  $\varepsilon$  tends to the new invariant scales [31,39].

### (3.2.3) Scale Dynamics:

Nottale [30-32] has taken non-linearity in scale into account. Such distortions may be attributed to the effect of scale dynamics, i.e., to a scale-field. Dynamic scale acts on the scale axis, not in space-time. In this case, Newton's equation of dynamics that comes from the Lagrange scale-equation is [30-32]:

$$\mathbf{F} = \mu \frac{d^2 \ln \mathcal{L}}{d\delta^2} \quad \text{-----} \quad (3.15)$$

where  $\mu$  is a scale-mass and  $\mathbf{\Gamma} = \frac{d^2 \ln \mathcal{L}}{d\delta^2} = \frac{d \ln(\lambda / \varepsilon)}{d\delta}$  is a scale-acceleration. When the scale-force  $\mathbf{F}$  is constant, eqn. (3.15) can be rewritten as:

$$\frac{d^2 \ln \mathcal{L}}{d\delta^2} = \mathbf{G} \quad \text{-----} \quad (3.16)$$

where  $\mathbf{G} = \mathbf{F}/\mu = \text{constant}$ . Eqn. (3.16) can be integrated as [30,31,36]:

$$\left. \begin{aligned} \mathbf{V} &= \mathbf{V}_0 + \mathbf{G} \delta \\ \ln \mathcal{L} &= \ln \mathcal{L}_0 + \mathbf{V}_0 \delta + \frac{1}{2} \mathbf{G} \delta^2 \end{aligned} \right\} \quad \text{-----} \quad (3.17)$$

Nottale [31,36] redefines the integration constant, and finds:

$$\left. \begin{aligned} \delta &= \delta_0 + \frac{1}{\mathbf{G}} \ln(\lambda / \varepsilon) \\ \ln \frac{\mathcal{L}}{\mathcal{L}_0} &= \frac{1}{2\mathbf{G}} \ln^2(\lambda / \varepsilon) \end{aligned} \right\} \quad \text{-----} \quad (3.18)$$

Then, the scale dimension  $\delta$  becomes a linear function of resolution  $\varepsilon$  [30-32].

### **(3.2.4) Quantum Scale-Relativity:**

The previous two cases assume differentiability of scale transformations. If one assumes them to be continuous but non-differentiable for space-time, one is confronted for scale laws with the same conditions that lead to quantum mechanics in space-time [31,36,38] (This will be discussed in more details in Secs. (3.4) and (3.5)).

In addition to pure scale laws, Nottale explains the scale motion coupling and gauge [30,66,67] by the ScR theory as well.

### **(3.3) Domains of Application of ScR Theory:**

The three fields of microphysics, cosmology and complex systems correspond to privileged fields of application of ScR theory. They can be described briefly as follows:

#### **(3.3.1) Microphysics:**

In this field,  $dx \rightarrow 0$  and  $dt \rightarrow 0$ ; one expects  $\hbar$  to have an effective value that varies with scale beyond the top quark energy ( $\sim 172.6$  GeV) [30-32]. Also, there is a new experiment that can be explained: associated with the free fall reference system for gravitation is an accelerating system. One may expect that some particle-fields could be absorbed in coordinate systems characterized by a "scale-acceleration" [30-32,36]. The resolution is defined with

scale-velocity which is a derived quantity, then, one can introduce a second-derived quantity which is the scale-acceleration. In such a new experiment, the resolution of the measurement apparatus should be variable in space-time, while scale-dependence should be no longer self-similar [30,31,36,38].

### **(3.3.2) Cosmology:**

In this field,  $dx \rightarrow \infty$  and  $dt \rightarrow \infty$ ; these are very large scales. Here the Lorentzian scale laws could be valid. In this domain, the resolution can be defined with the scale of the cosmological constant ( $\sim 10^{-47}$  GeV) [31,36,39]. Here, new solutions can be brought to the problem of the vacuum energy density [31,36], of the Mach principle [1-5] and of the large number hypothesis [30,39].

### **(3.3.3) Complex systems:**

For describing systems which have structures of density waves rather than solid objects, such as in the biological domain, one deals instead with the individual trajectories in the overall structure. In ScR theory, the complex structures can be described as density waves in terms of probability amplitudes which are solutions of a generalized Schrödinger equation [30,31,68]. This approach can be applied to the gravitational structures, that give several results, at scales ranging from planetary systems to large scale structure of the universe: Solar system [41], Extra-Solar, Planetary systems [42], Satellites of giant Planets [47] Planets around Pulsars [43], binary stars [31,36] and other systems .

### **(3.4) The Fractal Approach to Quantum Mechanics:**

Feynman [21] studied the geometrical structure of quantum paths. He showed that typical trajectories of quantum particles are continuous but non-differentiable and may be characterized by a fractal dimension 2. Though, Feynman evidently did not use the word "fractal", which was coined in 1975 by Mandelbrot (see Appendix A). Abbott and Wise [25], also studied the problem of the geometrical structure of quantum paths in terms of the concept of fractals. They showed that the length of a quantum mechanical trajectory varies with space resolutions as  $\mathcal{L} \propto \delta x^{-1}$  when  $\delta x \ll \lambda_{dB}$  (de Broglie length), and becomes independent of scale when  $\delta x \gg \lambda_{dB}$ . There are two points contained in this result. The first derives from the known expression for the scale divergence of a fractal curve [31,36,38]:

$$\mathcal{L} = \mathcal{L}_0 (\lambda_{dB} / \delta x)^{D-1} \quad \text{----- (3.19)}$$

This leads to the fractal dimension  $D=2$  which agrees with Feynman and Abbott-Wise results. The second point is that the fractal structure does not persist whatever the scale, and that there is a fast transition from fractal to non-fractal behavior ( $D = 2$  to  $D = 1$ ) at about the de Broglie scale. Abbott and Wise [25] identify this transition with a

quantum to classical transition [31,36]. Omitting fluctuations during the transition, i.e.,  $\delta x \approx \lambda_{dB}$ , the scale dependence reads [31,38]:

$$\mathcal{L} = \mathcal{L}_0 [1 + (\lambda_{dB}/\delta x)^{2(D-1)}]^{1/2} \quad \text{-----} \quad (3.20)$$

$\mathcal{L}$  is considered as a curvilinear coordinate along the fractal curve. Its scale diverges as  $\mathcal{L} \propto \delta t^{(1/D)-1}$  in the fractal regime [31,38]. Nottale [38] introduced a renormalized coordinate  $\mathring{t} = \mathcal{L}(\delta t/\tau_0)^{1-(1/D)}$  which remains finite. Each of the three coordinates can now be described as a fractal function of  $\mathring{t}$  and of the resolution  $\delta t$ , i.e., [38]:

$$x^i = x^i(\mathring{t}, \delta t) \Rightarrow \delta x^i = \mathbf{V}^i \delta t + \mathbf{V}(\mathring{t}, \delta t)(\delta t/\tau_0)^{1/D} \quad \text{---} \quad (3.21)$$

From this equation  $\mathcal{L}$  can be recomputed, and this yields essentially the result of eqn. (3.20). The curvilinear coordinate  $\mathring{t}$  is a monotonous function of time, so that the functions of  $(\mathring{t}, \delta t)$  can be replaced by functions of  $(t, \delta t)$ .

This discussion holds in space–time; the four fractal functions depending on an invariant but scale-dependent proper time  $S$ , then,  $\mathcal{L}$  can be renormalized in order to obtain a finite invariant  $s = S(\delta S/\tau_0)^{1-(1/D)}$ , where  $S$  is the classical invariant [30,37]. There is a difference between the classical invariant  $S$  and the new invariant  $s$ . The proper time  $S$  is defined along the fractal trajectory which is allowed to run backward in classical time at very small scales, while the classical invariant  $S$  is calculated only on classical differentiable trajectories for which all time intervals remain positive [31,38].

Nottale [31,36,38] introduced a new account of a compensation between the special relativistic contraction and the quantum scale-divergence issuing from Heisenberg's relation. Accordingly, the element of proper time  $S$  varies as [31,38]:

$$\delta S \propto \delta t^{1/D} = \left\{ c \delta t (1 - v^2/c^2)^{1/2} \right\}^{1/D} \quad \text{----- (3.22)}$$

Then from Heisenberg's relation, the term  $(1 - v^2/c^2)^{1/2}$  can be written as [31,38]:

$$(1 - v^2/c^2)^{1/2} = E_0/E \approx (\delta t / \tau_0) \quad \text{----- (3.23)}$$

This equation leads to:

$$\delta S \propto \delta t^{2/D} \quad \text{----- (3.24)}$$

i.e.,

$$\delta S \propto \delta t \quad \text{for } D=2,$$

while the limit  $v \rightarrow c$  leads to  $\delta S = 0$ .

These formulas are expressed in terms of the finite differences  $\delta f$ , identified with resolutions when dealing with space and time variables. Eqn. (3.21) for  $D=2$  is nothing but the basic relation describing a Wiener process [31,36,38]. This description leads to a reformulation of Nelson's stochastic mechanics [69,70] as shown in the next section.

### **(3.5) Quantum Mechanics as Mechanics in Non-Differentiable Space:**

Assuming space is continuous and non-differentiable, one can express the position vector of a particle by a finite, continuous fractal function  $x(t, \delta t)$  [31,38]. Adopting the non-standard analysis (NSA) formulation, Nottale [31,32] replaced  $\delta t$  by the differential  $dt$ . Then, the position vector between  $t$  and  $t + dt$  varies as [31,32]:

$$x(t + dt, dt) - x(t, dt) = b_+(x, t) dt + \zeta_+(t, dt) (dt / \tau_0)^\beta \quad \text{--- (3.25)}$$

where  $\beta = 1/D$  ( $\beta = 1/2$  in the quantum and Brownian motion),  $b_+$  is a forward velocity and  $\zeta_+$  is a fractal function .

The variation of  $x$  between  $t-dt$  and  $t$  is then [31,32,38]:

$$x(t,dt) - x(t-dt,dt) = b_-(x,t)dt + \zeta_-(t,dt)(dt/\tau_0)^\beta \quad \text{----- (3.26)}$$

where  $b_-$  is the backward velocity .

Eqns. (3.25) and (3.26) can be rewritten in terms of instantaneous velocities [31,32,36,38]:

$$v_+(x,t,dt) = b_+(x,t) + \zeta_+(t,dt)(dt/\tau_0)^{\beta-1} \quad \text{----- (3.27)}$$

and

$$v_-(x,t,dt) = b_-(x,t) + \zeta_-(t,dt)(dt/\tau_0)^{\beta-1} \quad \text{----- (3.28)}$$

The non-differentiability is evident in these expressions, since in the quantum case  $\beta-1=-1/2$  so that  $dt^{\beta-1}$  is an infinite quantity. Eqns. (3.27) and (3.28) in NSA can be defined as [31,32,38]:

$$\text{and} \quad \left. \begin{aligned} V_+ &= v_+(dt/\tau_0)^{1-\beta} \\ V_- &= v_-(dt/\tau_0)^{1-\beta} \end{aligned} \right\} \quad \text{----- (3.29)}$$

Then, each component of  $V_+$  and  $V_-$  is a finite number of the set  $\mathbb{R}^*$  of non-standard reals [71]: in NSA any finite number of  $\mathbb{R}^*$  can be decomposed in a unique way into the sum of a real (standard) number and an infinitesimal number [71]. Then, eqn. (3.29) becomes [31,32,38]:

$$\left. \begin{aligned} V_+ &= \zeta_+ + b_+(dt/\tau_0)^{1-\beta} \\ \text{and} \\ V_- &= \zeta_- + b_-(dt/\tau_0)^{1-\beta} \end{aligned} \right\} \quad \text{----- (3.30)}$$



where  $b_+$  and  $b_-$  being finite real numbers .

In the differentiable case, only the classical part of the velocity remains, i.e.,  $\zeta_+ = \zeta_- = 0$ , and the forward and backward velocities are equal [69]:

$$\lim_{t \rightarrow 0} \{x(t+dt, dt) - x(t, dt)\} = \lim_{t \rightarrow 0} \{x(t, dt) - x(t-dt, dt)\} \text{ ---(3.31)}$$

In the non-differentiable space-time, there is an infinity of geodesics between any couple of points, each of them having fractal properties, i.e., scale dependent. Their ensemble will define a probability amplitude. Fig. (3.2) shows the construction a non-differentiable function by successive dissections. Its length tends to infinity when the resolution interval tends to zero [36]. Nelson [69,70], in his stochastic quantum mechanics, assumes an underlying Brownian motion of unknown origin which acts on particles in a still Minkowskian space-time, and then introduces non-differentiability. Nottale [31,32] assumes that the space-time itself is no longer Minkowskian nor differentiable. His hypothesis of non-differentiability is essential and should hold down to the smallest possible length scales.

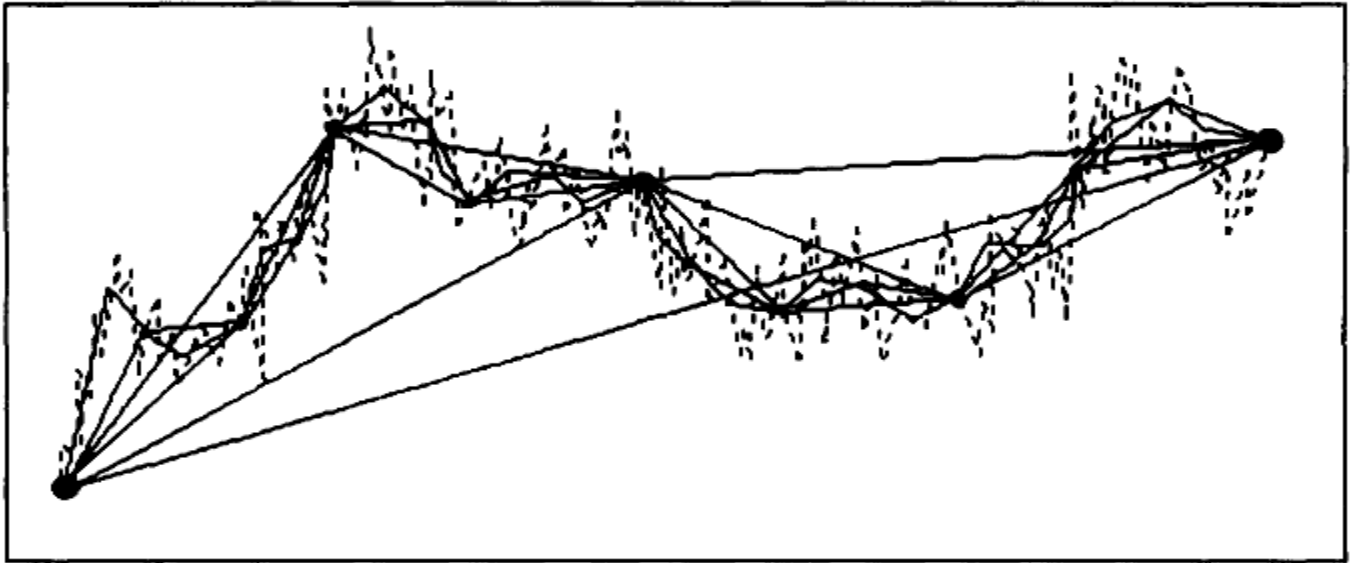


Fig. (3.2) Construction of a non-differentiable function by successive dissections [36].

Nelson [69,70] defines mean forward and backward derivatives  $d_+/dt$  and  $d_-/dt$  as:

$$\frac{d_{\pm}}{dt} Y(t) = \lim_{\Delta t \rightarrow 0_{\pm}} \left\langle \frac{Y(t + \Delta t) - Y(t)}{\Delta t} \right\rangle \quad \text{----- (3.32)}$$

where  $Y(t)$  is any arbitrary function of  $t$  and  $\langle \rangle$  is the mean .

Applying this equation to the position vector, one can introduce forward and backward mean velocities as [31,38,72,73]:

$$\frac{d_+}{dt}x(t)=b_+ \quad ; \quad \frac{d_-}{dt}x(t)=b_- \quad \text{-----} \quad (3.33)$$

By combining the forward and backward derivatives of eqn. (3.32) in a complex derivative operator one obtains [31,32,36,38]:

$$\frac{\delta}{dt} = \frac{(d_+ + d_-) - i(d_+ - d_-)}{2dt} \quad \text{-----} \quad (3.34)$$

Applying this equation to the position vector yields a complex velocity [31,32,36,38]:

$$\vec{\mathbf{V}} = \frac{\delta}{dt}x(t) = \vec{V} - i\vec{U} = \frac{b_+ + b_-}{2} - i\frac{b_+ - b_-}{2} \quad \text{-----} \quad (3.35)$$

One can also define [10,11,18]:

$$\frac{d_v}{dt} = \frac{1}{2} \frac{d_+ + d_-}{dt} \quad ; \quad \frac{d_u}{dt} = \frac{1}{2} \frac{d_+ - d_-}{dt} \quad \text{-----} \quad (3.36)$$

such that:

$$\vec{V} = \frac{d_v}{dt}x \quad ; \quad \vec{U} = \frac{d_u}{dt}x \quad \text{-----} \quad (3.37)$$

where  $\vec{V}$  is the real part of the complex velocity  $\vec{\mathbf{V}}$  or,  $\vec{V}$  is the classical velocity and,  $\vec{U}$  is the imaginary part of the complex velocity; it is a new quantity arising from the non-differentiability [31,36,38] . In a statistical representation, the position vector  $x(t)$  is assimilated into a stochastic process which satisfies the relation [38]:

$$\left. \begin{array}{l} dx(t) = b_+(x(t))dt + d\xi_+(t) \quad \text{for } dt > 0(\text{forward}) \\ \text{and} \\ dx(t) = b_-(x(t))dt + d\xi_-(t) \quad \text{for } dt > 0(\text{backward}) \end{array} \right\} \text{-----} \quad (3.38)$$

where  $d\xi(t)$  is the fluctuation about the classical part  $b_{\pm}$  which is Gaussian with mean zero, mutually and such that [31,34,38]:

$$\langle d\xi_{\pm i} d\xi_{\pm j} \rangle = \pm 2 \mathcal{D} \delta_{ij} dt \quad \text{-----} (3.39)$$

where  $\mathcal{D}$  stands for a diffusion coefficient,  $\mathcal{D} = \frac{\hbar}{2m}$  and  $\delta_{ij}$  is the Kronecker symbol defined previously. Also,  $d\xi$  can be defined as [31,34,38]:

$$d\xi = \eta \sqrt{2 \mathcal{D} (dt^2)^{1/2D}} \quad \text{-----} (3.40)$$

where  $\eta$  is a stochastic variable such that  $\langle \eta \rangle = 0$  and  $\langle \eta^2 \rangle = 1$ . Eqn. (3.39) allows one to get a general expression for the complex derivative  $\delta/dt$ . Consider a function  $f(x, t)$ , and expand its total differential to second order. One obtains [36]:

$$df = \frac{\partial f}{\partial t} dt + \vec{\nabla} f \cdot dx + \frac{1}{2} \frac{\partial^2 f}{\partial x_i \partial x_j} dx_i dx_j \quad \text{-----} (3.41)$$

To compute the forward and backward derivatives of  $f$ , the mean value  $\langle dx_i dx_j \rangle$  reduces to  $\langle d\xi_{\pm i} d\xi_{\pm j} \rangle$ ; eqn. (3.41) becomes:

$$d_{\pm} f / dt = \left( \frac{\partial}{\partial t} + b_{\pm} \cdot \vec{\nabla} \pm \mathcal{D} \Delta \right) f \quad \text{-----} (3.42)$$

where  $\Delta$  is the Laplacian ( $\Delta \equiv \vec{\nabla}^2$ ). Using eqn. (3.42), the expression for the complex time derivative operator becomes [31,34,38]:

$$\frac{\delta}{dt} = \frac{\partial}{\partial t} + \vec{\nabla} \cdot \vec{v} - i \mathcal{D} \Delta \quad \text{-----} (3.43)$$

Then, the passage from classical (differentiable) mechanics to the new non-differentiable mechanics can be achieved by replacing the

standard time derivative  $d/dt$  by the new complex operator  $\delta/dt$ .  $\delta/dt$  plays the role of a quantum covariant derivative [31,36]. In terms of this new correspondence principle, the main steps which generalize classical mechanics can be indicated as follows [31,38]:

Any mechanical system can be characterized by a Lagrange function  $\mathbf{L}(x, \vec{\mathbf{V}}, t)$ ; then, the average stochastic action  $\mathbf{S}$  is defined as [31,36,38]:

$$\mathbf{S} = \int_{t_1}^{t_2} \langle \mathbf{L}(x, \vec{\mathbf{V}}, t) \rangle dt \quad \text{----- (3.44)}$$

Applying  $d/dt$  on the Lagrange function and replacing  $d/dt$  by  $\delta/dt$ , leads to the generalized Euler-Lagrange equation [31,34,36,38]:

$$\frac{\delta}{dt} \frac{\partial \mathbf{L}}{\partial \mathbf{V}_i} = \frac{\partial \mathbf{L}}{\partial x_i} \quad \text{----- (3.45)}$$

Other fundamental results of classical mechanics are also generalized in the same way. Assuming homogeneity of space in the mean, leads one to define a complex momentum as [31,34,36,38]:

$$\vec{\mathbf{P}} = \frac{\partial \mathbf{L}}{\partial \mathbf{V}} \quad \text{----- (3.46)}$$

The variation of the action from a trajectory to another close-by trajectory, when combined with eqn. (3.45), yields, a generalization of another form of complex momentum as:

$$\vec{\mathbf{P}} = \vec{\mathbf{V}} \mathbf{S} \quad \text{----- (3.47)}$$

In Newtonian mechanics, the Lagrange function of a closed system can be generalized to [31,33,34,36]:

$$\mathbf{L}(x, \vec{\mathbf{V}}, t) = \frac{1}{2} m \vec{\mathbf{V}}^2 - \mathcal{U} \quad \text{----- (3.48)}$$

where  $\mathcal{U}$  is a scalar potential . The Euler-Lagrange equations keep the form of Newton's fundamental equation of dynamics as [31,33,36,38,68]:

$$-\vec{\nabla} \mathcal{U} = m \frac{\partial}{\partial t} \vec{\mathbf{V}} \quad \text{----- (3.49)}$$

which is written in terms of complex variables and derivative operator.

### **(3.6) The Schrödinger Equation in a New Perspective:**

The concepts of fractal space-time and complex time derivative operator allow to recover the Schrödinger equation, then to generalize it [45,38,68]. The probability amplitude is defined by the relation [31,68]:

$$\psi = e^{i\mathbf{s}/2m \mathcal{D}} \quad \text{----- (3.50)}$$

The complex velocity  $\vec{\mathbf{V}}$  appears as a gradient; the gradient for the complex action as [38,68]:

$$\vec{\mathbf{V}} = \vec{\nabla} \mathbf{S} / m \quad \text{----- (3.51)}$$

Then,  $\psi$  is related to the complex velocity by [68,73]:

$$\vec{\mathbf{V}} = 2i \langle \mathcal{D} \rangle \vec{\nabla} (\ln \psi) \quad \text{----- (3.52)}$$

Now, the generalized Newton equation, eqn. (3.49), takes the form [31,38]:

$$\vec{\nabla} \mathcal{U} = 2i\text{im}\langle \mathcal{D} \rangle \frac{\delta}{dt} (\vec{\nabla} \ln \psi) \quad \text{----- (3.53)}$$

where  $\delta$  and  $\vec{\nabla}$  do not commute, and  $\mathcal{D}$ , which appears in the expression for  $\frac{\delta}{dt}$ , is now a function of  $x$ . Both  $\mathcal{D}$  and its mean  $\langle \mathcal{D} \rangle$  lead to the relation [36,38,68]:

$$\mathcal{D}(x, t) = \langle \mathcal{D} \rangle + \delta \mathcal{D}(x, t) \quad \text{----- (3.54)}$$

where  $\langle \mathcal{D} \rangle$  is a constant with respect to the variables  $x$  and  $t$ , but may include an explicit scale-dependence in terms of time resolution  $\delta t$ . Eqn. (3.53), then, can be written as:

$$\vec{\nabla} \mathcal{U} = 2i\text{im}\langle \mathcal{D} \rangle \left[ \frac{\partial}{\partial t} + \vec{\mathbf{V}} \cdot \vec{\nabla} - i \mathcal{D}(x, t) \Delta \right] \vec{\nabla} (\ln \psi) \quad \text{---- (3.55)}$$

Substituting eqns. (3.52) and (3.54) into eqn. (3.55) gives [31,38,68]:

$$\vec{\nabla} \mathcal{U} = 2i\text{im}\langle \mathcal{D} \rangle \left[ \frac{\partial}{\partial t} - 2i\langle \mathcal{D} \rangle \vec{\nabla} (\ln \psi) \cdot \vec{\nabla} - i(\langle \mathcal{D} \rangle + \delta \mathcal{D}(x, t)) \Delta \right] \vec{\nabla} (\ln \psi) \quad \text{--(3.56)}$$

Using the three identities [31,68]:

$$\left. \begin{aligned} (\vec{\nabla} \ln \psi)^2 + \Delta \ln \psi &= \frac{\vec{\nabla} \psi}{\psi} \\ (\vec{\nabla} \ln \psi)^2 &= 2(\vec{\nabla} \ln \psi \cdot \vec{\nabla})(\vec{\nabla} \ln \psi) \\ \Delta \vec{\nabla} &\equiv \vec{\nabla} \Delta \end{aligned} \right\} \quad \text{----- (3.57)}$$

then, eqn. (3.56) can be given in the form of a generalized Schrödinger equation [30,35,62]:

$$\vec{\nabla} \left\{ \frac{\mathcal{U}}{2m\langle \mathcal{D} \rangle} - \frac{1}{\psi} \left[ \mathcal{D} \Delta \psi + i \frac{\partial \psi}{\partial t} \right] + \delta \mathcal{D} (\vec{\nabla} \ln \psi)^2 \right\} = -\vec{\nabla} (\delta \mathcal{D}) \Delta \ln \psi \quad \text{----(3.58)}$$

Nottale [31,36,68], considered some special simplified cases:

1-  $\mathcal{D} = \text{constant} = \frac{\hbar}{2m}$  : in this case  $\delta\mathcal{D}=0$ ; the last two terms of eqn. (3.58) disappear. Eqn. (3.58) can be integrated and yields the Schrödinger equation[31,36,68]:

$$\mathcal{D} \Delta \psi + i \mathcal{D} \frac{\partial}{\partial t} \psi = \frac{\mathcal{U}}{2m} \psi \quad \text{----- (3.59)}$$

2-  $\mathcal{D} = \mathcal{D}(\delta t) = \mathcal{D}(\delta t/\tau)^{(2/D)-1}$  : this is the opposite case; the diffusion coefficient remains constant in terms of position and time, but it includes the effect of a fractal dimension different from 2. Then, the last two terms of eqn. (3.58) disappear. In this case Schrödinger's equation has the form:

$$\mathcal{D}^2(\delta t) \Delta \psi + i \mathcal{D}(\delta t) \frac{\partial \psi}{\partial t} = \frac{\mathcal{U}}{2m} \psi \quad \text{----- (3.60)}$$

3-  $\vec{\nabla}(\delta\mathcal{D}) = 0$  or  $\vec{\nabla}(\delta\mathcal{D}) \ll 1$ : in this case the diffusion coefficient depends on time but not on position . Then, the right hand side of eqn. (3.58) vanishes , so that it may be integrated to get:

$$\left[ \frac{\mathcal{U}}{2m \langle \mathcal{D} \rangle} + a + \delta \mathcal{D} (\vec{\nabla} \ln \psi)^2 \right] \psi = \mathcal{D} \Delta \psi + i \frac{d\psi}{dt} \quad \text{----- (3.61)}$$

where  $a$  is a constant of integration . Assuming that  $\delta\mathcal{D}/\mathcal{D}$  remains  $\ll 1$ , the effect of the term  $\delta\mathcal{D} \psi (\vec{\nabla} \ln \psi)^2$ , which is extra to the standard Schrödinger equation, and the effect of  $\mathcal{D}$  being a function of  $x$  and  $t$ , can be treated by perturbation. One gets an equation of the form [31,36,67]:

$$\left[ \frac{\mathcal{U}(x, t)}{2m} + a + \delta \mathcal{D}(x, t) \right] \psi = \langle \mathcal{D} \rangle^2 \Delta \psi + i \langle \mathcal{D} \rangle \frac{d\psi}{dt} \quad \text{----- (3.62)}$$



where  $a$  and  $b$  are constants. The behavior of eqn. (3.62) is of interest to the future development of scale relativity into a field theory [31,38,67].

The statistical interpretation of the wave function  $\psi$  in eqn. (3.58) in terms of  $P = \psi\psi^*$ , giving the probability of presence of the particle, remains correct, since the imaginary part of the Schrödinger equation is the equation of continuity [38]:

$$\frac{\partial P}{\partial t} + \text{div}(P\vec{V}) = 0 \quad \text{-----}(3.63)$$

where  $\vec{V}$  is a generalized classical velocity .

### **(3.7) The Energy at Quantum Scales in the Non-Relativistic Case:**

The quantity which plays the role of energy in the present fractal approach to quantum mechanics does not have a quadratic form [48]. It is well known that the equation of motion for a free particle is given by [45]:

$$\frac{dV}{dt} = 0 \quad \text{-----} (3.64)$$

In this case, the energy is  $E_{free} = \frac{1}{2}m_0V^2$ , which corresponds to the kinetic energy  $\mathcal{E} = E - \mathcal{U}$  of the particle. In the presence of an external potential  $\mathcal{U}(x)$ , eqn. (3.64) becomes  $m \frac{dV}{dt} = -\nabla \mathcal{U}$  and the total energy is written as [31,46]:

$$E = \frac{1}{2}mV^2 + \mathcal{U} \quad \text{----- (3.65)}$$

This quantity satisfies [46]:

1- The conservation equation  $\frac{dE}{dt} = 0$ .

2- The Hamilton–Jacobi [45] equation  $\frac{\partial \mathcal{S}}{\partial t} = -H$  where  $H = \frac{p^2}{2m} + \mathcal{U}$

and  $p = mV$ .

In the framework of scale-relativity, the Hamilton function  $\mathcal{H}$  is a complex quantity which satisfies the complex Hamilton-Jacobi equation [50]:

$$\frac{\partial \mathcal{S}}{\partial t} = \mathcal{H} \quad \text{----- (3.66)}$$

which corresponds to the equations of motion  $\frac{\delta \vec{\mathbf{P}}}{dt} = -\vec{\nabla} \mathcal{U}$  after differentiation . Pissondes [50] found that  $\mathcal{H} = \frac{\vec{\mathbf{P}}^2}{2m} - i \frac{c\lambda_{dB}}{2} \vec{\nabla} \cdot \vec{\mathbf{P}} + \mathcal{U}$ . Therefore, the complex quantity  $\mathbf{E}$  which satisfies the conservation equation:

$$\frac{\delta}{dt} \mathbf{E} = 0 \quad \text{----- (3.67)}$$

when  $\mathcal{H} = \mathbf{E}$  and  $\vec{\mathbf{P}} = m \vec{\mathbf{V}}$  , is:

$$\mathbf{E} = \frac{1}{2}m \vec{\mathbf{V}}^2 - i \frac{mc\lambda_{dB}}{2} \vec{\nabla} \cdot \vec{\mathbf{V}} + \mathcal{U} \quad \text{----- (3.68)}$$

Eqn. (3.68) is the equivalent of the equation of total energy which is obtained by applying the concepts of the ScR theory[50].

### **(3.8) The Relativistic Case:**

In this case, starting from the hypothesis that space-time is non-differentiable, one can see as in Secs. (3.4) and (3.5) that the trajectories of particles are fractals [31,38]. Hence one can define a scale-dependent invariant which is a proper time  $S$  on these trajectories [46,50]. In the relativistic case all equations that one gets for the non-relativistic case can be re-written by replacing [46,50,51]:

$$\left. \begin{aligned} x &\rightarrow x^\mu \text{ (four - vector)} \\ t &\rightarrow S \end{aligned} \right\} \text{----- (3.69)}$$

Therefore, one can write [45,49,50] :

$$(dx^\mu)_\pm = b_\pm^\mu dS + d\xi_\pm^\mu \text{----- (3.70)}$$

with

$$\langle d\xi_\pm^\mu d\xi_\pm^\nu \rangle = \pm 2 \mathcal{D} \delta^{\mu\nu} dS \text{----- (3.71)}$$

$x$

where  $\mathcal{D} = \frac{\hbar}{2mc}$  .

The quantum - covariant derivative then becomes [46,50,51]:

$$\frac{\delta}{dS} = \frac{\partial}{\partial S} \mathbf{V}^\mu \partial_\mu - i \mathcal{D} \partial^\mu \partial_\mu \text{----- (3.72)}$$

$x$

where  $\mathbf{V}^\mu$  is the four-dimensional complex velocity. As for the Schrödinger equation, one can get the free particle Klein-Gordon equation [31,36,46] using this approach. Also, using the definition of gauge invariance [31,66,67], one can get the Klein-Gordon equation with electro-magnetic field [50,51] in a similar manner. Finally, the Dirac equation is derived when the Klein-Gordon equation is re-written in a quaternionic form [50,51].

# Chapter Four

## Application of ScR Theory to Problems of a Particle in Potential Wells

### (4.1) Potential Wells:

The one-dimensional square well potential is a simple example which shows discrete energy levels of a particle in quantum mechanics [8-12]. There are two simple types of square well potentials, namely; the infinite square well and the finite square well. In the first type, the potential energy  $\mathcal{U}(x)$  in the region  $-a < x < a$ , as shown in Fig. (4.1-a), is equal to zero while  $\mathcal{U}(x) = \infty$  for  $|x| > a$ . The second type has a sudden jump in the potential energy at the walls,  $\mathcal{U}(x) = \mathcal{U}_0$  for  $|x| > a$  as shown in Fig. (4.1-b) [8-12]:

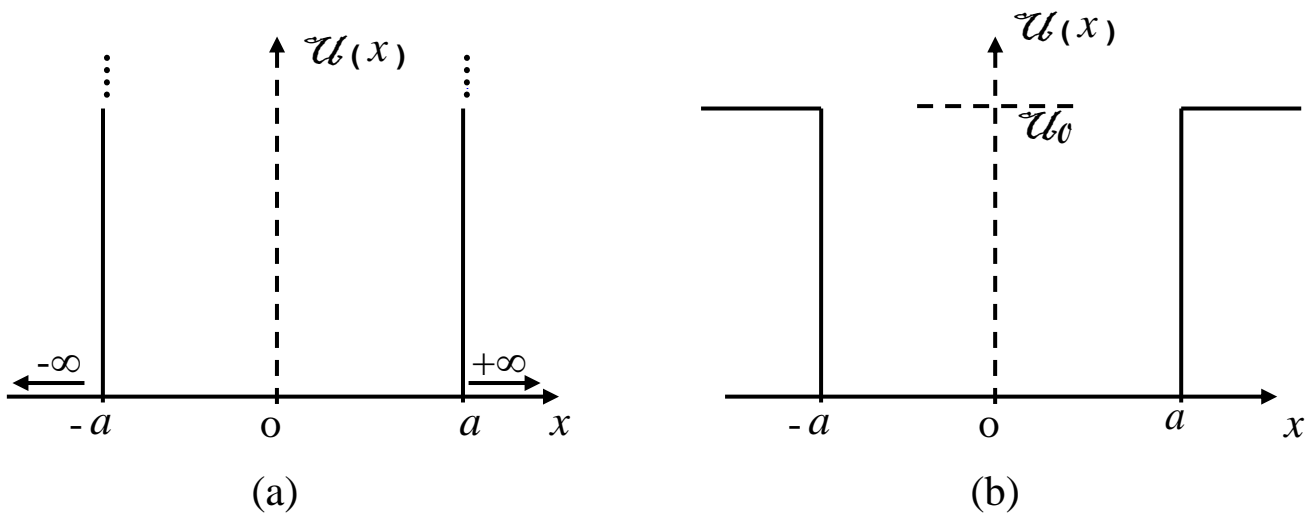


Fig. (4.1) Two types of square well potentials [1,2,3]:

*a- infinite square well*

*b- finite square well*

In this chapter, a review of Hermann's work (HScR) [53], who applied the principle of ScR theory to the infinite square well will be given. Also, the prediction the behavior of a quantum particle in a one-dimensional finite square well potential that can be obtained without writing explicitly the Schrödinger equation nor using any conventional quantum axiom, along the lines of Hermann, will be obtained using HScR .

## **(4.2) Review of ScR Theory Applied to a Particle in an Infinite One-Dimensional Square Well Potential (IODSW):**

Hermann [53] obtained, by means of numerical simulation, the behavior of a quantum particle in an infinite one-dimensional square well (IODSW) potential. The one-dimensional infinite square well potential used by Hermann [53] extends from  $x=0$  to  $x=a$  in contrast with that shown in Fig. (4.1) which extends from  $x = -a$  to  $x = a$  . He achieved this by using the non-differentiability hypothesis, not going further in the scale relativistic description. Hermann found that it is possible to simulate some simple quantum mechanical problems by using the equivalence of non-differentiable mechanics and quantum mechanics that was showed by Nottale [31,36,38]. In this application, Hermann started from the complex Newton equation (eqn. (3.49)) and separated this equation into real and imaginary parts. Since the potential  $\mathcal{U}$  is a real quantity, then the equations of motion are:

$$m\left(\frac{\partial}{\partial t}\vec{V} - \mathcal{D}\Delta\vec{U} + (\vec{V}\cdot\vec{V})\vec{V} - (\vec{U}\cdot\vec{V})\vec{U}\right) = \vec{V} \mathcal{U} \quad \text{----- (4.1)}$$

and

$$m\left(\frac{\partial}{\partial t}\vec{U} + \mathcal{D}\Delta\vec{V} + (\vec{V}\cdot\vec{V})\vec{U} + (\vec{U}\cdot\vec{V})\vec{V}\right) = 0 \quad \text{----- (4.2)}$$

Since  $\mathcal{U}$  is constant for  $-a < x < a$  and the average classical velocity  $V$  of such a particle, which is the sum of the forward and backward velocity is expected to be zero, then Hermann reduced the equations of motion to the form [53]:

$$\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \mathcal{U}(x) + \frac{1}{2} \vec{U}^2(x) \right) = 0 \quad \text{----- (4.3)}$$

and

$$\frac{\partial}{\partial t} \vec{U}(x) = 0 \quad \text{----- (4.4)}$$

Eqn. (4.4) shows that  $U$  is a function of  $x$  alone, and eqn. (4.3) can be solved in one-dimension as:

$$U(x) = \sqrt{2c_1} \tan\left(-\frac{\sqrt{2c_1}}{2\mathcal{D}} x + c_2\right) \quad \text{----- (4.5)}$$

where  $c_1$  and  $c_2$  are integration constants. In HScR,  $U$  is considered as a difference of velocities and, hence, interpreted it as a kind of acceleration [53]. The boundary conditions can then be used to calculate the integration constants. Hence, eqn. (4.5) becomes:

$$U(x) = \frac{2\mathcal{D}n\pi}{a} \tan\left(-\frac{n\pi x}{a} + \frac{\pi}{2}\right) \quad \text{----- (4.6)}$$

where the infinite square well is of size  $a$ . Eqn. (3.38) was then used to define the position vector as:

$$d x(t) = \frac{2 \mathcal{D} n \pi}{a} \tan\left(-\frac{n \pi x}{a} + \frac{\pi}{2}\right) dt + d \xi_{+}(t) \quad \text{----- (4.7)}$$

where  $d \xi_{+}(t)$  is now a random variable of Gaussian distribution and is of width  $\sqrt{2 \mathcal{D} dt}$ . Taking  $2 \mathcal{D} dt = 1$  as done by Hermann [53], then eqn. (4.7) becomes:

$$dx(t) = \frac{n \pi}{a} \tan\left(-\frac{n \pi}{a} x + \frac{\pi}{2}\right) + N(0,1) \quad \text{----- (4.8)}$$

where  $N(0,1)$  is a normalized random variable. Also, Hermann [53] used the following expression for the energy based on the previous work of Pissondes [50] as:

$$E = c_1 m = \frac{2 n^2 \pi^2 \mathcal{D}^2}{a^2} \quad \text{----- (4.9)}$$

which is exactly the quantum energy for particle in an infinite square well of size  $a$  when the substitution  $\mathcal{D} \rightarrow \hbar/2m$  is made.

The HScR numerical simulations were performed using eqn. (4.8). The output of these simulations give the probability density  $f(x)$  of the presence of the particle in the infinite potential well. These simulations were done by dividing the box of size  $a$  into 600 pieces and counting the number of time steps the particle is in each specific sub box. In his scheme, the  $x$  position in the one-dimensional box is drawn horizontally, and number of occurrences vertically. The results are then compared with conventional quantum mechanics ( $P(x) = \sin^2\left(\frac{n \pi x}{a}\right)$ ) [8-12] by calculating the standard deviation  $\sigma$  and the correlation coefficient  $\rho$  which are defined as [53]:

$$\sigma\sigma = \sqrt{\frac{\sum_{i=1}^N (P(i) - f(i))^2}{N}} \quad \text{----- (4.10)}$$

and

$$\rho\rho = \frac{\sum_{i=1}^N (P(i) - \langle P \rangle)(f(i) - \langle f \rangle)}{\sum_{i=1}^N (P(i) - \langle P \rangle)^2 \sum_{i=1}^N (f(i) - \langle f \rangle)^2} \quad \text{----- (4.11)}$$

where N is the number of pieces ,  $P(i) \equiv P(x)$  and  $f(i) \equiv f(x)$  .

In this section, the results of applying a computer program (see Appendix D) built following the HScR method are presented. The same results that Hermann obtained are achieved again. Fig. (4.2) shows the results of first attempt modeling with  $n=3$  for  $5 \times 10^8$  steps and with  $n=9$  for  $10^8$  steps. In the HScR method, two ways to improve the results were suggested [53]. They are:

- 1- using more steps in time .
- 2- restarting the simulation after many steps in time with a new starting position . This leads to a better thermalization of the system .

Fig. (4.3) shows the improved results obtained in the present work with  $n=3$  and  $n=9$  for  $10^8$  steps by using the thermalization process. The convergence between the HScR results and conventional quantum mechanics is clear by the values of  $\sigma\sigma$  (approaching zero) and  $\rho\rho$  (approaching one).

The results of this application, which were originally obtained by Hermann [53], are important since they show the importance of the direct application of ScR theory to quantum mechanics in revealing



the validity of this theory. Hermann [53] promised to do other similar applications to further establish this validity, but survey of literature did not reveal any such applications by him or other researchers in the field. Direct correspondence with him about this subject confirmed this and emphasized the importance of pursuing further applications along the same lines [54].

It is believed that performing such applications is important to prove the direct validity of ScR theory in the more general sense. Besides, Hermann [53] did not refer to the interaction with Riccati equation which will be presented in Sec.(4.3) as an original contribution in the present work.

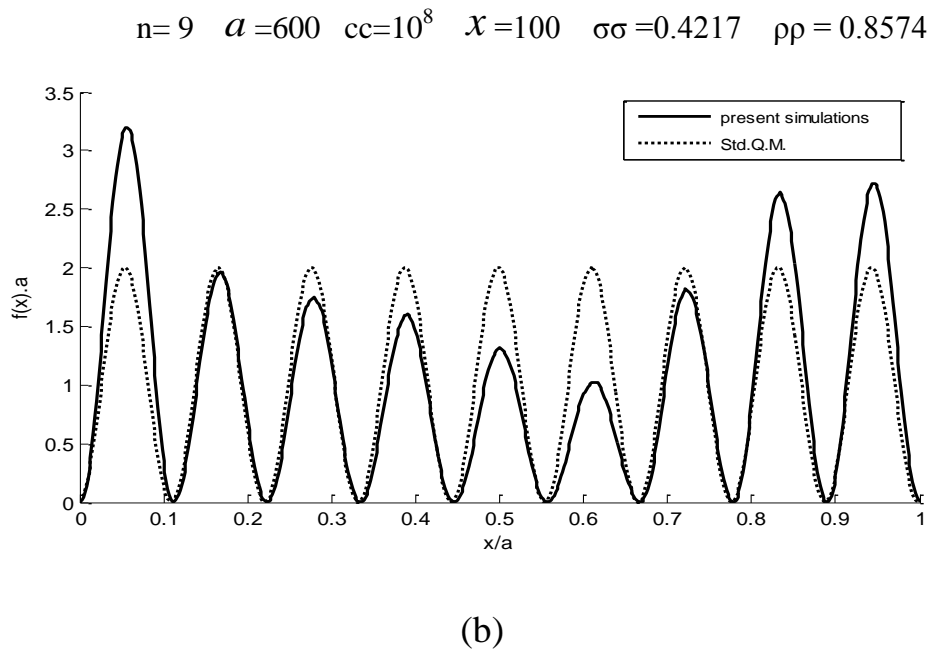
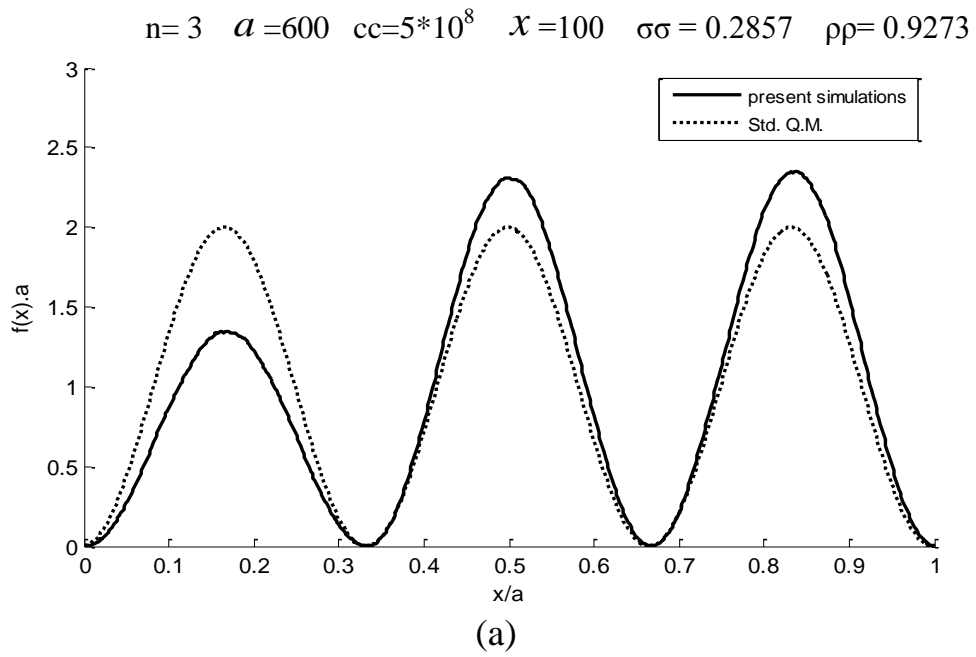


Fig. (4.2) Probability density for a particle in IODSW potential (a)  $n=3$  and (b)  $n=9$ , without the thermalization process, obtained by following the same lines of calculations as Hermann [53].

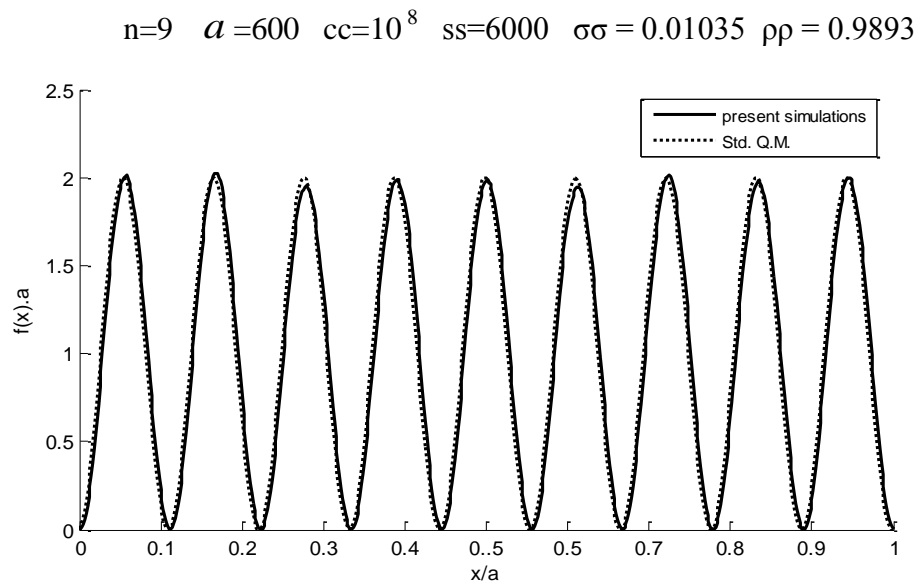
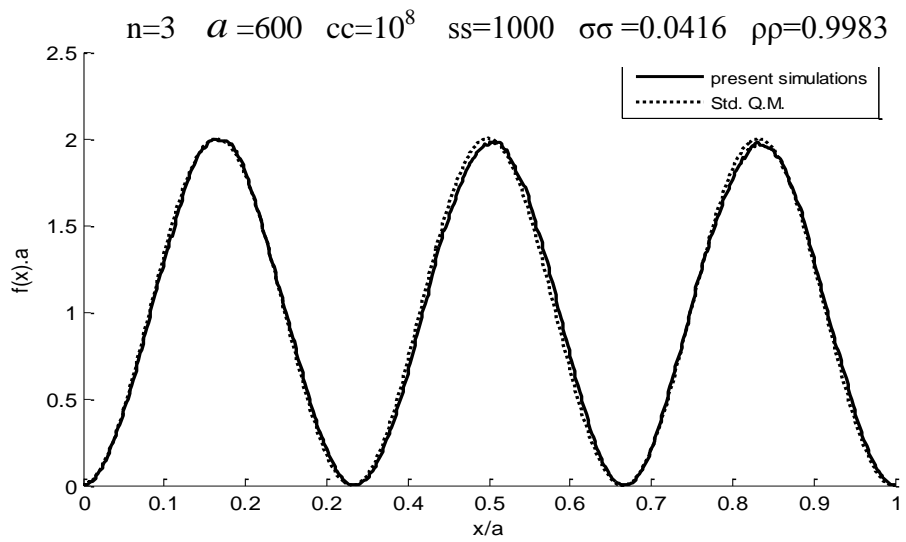


Fig. (4.3) Probability density for a particle in IODSW potential (a)  $n=3$  and (b)  $n=9$ , with the thermalization process, obtained by following the same lines of calculations as Hermann [53].

### **(4.3) Application of ScR Theory to the Problem of a Particle in a Finite One-Dimensional Square Well (FODSW) Potential:**

The energy diagram for the finite one-dimension square well (FODSW) potential is as shown in Fig. (4.1.b). The quantum mechanical problem of a particle moving in this potential well has served as a test ground for the basic findings of quantum mechanics since its discovery [8-12]. The solvable nature of this problem on the mathematical side is one reason for its adoption as a model for many real physical situations [9-11]. This section is devoted to the treatment of this problem on the basis of the direct application of ScR theory along the lines of Hermann [53] reviewed for the infinite analogue of this problem in the previous section.

#### ***(4.3.1) Solution of the equation of motion:***

As for a particle in an infinite square well potential, one may start with the complex Newton equation (eqn. (3.49)), and separate this equation into real and imaginary parts. Also, for this problem the average classical velocity  $V$  of the particle is expected to be zero [53]. Then the equations of motion reduce to the forms of equations (4.3) and (4.4) as:

$$\left. \begin{aligned} -\mathcal{D}\Delta U - (\vec{U} \cdot \vec{\nabla})\vec{U} &= -\vec{\nabla}\mathcal{U} \\ \frac{\partial}{\partial t} U &= 0 \end{aligned} \right\} \text{----- (4.12)}$$

If one takes the 1<sup>st</sup> of eqns. (4.12) and rewrite it for one-dimension as :

$$\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \mathcal{D} U(x) + \frac{1}{2} U^2(x) \right) = \frac{1}{m} \frac{\partial}{\partial x} \mathcal{U}(x) \text{----- (4.13)}$$

then, integrating, one obtains:

$$\mathcal{D} \frac{\partial}{\partial x} U(x) + \frac{1}{2} U^2(x) + c_3 = \frac{1}{m} \mathcal{U}(x) \quad \text{----- (4.14)}$$

where  $c_3$  is a constant of integration . According to the HScR method [53],  $c_3=E/m$ . Then eqn. (4.14) can be written in the form:

$$\frac{d}{dx} U(x) = -\frac{m}{\hbar} U^2(x) + \frac{2}{\hbar} (\mathcal{U}(x) - E) \quad \text{----- (4.15)}$$

where  $\mathcal{D} = \frac{\hbar}{2m}$  . Eqn. (4.15) has the form of a Riccati equation [55,56] (see Appendix B) . To solve this equation, one may transform it into a 2<sup>nd</sup> order differential equation [55,56] which is:

$$ry''(x) + r^2 q(x)y(x) = 0 \quad \text{----- (4.16)}$$

where [55,56],

$$U(x) = -\frac{1}{r} \frac{y'(x)}{y(x)} \quad \text{----- (4.17)}$$

and  $y(x)$  is an arbitrary function of  $x$  .

From eqn. (4.15), it follows that:

$$r = -\frac{m}{\hbar} \quad ; \quad q(x) = \frac{2}{\hbar} (\mathcal{U}(x) - E) \quad \text{----- (4.18)}$$

Using eqn. (4.18), eqn. (4.16) becomes:

$$\frac{d^2}{dx^2} y(x) - \frac{2m}{\hbar^2} (\mathcal{U}(x) - E)y(x) = 0 \quad \text{----- (4.19)}$$

Depending on the values of  $E$ , there are two general classes for the solution of eqn. (4.19) [8,9,74] which are:

1- bound state solution if  $E < \mathcal{U}_0$ ; the particle is confined to the region of potential well .

2- free particle state solution if  $E > \mathcal{U}_0$  ; the particle is free to reach  $x = \pm \infty$  .

In this problem, the case  $E < \mathcal{U}_0$  will be taken. As shown in Sec.(4.1), there are three regions of potential in the problem of a finite square well that are [8-12]:

$$\mathcal{U}(x) = \begin{cases} \mathcal{U}_0 & \text{at } a < x \\ 0 & \text{at } -a < x < a \\ \mathcal{U}_0 & \text{at } x > -a \end{cases} \quad \text{----- (4.20)}$$

Then, the general solutions of eqn. (4.19) are given by [9-12,74]:

$$\left. \begin{aligned} y_1(x) &= Ge^{Kx} + G'e^{-Kx} & \text{for } x > -a \\ y_2(x) &= A\cos \kappa x + B\sin \kappa x & \text{for } -a < x < a \\ y_3(x) &= H'e^{Kx} + He^{-Kx} & \text{for } a < x \end{aligned} \right\} \quad \text{----- (4.21)}$$

where G, G', A, B, H' and H are arbitrary constants,  $\kappa = \sqrt{2mE / \hbar^2}$  and

$K = \sqrt{2m(\mathcal{U}_0 - E) / \hbar^2}$  . Applying the boundary conditions for  $x \rightarrow \pm\infty$  ,

this leads to  $y(x) \rightarrow 0$  . Then, one can rewrite eqn. (4.21) as:

$$\left. \begin{aligned} y_1(x) &= Ge^{Kx} \\ y_2(x) &= A\cos \kappa x + B\sin \kappa x \\ y_3(x) &= He^{-Kx} \end{aligned} \right\} \quad \text{----- (4.22)}$$

The next step is to apply the matching conditions at the boundaries between regions, which requires that both function and its derivative

be continuous. In this way, one gets a set of four homogeneous linear equations with four unknowns [74]:

(i) for  $x = -a$  :

$$\left. \begin{aligned} Ge^{-Kx} &= A \cos \kappa a - B \sin \kappa a \\ KGe^{-Ka} &= \kappa A \sin \kappa a + \kappa B \cos \kappa a \end{aligned} \right\} \text{----- (4.23)}$$

(ii) for  $x = a$  :

$$\left. \begin{aligned} A \cos \kappa a + B \sin \kappa a &= He^{-Ka} \\ -\kappa A \sin \kappa a + \kappa B \cos \kappa a &= -KHe^{-Ka} \end{aligned} \right\} \text{----- (4.24)}$$

These equations can be rewritten in matrix form as:

$$\begin{pmatrix} \cos \kappa a & -\sin \kappa a & -e^{-Ka} & 0 \\ \kappa \sin \kappa a & \kappa \cos \kappa a & -Ke^{-Ka} & 0 \\ \cos \kappa a & \sin \kappa a & 0 & e^{-Ka} \\ -\kappa \cos \kappa a & \kappa \cos \kappa a & 0 & Ke^{-Ka} \end{pmatrix} \begin{pmatrix} A \\ B \\ G \\ H \end{pmatrix} = M \begin{pmatrix} A \\ B \\ G \\ H \end{pmatrix} = 0 \text{----- (4.25)}$$

where the matrix M is given by:

$$M = \begin{pmatrix} \cos \kappa a & -\sin \kappa a & -e^{-Ka} & 0 \\ \kappa \sin \kappa a & \kappa \cos \kappa a & -Ke^{-Ka} & 0 \\ \cos \kappa a & \kappa \sin \kappa a & 0 & e^{-Ka} \\ -\kappa \cos \kappa a & \kappa \cos \kappa a & 0 & Ke^{-Ka} \end{pmatrix} \text{----- (4.26)}$$

The trivial solution of eqn. (4.25) is  $A=0$  ,  $B=0$  ,  $G=0$  and  $H=0$  [74] .

While for a non-trivial solution to exist the condition [74]:

$$\det M=0 \text{----- (4.27)}$$

must be satisfied. To simplify, one eliminates coefficients G and H.

Then eqn. (4.25) becomes the 2×2 matrix equation [74]:

$$\begin{pmatrix} \kappa \tan \kappa a - K & K \tan \kappa a + \kappa \\ -\kappa \tan \kappa a + K & K \tan \kappa a + \kappa \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = M' \begin{pmatrix} A \\ B \end{pmatrix} = 0 \quad \text{----- (4.28)}$$

For this equation to have a non-trivial solution, the determinant of the coefficients must be equal to zero, or:

$$2(\kappa \tan \kappa a - K)(K \tan \kappa a + \kappa) = 0 \quad \text{----- (4.29)}$$

Then , there are two solutions which are [74]:

$$\text{a- } \kappa \tan \kappa a = K, \text{ this means } B=0 \text{ and } y_2(x) = A \cos \kappa x \quad \text{----- (4.30)}$$

$$\text{b- } K \tan \kappa a = \kappa, \text{ this means } A=0 \text{ and } y_2(x) = B \sin \kappa x \quad \text{----- (4.31)}$$

Eqn. (4.30) corresponds to even parity solutions while eqn. (4.31) corresponds to odd parity solutions. These equations can be simplified by introducing the new dimensionless variables:

$$\chi = \kappa a \text{ and } \eta = K a \quad \text{----- (4.32)}$$

From the definition of  $\kappa$  and  $K$ , one can write:

$$\kappa^2 + K^2 = \frac{2m}{\hbar^2} \mathcal{U}_0 \quad \text{----- (4.33)}$$

Using eqn. (4.32), one can rewrite eqns. (4.30), (4.31) and (4.32) in the forms:

$$\eta = \chi \tan \chi \quad \text{----- (4.34)}$$

$$\eta = -\chi \cot \chi \quad \text{----- (4.35)}$$

$$\eta^2 + \chi^2 = \frac{2m}{\hbar^2} \mathcal{U}_0 a^2 = \alpha^2 \quad \text{----- (4.36)}$$



where the dimensionless parameter  $\alpha$  measures the volume of the potential  $\mathcal{U}_0 a^2$  in unit of  $\hbar^2/2m$  .

To determine the values of  $\kappa$  and  $K$  in eqns. (4.34) and (4.35), one may solve these equations graphically together with eqn. (4.36) [8-12,74] .

Figs. (4.4) and (4.5) give the intercepts for the even parity solution (eqn. (4.34)) and odd parity solution (eqn. (4.35)) for two set of values of the potential volume parameter ( $\alpha=1$  and  $4$ ) and ( $\alpha=2$  and  $6$ ) for the even and odd parity solutions respectively . In these figures,  $\kappa$  is drawn horizontally and  $\eta$  vertically. The dashed curve is that of  $\chi \tan \chi$  (for even parity) or  $\chi \cot \chi$  (for odd parity). The continues curve is that of  $\eta^2 + \chi^2 = \alpha^2$ .

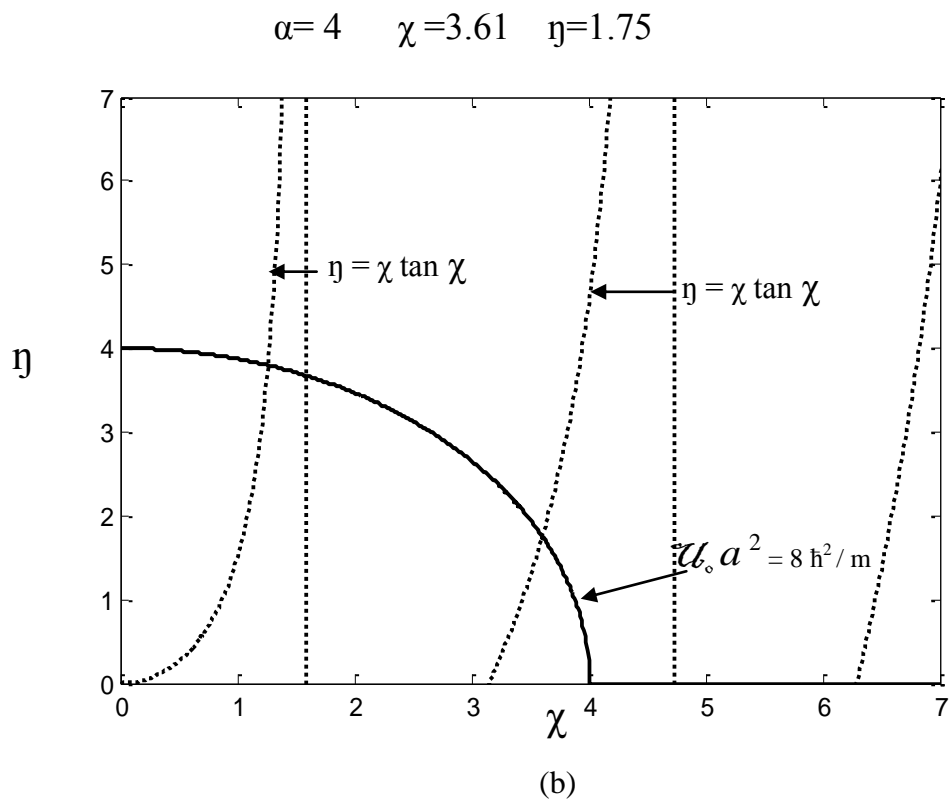
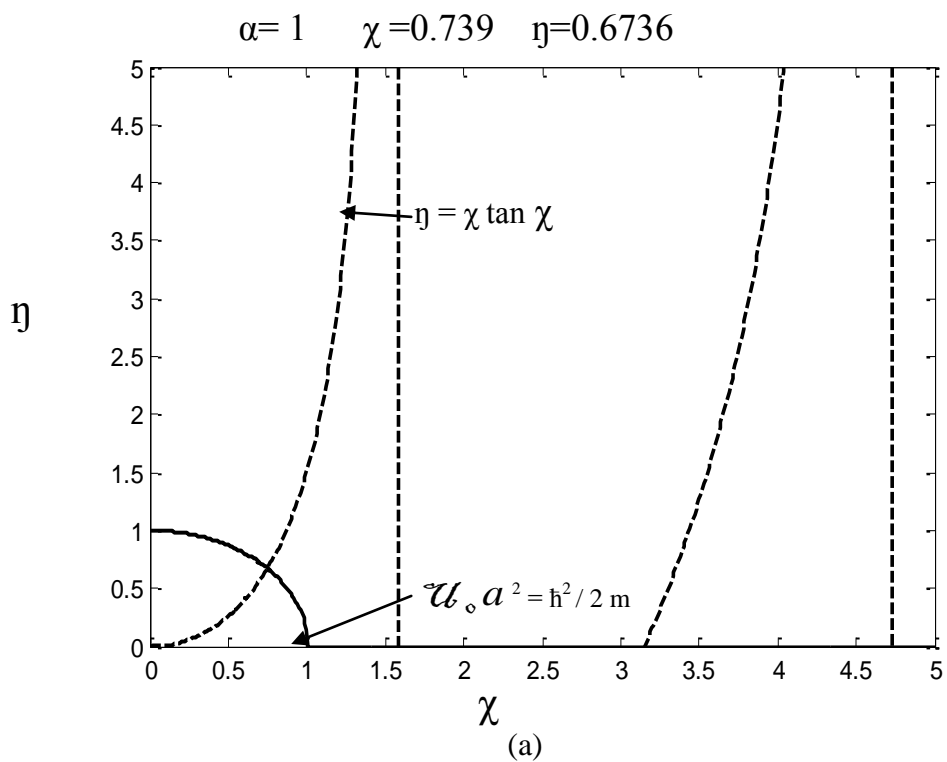


Fig. (4.4) Graphical solution of Eqn. (4.32) (even parity solution), for  
 (a)  $\alpha = 1$  and (b)  $\alpha = 4$ .

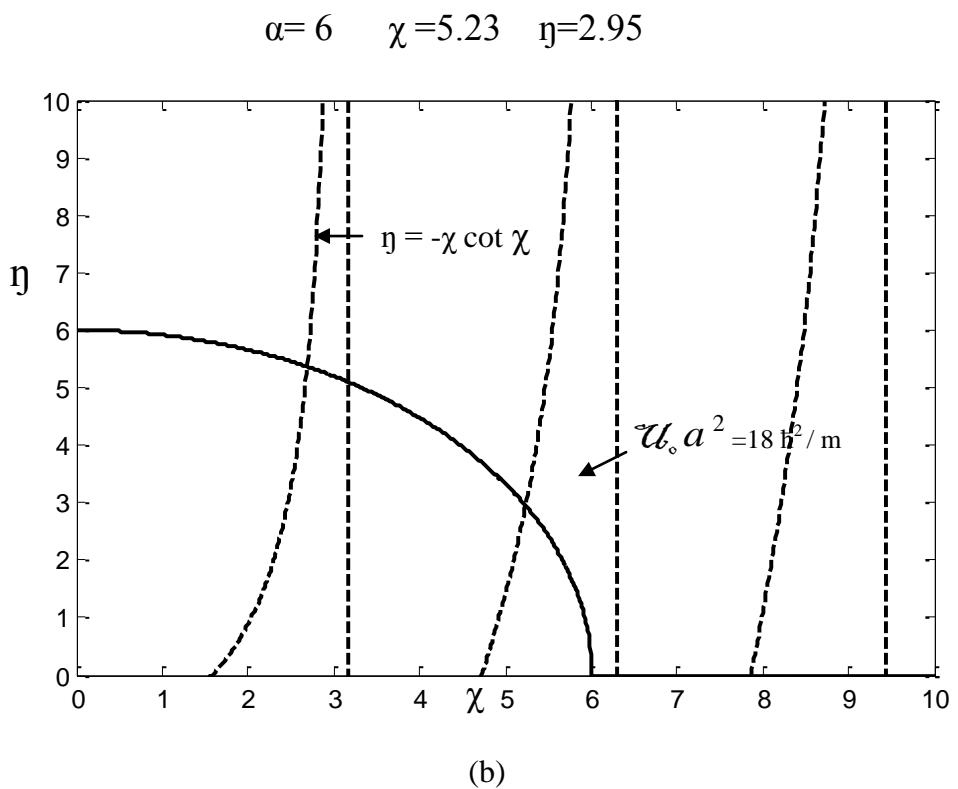
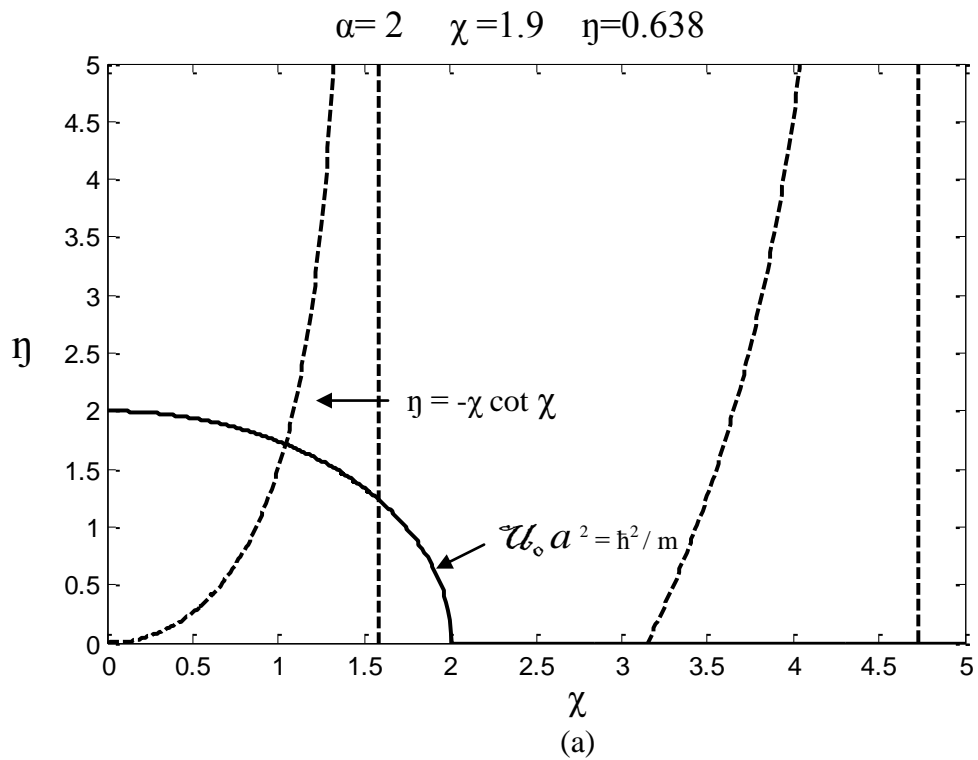


Fig. (4.5) Graphical solution of Eqn. (4.33) (odd parity solution), for (a)  $\alpha = 2$  and (b)  $\alpha = 6$ .

The values of  $\kappa$  and  $K$  ( $\chi$  and  $\eta$ ) corresponding to the solutions of eqns. (4.34), (4.35) and (4.36) can be determined from Figs. (4.4) and (4.5). Then, one can calculate the state energy and the function  $y(x)$  for different values of  $\alpha$  in the following way:

- (i) for  $\alpha = 1$  (equivalent to  $n=1$ ),  $\chi \simeq 0.7391$  and  $\eta = 0.673$ .

This is called the ground state energy, which is:

$$E_{gs} \approx (0.7391)^2 \frac{\hbar^2}{2ma^2} = 0.273 \frac{\hbar^2}{ma^2} \quad \text{----- (4.37)}$$

and eqn. (4.20) can be re-written for even parity solutions as:

$$y(x) = \begin{cases} G \exp\left(\frac{0.673}{a} x\right) & \text{for } x < -a \\ A \cos\left(\frac{0.7391}{a} x\right) & \text{for } -a < x < a \\ H \exp\left(-\frac{0.673}{a} x\right) & \text{for } x > a \end{cases} \quad \text{----- (4.38)}$$

According to eqn. (4.17), the function  $U(x)$  can be defined by using eqn. (4.36) as:

$$U(x) = \frac{\hbar}{ma} \begin{cases} 0.673 & \text{for } x < -a \\ -0.739 \tan\left(\frac{0.739}{a} x\right) & \text{for } -a < x < a \\ -0.673 & \text{for } x > a \end{cases} \quad \text{----- (4.39)}$$

As in Hermann [53],  $U(x)$  is treated as a difference of velocities, i.e., it is a kind of acceleration. Thus, the equation of position coordinate (eqn. (3.38)) has the following form, which is a stochastic process [53]:

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 0.673.dt + d\xi_+(t) & \text{for } x < -a \\ -0.739 \tan\left(\frac{0.739}{a}x\right)dt + d\xi_+(t) & \text{for } -a < x < a \\ -0.673.dt + d\xi_+(t) & \text{for } x > a \end{cases} \quad \text{-----(4.40)}$$

(ii)  $\alpha = 2$  (equivalent to  $n = 2$ ),  $\chi \simeq 1.9$  and  $\eta = 0.638$ , the energy is:

$$E \approx (1.9)^2 \frac{\hbar^2}{2ma^2} = 1.805 \frac{\hbar^2}{ma^2} \quad \text{----- (4.41)}$$

and eqn. (4.20) can be re-written for odd parity solutions as:

$$y(x) = \begin{cases} G \exp\left(\frac{0.638}{a}x\right) & \text{for } x < -a \\ B \sin\left(\frac{1.9}{a}x\right) & \text{for } -a < x < a \\ H \exp\left(-\frac{0.638}{a}x\right) & \text{for } x > a \end{cases} \quad \text{----- (4.42)}$$

Also,

$$U(x) = \frac{\hbar}{ma} \begin{cases} 0.638 & \text{for } x < -a \\ 1.9 \cot\left(\frac{1.9}{a}x\right) & \text{for } -a < x < a \\ -0.638 & \text{for } x > a \end{cases} \quad \text{----- (4.43)}$$

and,

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 0.638.dt + d\xi_+(t) & \text{for } x < -a \\ 1.9 \cot\left(\frac{1.9}{a}x\right)dt + d\xi_+(t) & \text{for } -a < x < a \\ -0.638.dt + d\xi_+(t) & \text{for } x > a \end{cases} \quad \text{-----(4.44)}$$

(iii)  $\alpha = 4$  (equivalent to  $n = 3$ ),  $\chi = 3.61$  and  $\eta = 1.75$ , the energy is:

$$E \approx 6.51 \frac{\hbar^2}{ma^2} \quad \text{----- (4.45)}$$

and eqn. (4.20) for even parity solutions becomes:

$$y(x) = \begin{cases} G \exp\left(\frac{1.75}{a} x\right) & \text{for } x < -a \\ A \cos\left(\frac{3.61}{a} x\right) & \text{for } -a < x < a \\ H \exp\left(-\frac{1.75}{a} x\right) & \text{for } x > a \end{cases} \quad \text{----- (4.46)}$$

Also,

$$U(x) = \frac{\hbar}{ma} \begin{cases} 1.75 & \text{for } x < -a \\ -3.61 \tan\left(\frac{3.61}{a} x\right) & \text{for } -a < x < a \\ -1.75 & \text{for } x > a \end{cases} \quad \text{----- (4.47)}$$

and,

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 1.75dt + d\xi_+(t) & \text{for } x < -a \\ -3.61 \tan\left(\frac{3.61}{a} x\right)dt + d\xi_+(t) & \text{for } -a < x < a \\ -1.75dt + d\xi_+(t) & \text{for } x > a \end{cases} \quad \text{----- (4.48)}$$

(iv)  $\alpha = 6$  (equivalent to  $n = 4$ ),  $\chi = 5.23$  and  $\eta = 2.95$ , the energy is:

$$E \approx 13.6 \frac{\hbar^2}{ma^2} \quad \text{----- (4.49)}$$

and eqn. (4.20) for odd parity solutions becomes:

$$y(x) = \begin{cases} G \exp\left(\frac{2.95}{a} x\right) & \text{for } x < -a \\ B \sin\left(\frac{5.23}{a} x\right) & \text{for } -a < x < a \\ H \exp\left(-\frac{2.95}{a} x\right) & \text{for } x > a \end{cases} \quad \text{----- (4.50)}$$

Also,

$$U(x) = \frac{\hbar}{ma} \begin{cases} 2.95 & \text{for } x < -a \\ 5.23 \cot\left(\frac{5.23}{a}x\right) & \text{for } -a < x < a \\ -2.95 & \text{for } x > a \end{cases} \quad \text{----- (4.51)}$$

and,

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 2.95dt + d\xi_+(t) & \text{for } x < -a \\ 5.23 \cot\left(\frac{5.23}{a}x\right)dt + d\xi_+(t) & \text{for } -a < x < a \\ -2.95dt + d\xi_+(t) & \text{for } x > a \end{cases} \quad \text{----- (4.52)}$$

### (4.3.2) Numerical Simulations

To simplify eqns. (4.40), (4.44), (4.48) and (4.52), one can take  $2\mathcal{D}dt=1$  [53], then, these equation become:

(i)  $\alpha = 1$

$$dx(t) = \frac{1}{a} \begin{cases} 0.673 + N(0,1) & \text{for } x < -a \\ -0.739 \tan\left(\frac{0.739}{a}x\right) + N(0,1) & \text{for } -a < x < a \\ -0.673 + N(0,1) & \text{for } x > a \end{cases} \quad \text{----- (4.53)}$$

(ii)  $\alpha = 2$

$$dx(t) = \frac{1}{a} \begin{cases} 0.638 + N(0,1) & \text{for } x < -a \\ 1.9 \cot\left(\frac{1.9}{a}x\right) + N(0,1) & \text{for } -a < x < a \\ -0.638 + N(0,1) & \text{for } x > a \end{cases} \quad \text{----- (4.54)}$$

$$(iii) \quad \alpha = 4$$

$$dx(t) = \frac{1}{a} \begin{cases} 1.75 + N(0,1) & \text{for } x < -a \\ -3.61 \tan\left(\frac{3.61}{a}x\right) + N(0,1) & \text{for } -a < x < a \\ -1.75 + N(0,1) & \text{for } x > a \end{cases} \quad \text{----- (4.55)}$$

$$(iv) \quad \alpha = 6$$

$$dx(t) = \frac{1}{a} \begin{cases} 2.95 + N(0,1) & \text{for } x < -a \\ 5.23 \cot\left(\frac{5.23}{a}x\right) + N(0,1) & \text{for } -a < x < a \\ -2.95 + N(0,1) & \text{for } x > a \end{cases} \quad \text{----- (4.56)}$$

Numerical simulations are performed using eqns. (4.53), (4.54), (4.55) and (4.56) which represent trajectory equations of the particle for different value of  $\alpha$ . The output of these simulations gives the probability density  $f(x)$  of the particle in a finite square well potential. To construct it, one divides the region into 1801 pieces (boxes), which give better results. This choice comes after many tests. Here, one choose the step of time cc equal to  $5 \times 10^8$  which gives better results after many tests. The  $x$  position in the region will be drawn horizontally and the number of occurrences vertically. So, a point of the curves to be drawn has to be understood as  $(x, y)$ ;  $x$  is the number of boxes and  $y$  is the number of steps for which the particle was in box  $x$ . The results are always normalized by multiplying the number of occurrences in each box by the total number of boxes which is  $a$ .



The probability density  $P(x)$  of conventional quantum mechanics which will be compared with the present results is given by:

(i) for even parity solutions:

$$P(x) = \begin{cases} \tilde{N}_1^2 \exp(2\eta \frac{x}{a}) & \text{for } x < -a \\ \tilde{N}_2^2 \cos^2(\chi \frac{x}{a}) & \text{for } -a < x < a \\ \tilde{N}_3^2 \exp(-2\eta \frac{x}{a}) & \text{for } x > a \end{cases}$$

and,

(ii) for odd parity solutions:

$$P(x) = \begin{cases} \tilde{N}_4^2 \exp(2\eta \frac{x}{a}) & \text{for } x < -a \\ \tilde{N}_5^2 \sin^2(\chi \frac{x}{a}) & \text{for } -a < x < a \\ \tilde{N}_6^2 \exp(-2\eta \frac{x}{a}) & \text{for } x > a \end{cases}$$

where  $\tilde{N}_1, \dots, \tilde{N}_6$  are normalization constants [8-12].

For  $\alpha = 1, 2, 4$  and  $6$  is given by [74]:

(i)  $\alpha = 1$

$$P(x) = \frac{1}{a} \begin{cases} 0.844 \exp(1.3 \frac{x}{a}) & \text{for } x < -a \\ 0.4019 \cos^2(0.739 \frac{x}{a}) & \text{for } -a < x < a \\ 0.844 \exp(-1.3 \frac{x}{a}) & \text{for } x > a \end{cases} \quad \text{----- (5.57)}$$

(ii)  $\alpha = 2$

$$P(x) = \frac{1}{a} \begin{cases} 1.4304 \exp(1.27 \frac{x}{a}) & \text{for } x < -a \\ 0.445 \sin^2(1.9 \frac{x}{a}) & \text{for } -a < x < a \\ 1.4304 \exp(-1.27 \frac{x}{a}) & \text{for } x > a \end{cases} \quad \text{----- (5.58)}$$

(iii)  $\alpha = 4$

$$P(x) = \frac{1}{a} \begin{cases} 16.828 \exp(3.5 \frac{x}{a}) & \text{for } x < -a \\ 0.638 \cos^2(3.61 \frac{x}{a}) & \text{for } -a < x < a \\ 16.828 \exp(-3.5 \frac{x}{a}) & \text{for } x > a \end{cases} \quad \text{----- (5.59)}$$

(iv)  $\alpha = 6$

$$P(x) = \frac{1}{a} \begin{cases} 227.37 \exp(5.9 \frac{x}{a}) & \text{for } x < -a \\ 0.8244 \sin^2(5.23 \frac{x}{a}) & \text{for } -a < x < a \\ 227.37 \exp(-5.9 \frac{x}{a}) & \text{for } x > a \end{cases} \quad \text{----- (5.60)}$$

The comparison between the present results and the results of conventional quantum mechanics is further facilitated by calculating the standard deviation  $\sigma$  and correlation coefficient  $\rho$  (eqns. (4.10) and (4.11)).

Figs. (4.6) and (4.7) show a first attempt of modeling for  $\alpha = 1$  and 4 (even parity solutions) and for  $\alpha = 2$  and 6 (odd parity solutions) respectively. Here, the time step has been chosen as  $5 \times 10^8$ . The numerical simulations start with arbitrary point which is  $x = 100$

(corresponding to box no. 100). The continuous curves indicate the results of the present simulations and the dashed curves the results of conventional quantum mechanics, with the same normalization as the numerical results. In these figures, there is a clear difference between the present results and the results of quantum mechanics, that is measured by  $\sigma\sigma$  and  $\rho\rho$ .

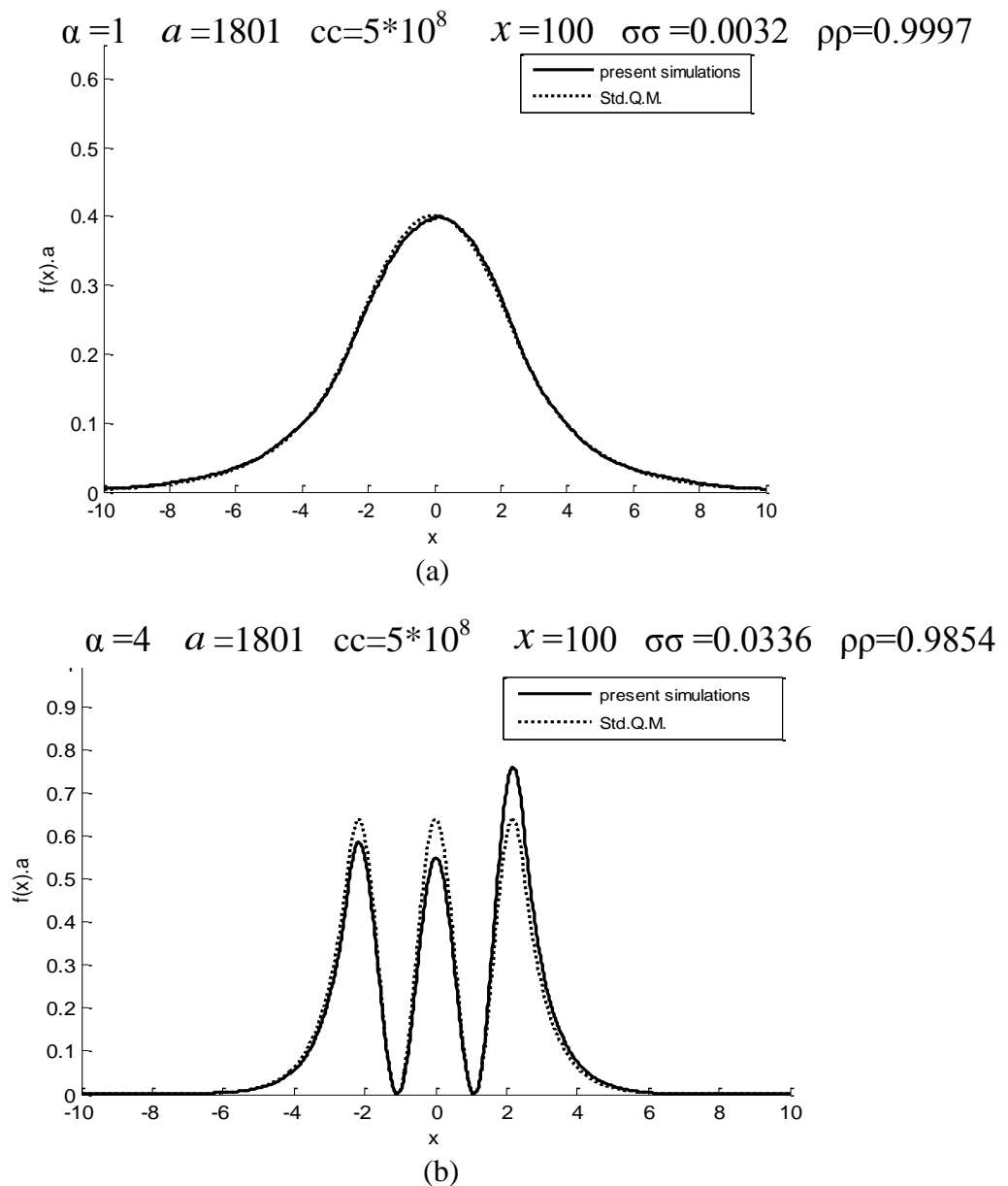
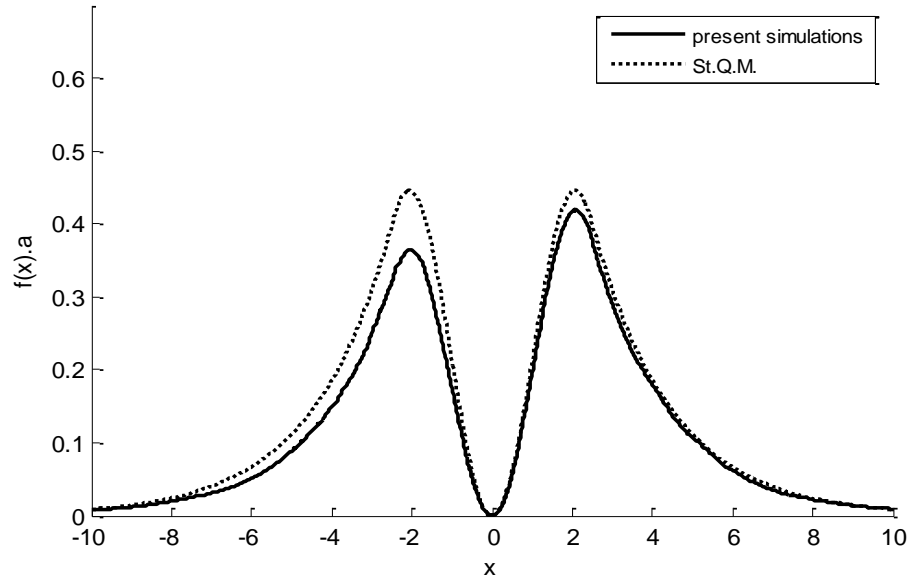


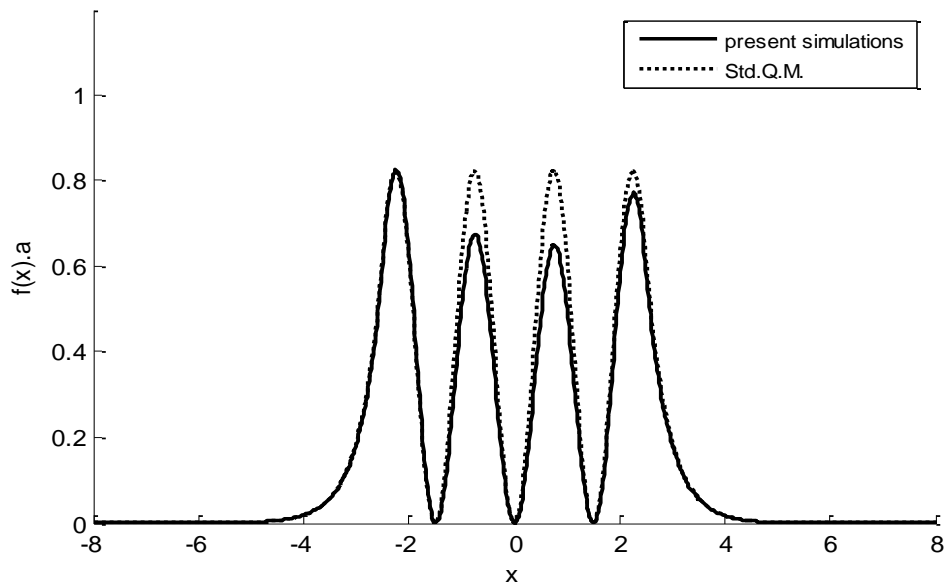
Fig. (4.6) Probability density for even parity solutions corresponding to a particle in a FODSW potential (a)  $\alpha=1$  and (b)  $\alpha=4$  without thermalization process.

$\alpha=2$   $a=1801$   $cc=5*10^8$   $x=100$   $\sigma\sigma=0.0214$   $\rho\rho=0.9945$



(a)

$\alpha=6$   $a=1801$   $cc=5*10^8$   $x=100$   $\sigma\sigma=0.037$   $\rho\rho=0.9938$



(b)

Fig. (4.7) Probability density for odd parity solutions corresponding to a particle in a FODSW potential (a)  $\alpha=2$  and (b)  $\alpha=6$ , without thermalization process.

Hermann [53] indicated in his work that the simulations were restarted after  $10^5$  steps, or more, with a new starting position, then, better thermalization of the system is obtained and convergence is increased. Tests in the present work indicated that the thermalization process as used by Hermann [53] cannot be applied here without fixing additional parameters. This required very long computer time and, therefore, was not adopted in the present work. However, these tests also indicated that the present results can be improved by increasing the number of divisions of  $a$  (i.e., number of boxes). Fig. (4.8) shows the results obtained for  $\alpha=6$  after increasing the number of boxes from 1801 to 2201.

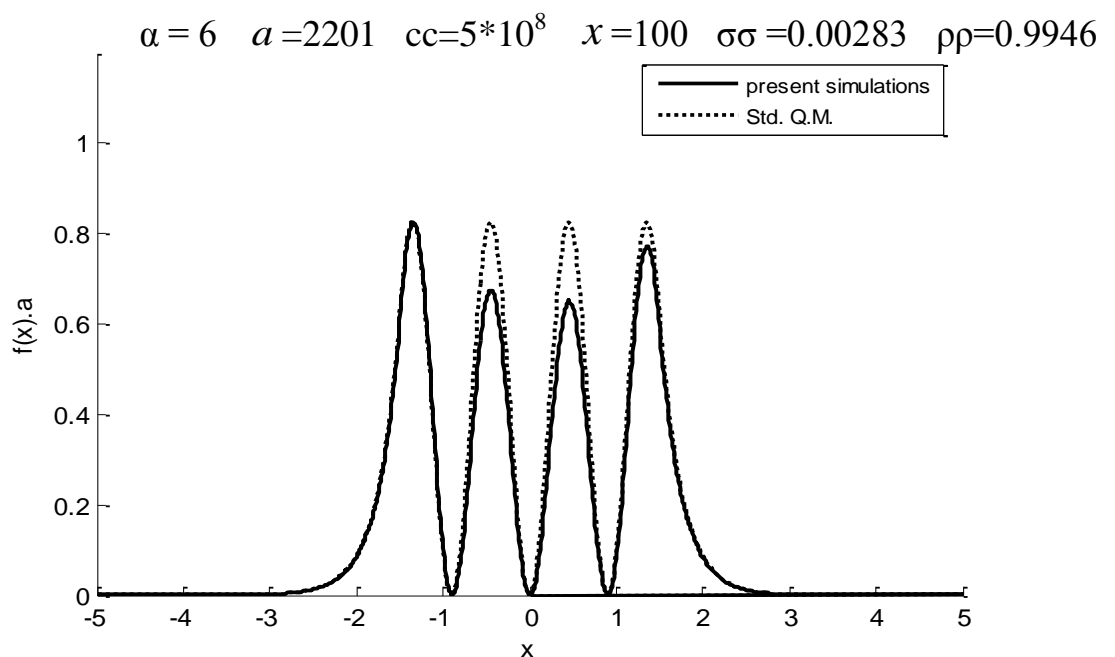


Fig.(4.8) Probability density for  $\alpha=6$  (odd parity solution) corresponding to a particle in a FODSW potential after increasing the number of boxes.

# Chapter Five

## Application of ScR Theory to the Problem of a Particle in a Simple Harmonic Oscillator Potential

### (5.1) The Simple Harmonic Oscillator Potential:

The one-dimensional system, known as linear or simple harmonic oscillator (SHO), is the system consisting of a particle of mass  $m$  moving on the  $x$ -axis under the influence of a restoring force that is proportional to the displacement of the particle from some fixed point on the axis. This system is conservative, and the force  $-kx$  (where  $k$  is the force per unit displacement) is the negative gradient of the potential function  $\mathcal{U}(x) = \frac{1}{2} kx^2$ . The energy diagram for the SHO is shown in Fig. (5.1) where the parabola is the potential function  $\frac{1}{2} kx^2$  and  $x_1$  and  $x_2$  are the classical limits of motion [9,10,11]. The one-dimensional SHO is very important for the quantum mechanical treatment of problems such as the vibration of individual atoms in molecules and in crystals [10,11].

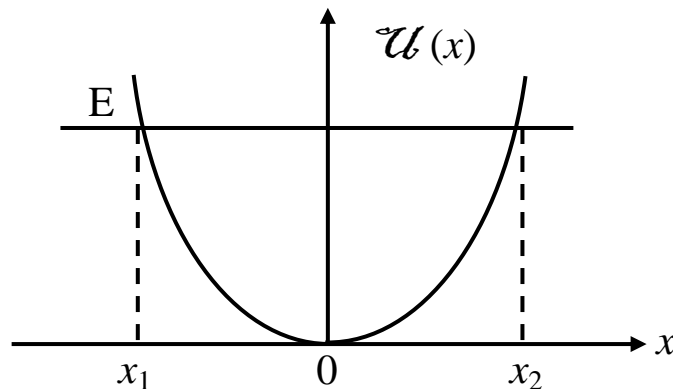


Fig. (5.1) Energy diagram of the SHO [9,10,11]

In this chapter, the problem of a particle moving in one dimensional SHO will be treated by applying the principle of ScR theory along the lines of Hermann [53]. To the best of our knowledge, this problem has not been treated elsewhere [53,54] .

## (5.2) Solution of the Equation of Motion:

As for the problem of a particle in an infinite square well (see Ch. 4), one may start from the complex Newton equation (eqn. (3.49)) and separate the equation into real and imaginary parts. Also, here the average classical velocity is expected to be zero because the SHO is a symmetric system. Then, the equation of motion becomes:

$$\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \mathcal{D} U(x) + \frac{1}{2} U^2(x) \right) = \frac{\partial}{\partial x} \mathcal{U} \quad \text{----- (5.1)}$$

The potential of the one-dimensional SHO can be written as  $\frac{1}{2} m \omega^2 x^2$ , where  $\omega$  is the angular frequency. Then, eqn. (5.1) becomes:

$$\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \mathcal{D} U(x) + \frac{1}{2} U^2(x) \right) = \frac{1}{2} m \omega^2 \frac{\partial}{\partial x} x^2 \quad \text{----- (5.2)}$$

Integrating and rearranging terms in the resulting equation, one obtains:

$$\frac{d}{dx} U(x) + \frac{1}{2\mathcal{D}} U^2(x) - \frac{1}{2\mathcal{D}} m \omega^2 x^2 + \frac{1}{\mathcal{D}} c_4 = 0 \quad \text{----- (5.3)}$$

where  $c_4$  is a constant of integration. Letting  $c_4 = E/m$  (according to Hermann's work) [53], then eqn. (5.3) becomes:

$$\frac{dU(x)}{dx} + \frac{m}{\hbar} U^2(x) - \frac{m^2}{\hbar} \omega^2 x^2 + \frac{2E}{\hbar} = 0 \quad \text{----- (5.4)}$$

where  $\mathcal{D} = \frac{\hbar}{2m}$ . The last equation has the form of a Riccati equation [55] (see Appendix B). As for a particle in a finite square well

potential (Sec. (4.3)), to solve this equation, one may transform it into a 2<sup>nd</sup> order differential equation [56] . Then, eqn. (5.4) becomes:

$$y''(x) + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 x^2 \right) y(x) = 0 \quad \text{----- (5.5)}$$

Its solution is [9,10,57]:

$$y_n(x) = A_n \exp\left(-\frac{x^2}{2}\right) H_n(x) \quad \text{----- (5.6)}$$

where  $A_n$  is a constant and  $H_n$  is a Hermite polynomial of order  $n$  [9,10,57] and  $n=0,1,2,\dots$  . Then,  $U_n(x)$  is given by:

$$U_n(x) = \frac{\hbar}{m} (-x H_n(x) + H'_n(x)) \quad \text{----- (5.7)}$$

Using the equality  $H'_n(x) = 2n H_{n-1}(x)$  [9,10,57] then, eqn. (5.7) becomes:

$$U_n(x) = \frac{\hbar}{m} (-x + 2n(H_{n-1}(x)/H_n(x))) \quad \text{----- (5.8)}$$

The equation of position coordinate (eqn. (3.38)) can then be written as:

$$dx(t) = \frac{\hbar}{m} (-x + 2n(H_{n-1}(x)/H_n(x))) dt + d\xi_+(t) \quad \text{----- (5.9)}$$

### **(5.3) Numerical Simulations:**

As before, eqn. (5.7) represents a stochastic process [53]. Here, in the problem of a one-dimensional SHO, it was found that the assumption  $2 \mathcal{D} dt=1$  is not useful for the present simulations since it gives bad results for the present application. Then, one starts to adjust the value of  $dt$  until one approaches a specific value for which meaningful results are obtained. It was found that a value of



$dt=10^{-3}(\frac{m}{\hbar})$  is suitable for the present simulations. It seems that this value of  $dt$  is related to the period of the motion in the SHO potential. It is expected that a suitable value which gives meaningful numerical simulation results is that which leads to a sufficient number of time steps during one period so as to give meaningful counts. This is a consequence of the statistical nature of these simulations which requires better statistics to be meaningful. Then, eqn. (5.9) becomes:

$$dx(t) = 10^{-3}(-x + 2n(H_{n-1}(x)/H_n(x)) + \sqrt{10^{-3}}N(0,1)) \quad -- (5.10)$$

where the choice of units was made such that  $\hbar = m = 1$ .

As for the case of the particle in an infinite square well, the numerical simulations are performed using eqn. (5.10) for different values of the quantum number  $n$  ( $n=0, 1, 2, 3, 4$  and  $5$ ). A total of 601 boxes and time steps of  $10^8$  and  $5 \times 10^8$  steps were used, as in Hermann's work [53]. The results of the present numerical simulations are compared with the probability density of conventional quantum mechanics, that is,  $P(x) = N_n^2 H_n^2(x) e^{-x^2}$  where  $N_n = 1/\sqrt{2^n n! \pi^{1/2}}$  is the normalization constant [9,11,12].

As for the case of a particle in an infinite square well potential, the output of the present simulations gives the probability density of a particle in a SHO potential. Figs. (5.2), (5.3) and (5.4) show the results of numerical simulations for  $n = 0, 1, 2, 3, 4$ , and  $5$  with  $10^8$  timesteps. These numerical simulations started with arbitrary particle at the position  $x=2$ . Also, the output of the simulations was normalized by multiplying it with a constant  $q$  whose value depends on the number of divisions of the region (here,  $q=50$ ).

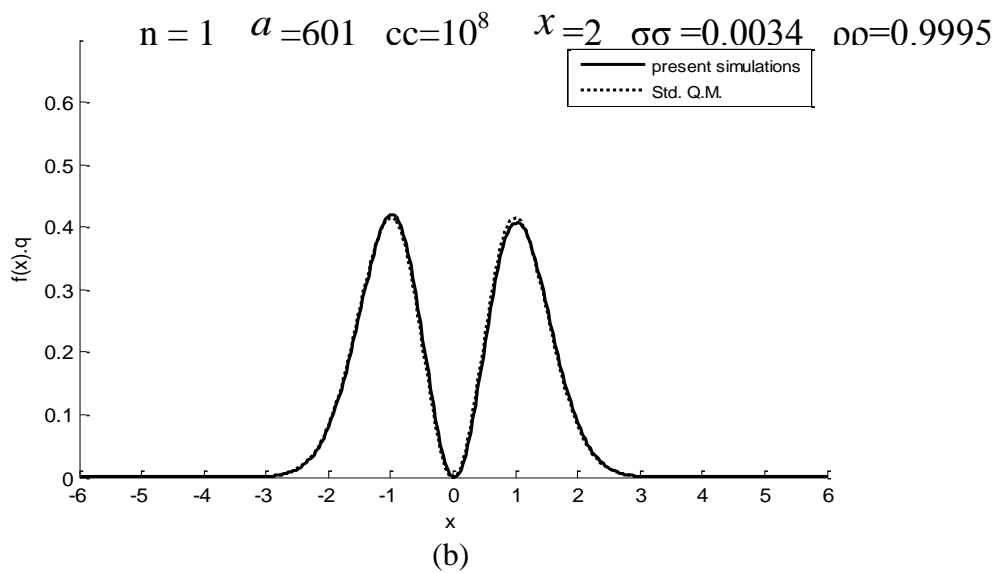
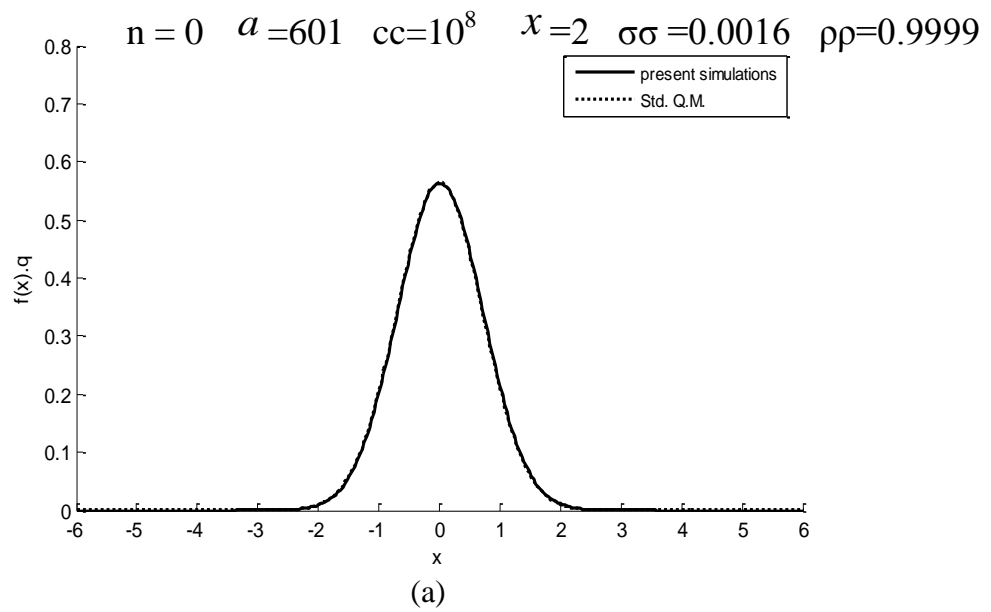


Fig. (5.2) Probability density for a particle in a SHO potential (a)  $n = 0$  and (b)  $n = 1$ , without thermalization process.

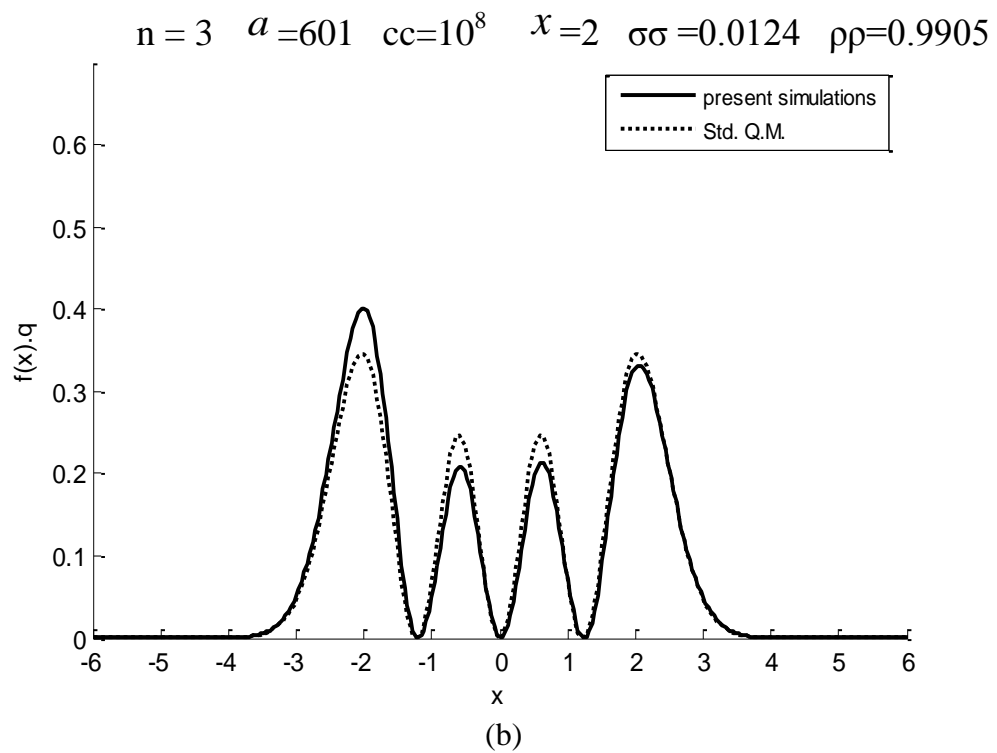
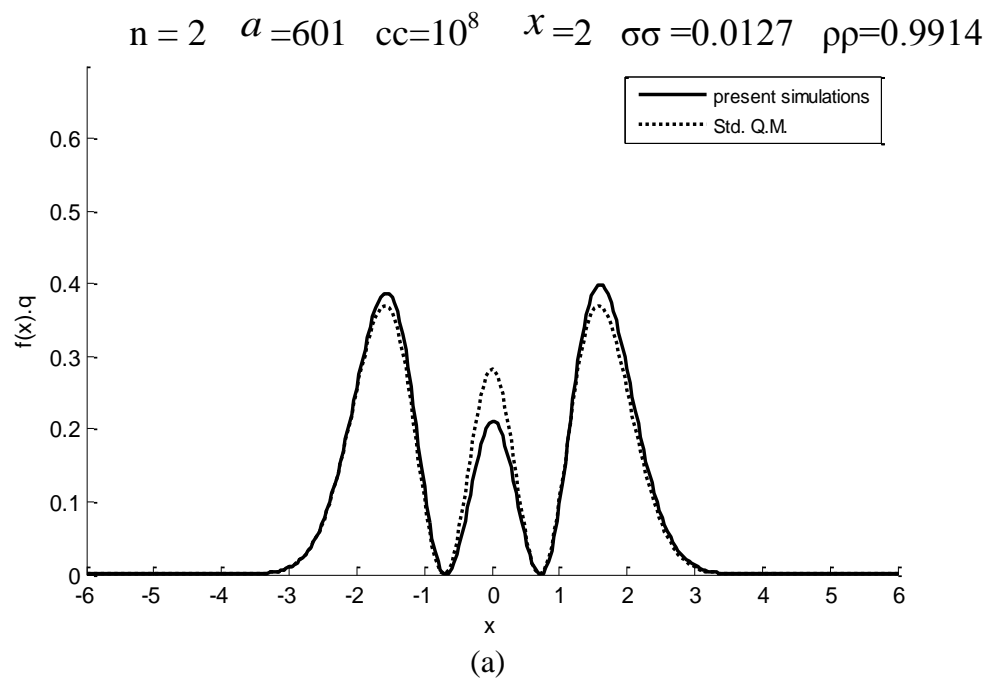


Fig. (5.3) Probability density for a particle in a SHO potential (a)  $n = 2$  and (b)  $n = 3$ , without thermalization process.

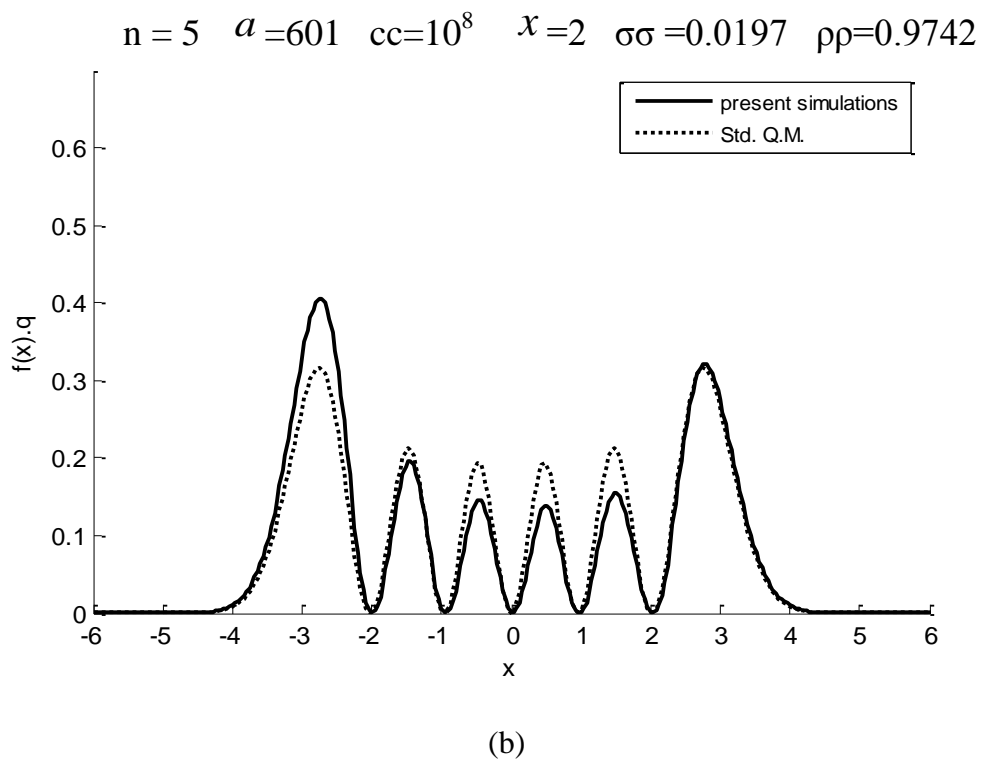
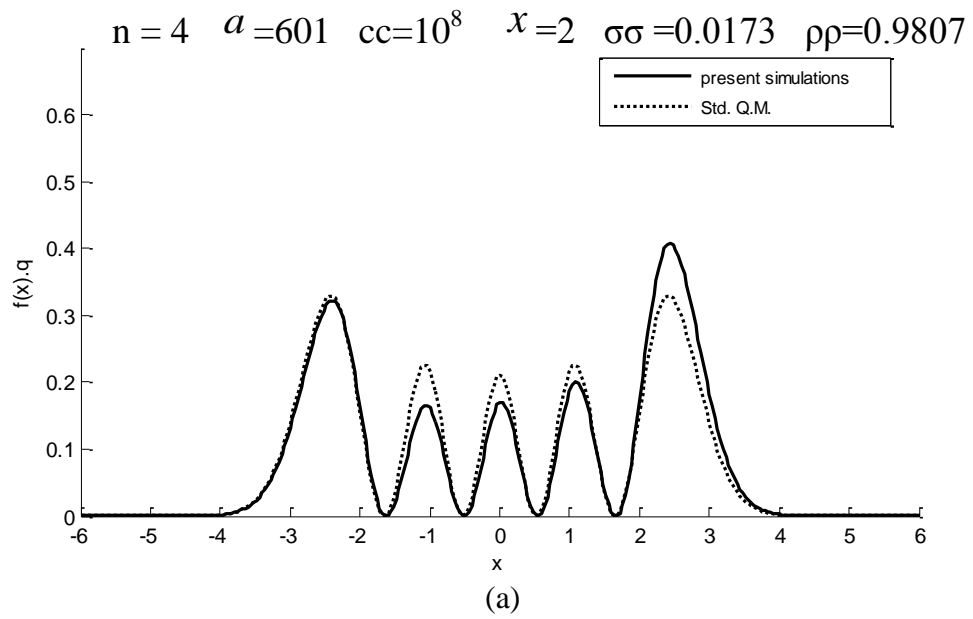


Fig. (5.4) Probability density for a particle in a SHO potential (a)  $n = 4$  and (b)  $n = 5$ , without thermalization process.

Here, it was found, after some numerical tests, that the thermalization process [53] is useful to improve the present results. Fig. (5.5) shows the results of such numerical tests for  $n=2, 3$  and  $5$  which have starting points  $ss = 100$  and  $200$ . These starting points are chosen after many attempts and were found to give better results from other choices. The improvement is clear from the values of  $\sigma\sigma$  and  $\rho\rho$  compared with Figs. (5.3) and (5.4).

Also, as stated in Ch.4, the present results can also be improved to increase convergence between them and the results of quantum mechanics by using more time steps. Fig. (5.6) shows the results obtained this way, for  $n = 3$ . It appears that there is a better agreement with the results of conventional quantum mechanics compared with the results from a thermalization process for  $n=3$  (see Fig. (5.5)).

It was also found that, in the present problem, convergence between the results of numerical simulations and those of conventional quantum mechanics can be improved by increasing the number of boxes. This is clear in Fig. (5.7), where it appears that there is better agreement between the two results for  $n=3$  when the number of boxes was increased to 1201.

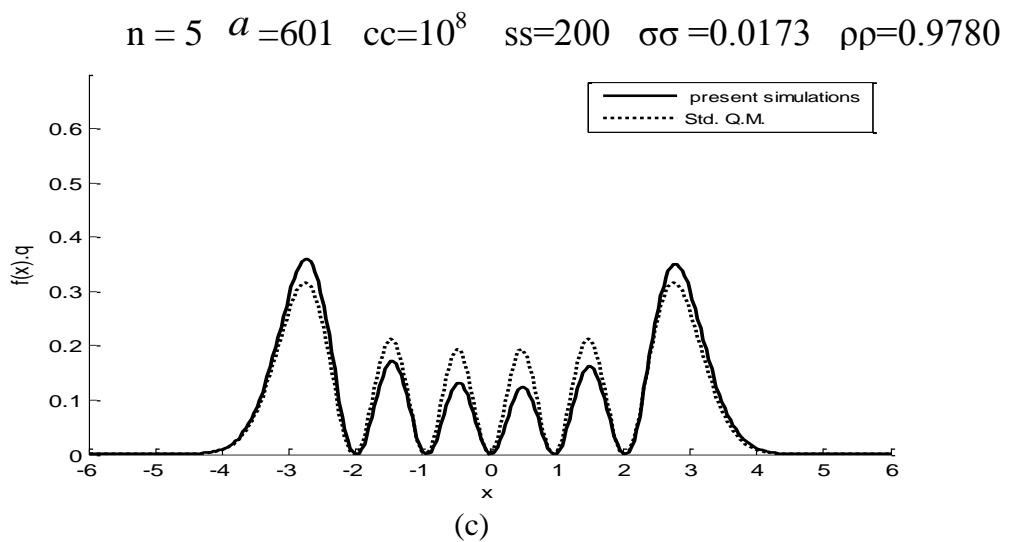
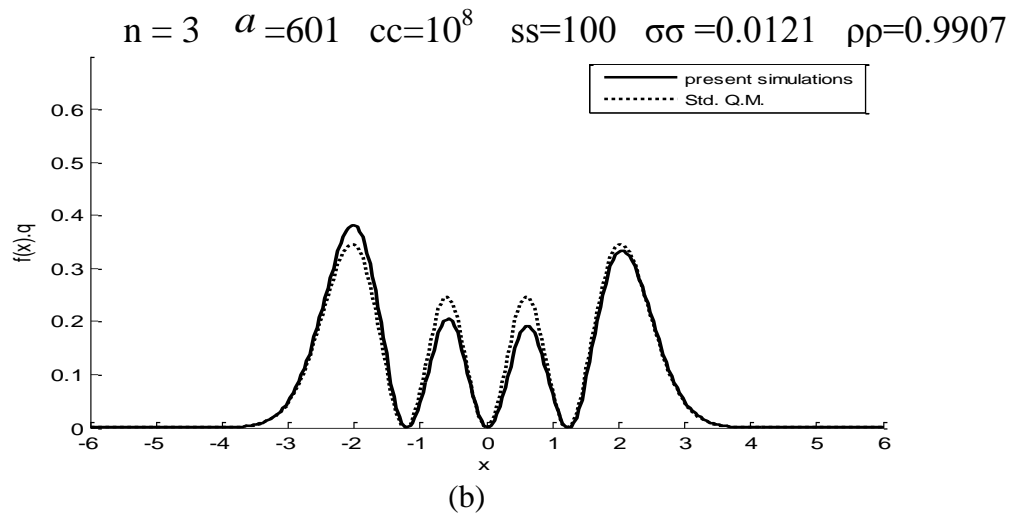
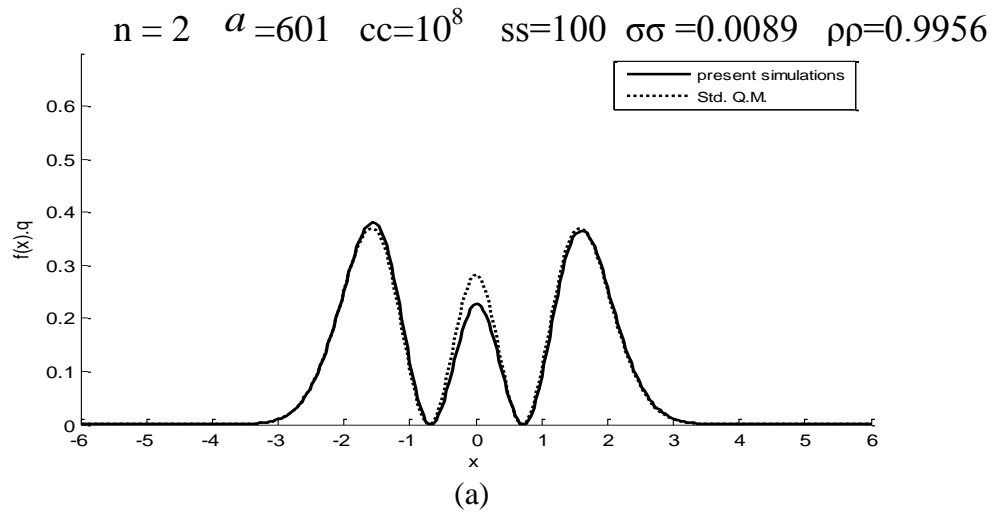


Fig. (5.5) Probability density for a particle in a SHO potential (a)  $n=2$ , (b)  $n=3$  and (c)  $n=5$ , with thermalization process.

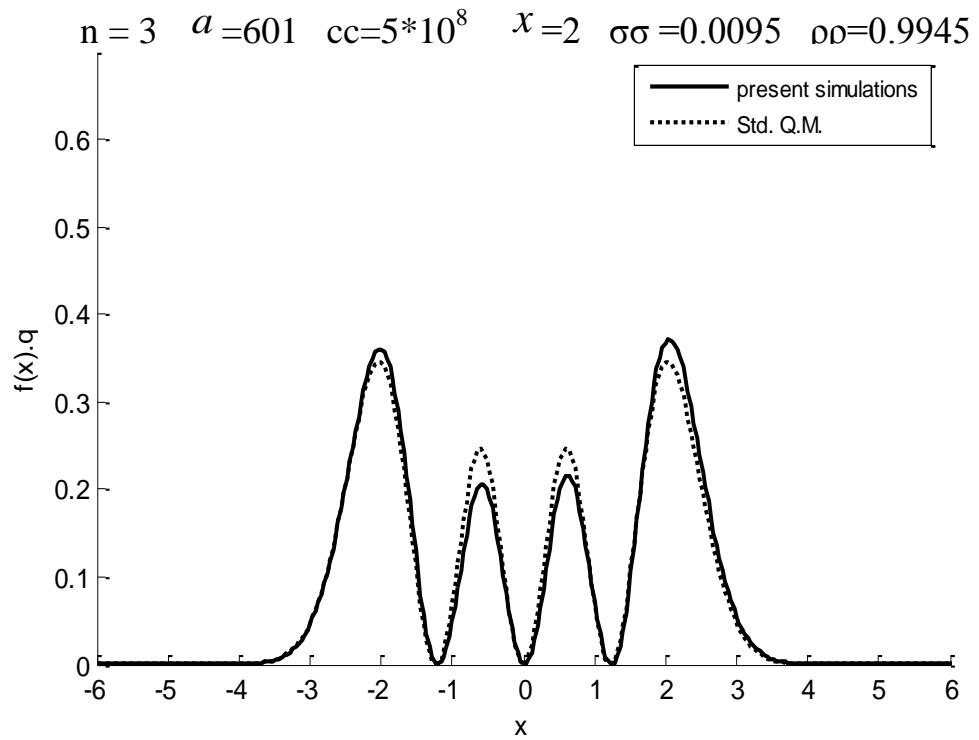


Fig. (5.6) Probability density for a particle in a SHO potential with  $n=3$  for longer time steps ( $cc=5 \times 10^8$ ).

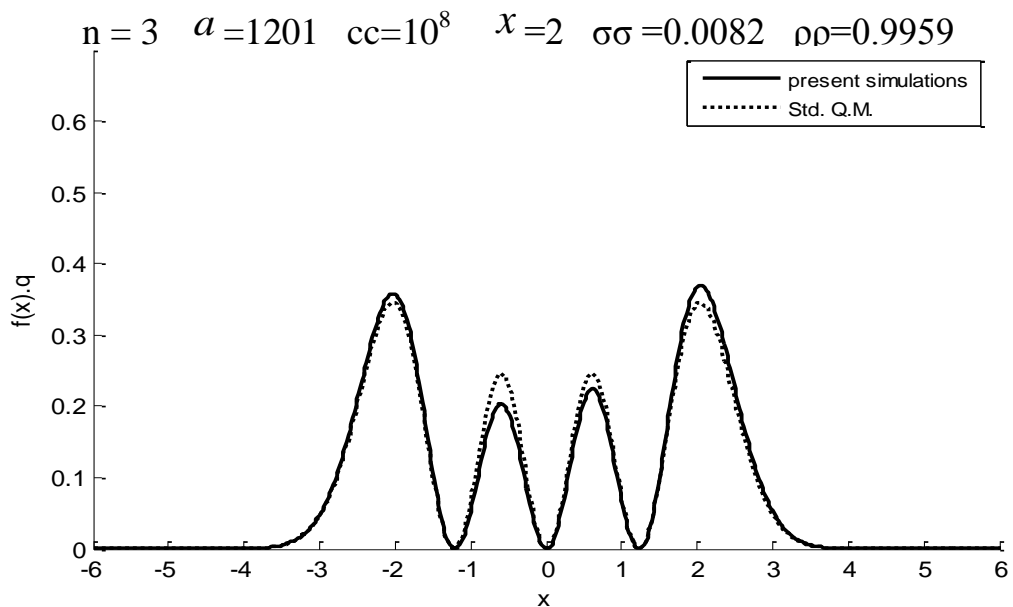


Fig. (5.7) Probability density for a particle in a SHO potential with  $n=3$  after increasing the number of boxes.

# Chapter Six

## Application of ScR Theory to the Problem of a Particle in a Double Well Potential

### (6.1) The Double Well Potential:

When a particle of mass  $m$  is moving in one-dimension in the presence of a potential that has the form [10,75]:

$$\mathcal{U}(x) = \begin{cases} \infty & \text{for } |x| > (a+b) \\ 0 & \text{for } (a+b) > |x| > (b-a) \\ \mathcal{U}_0 & \text{otherwise} \end{cases} \quad \text{----- (6.1)}$$

then, this system is called a double well potential. The energy diagram for this system is shown in Fig. (6.1) [75]. This potential is used as a one-dimensional model of molecules [10,75].

In this chapter, the application of ScR theory to problem of a particle in a double well potential for the case  $E < \mathcal{U}_0$  will be discussed.

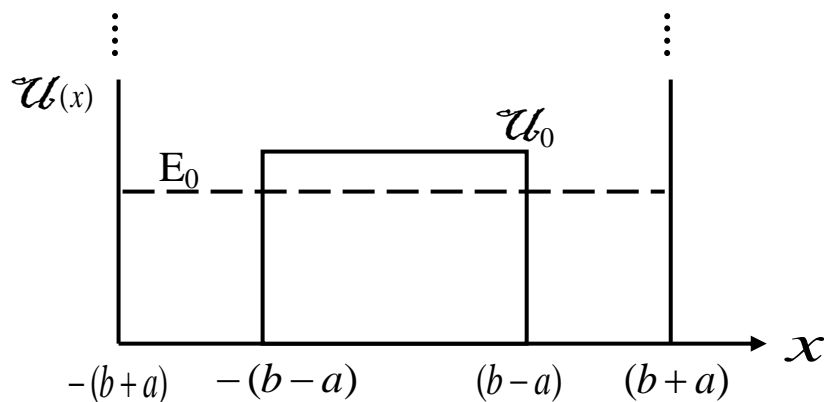


Fig. (6.1) The double well potential [75].



## (6.2) Solution of the Equation of Motion :

The solution of the equation of motion for this problem follows the same approach as for the problem of an infinite square well treated in chapter four. Again the average classical velocity is expected to be zero since the double well potential is a symmetric system. Then, the equation of motion becomes:

$$\frac{d}{dx}U(x) = -\frac{m}{\hbar}U^2(x) + \frac{2}{\hbar}(\mathcal{U}(x) - E) \quad \text{----- (6.2)}$$

Again, eqn. (6.2) has the form of a Riccati equation [55]. It can be rewritten in the form of a 2<sup>nd</sup> order differential equation (see Sec. (4.3)) as [56]:

$$\frac{d^2}{dx^2}y(x) - \frac{2m}{\hbar^2}(\mathcal{U}(x) - E)y(x) = 0 \quad \text{----- (6.3)}$$

But here, the potential  $\mathcal{U}(x)$  have the values that are shown in eqn. (6.1). Then, there are two solutions of eqn. (6.3); the even and odd parity solutions. This comes from following the same procedure that was followed in Sec. (4.3). Then, the solutions are [55]:

$$y(x) = \begin{cases} Q \sin \kappa(x - a - b) & \text{for } (a + b) > x > (b - a) \\ J \cosh Kx & \text{for } (b - a) > |x| \\ -Q \sin \kappa(x + a + b) & \text{for } -(b - a) > x > -(b + a) \end{cases} \quad \text{----- (6.4)}$$

for even parity , and

$$y(x) = \begin{cases} Q \sin \kappa(x-a-b) & \text{for } (a+b) > x > (b-a) \\ J \sinh \kappa x & \text{for } (b-a) > |x| \\ -Q \sin \kappa(x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{----- (6.5)}$$

for odd parity, where Q and J are arbitrary constants.

First, the even parity solutions of eqn. (6.4) will be discussed. The boundary conditions for these equations at  $x = \pm(b+a)$  lead to  $y(x) = 0$ , while the matching conditions at  $x = \pm(b-a)$  are [55]:

(i) at  $x = -(b-a)$ :

$$\left. \begin{aligned} Q \sin 2\kappa a &= J \cosh K(b-a) \\ -\kappa Q \cos 2\kappa a &= KJ \sinh K(b-a) \end{aligned} \right\} \quad \text{----- (6.6)}$$

(ii) and, at  $x = (b-a)$ :

$$\left. \begin{aligned} -Q \sin 2\kappa a &= J \cosh K(b-a) \\ \kappa Q \cos 2\kappa a &= KJ \sinh K(b-a) \end{aligned} \right\} \quad \text{----- (6.7)}$$

Eqns. (6.6) and (6.7) lead to the self-consistency equation for the even parity solutions which is [75]:

$$\kappa \cot 2\kappa a = -K \tanh K(b-a) \quad \text{----- (6.8)}$$

This equation, together with the relation  $\kappa^2 + K^2 = \frac{2m}{\hbar^2} \mathcal{U}_0 = \alpha^2$  (see eqn. (4.33)), can be solved graphically to determine the values of  $\kappa$  and K in a similar manner to Sec. (4.3). While, for the odd parity solutions, the self-consistency equation becomes:

$$\kappa \cot 2\kappa a = -K \coth K(b-a) \quad \text{----- (6.9)}$$

Fig. (6.2) shows the graphical solutions of the self-consistency equation for the double well potential, for  $\alpha = 3$ . If one lets  $b = 2a$  then, one can get from the graphical solutions that  $\chi = \kappa a = 1.35$  and  $\eta = K(b-a) = 2.679$  for  $\alpha = 3$ , for the even parity solutions. While, for the odd parity solutions one has  $\kappa a = 1.35$  and  $K(b-a) = 2.679$  too. Then, eqns. (6.4) and (6.5) become:

$$y(x) = \begin{cases} Q \sin \frac{1.35}{a}(x-a-b) & \text{for } (a+b) > x > (b-a) \\ J \cosh \frac{2.679}{a} x & \text{for } (b-a) > |x| \\ -Q \sin \frac{1.35}{a}(x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{---- (6.10)}$$

for even parity , and

$$y(x) = \begin{cases} Q \sin \frac{1.35}{a}(x-a-b) & \text{for } (a+b) > x > (b-a) \\ J \sinh \frac{2.679}{a} x & \text{for } (b-a) > |x| \\ Q \sin \frac{1.35}{a}(x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{---(6.11)}$$

for odd parity .

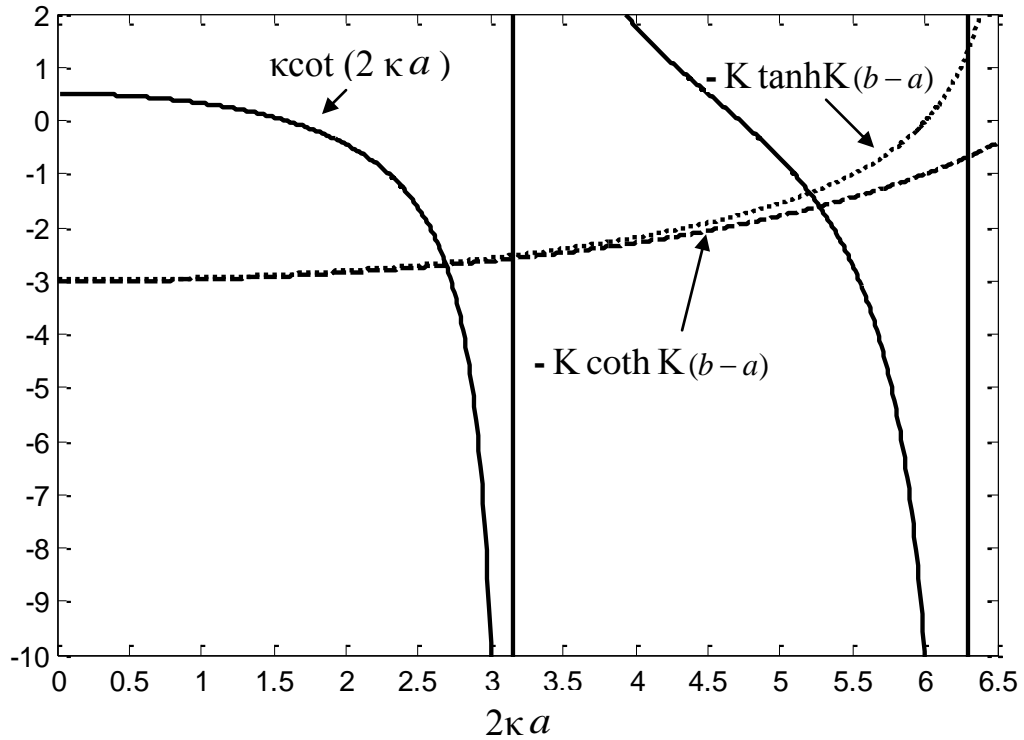


Fig. (6.2) The graphical solution of the self consistency condition for the double well potential ( $\alpha = 3$ ).

According to eqn. (4.17), the function  $U(x)$  is given in terms of an arbitrary function  $y(x)$  as  $U(x) = -\frac{1}{r} \frac{y'(x)}{y(x)}$ . Here, in this problem

$r = -m/\hbar$ , then,  $U(x)$  can be written as:

$$U(x) = \frac{\hbar}{ma} \begin{cases} 1.35 \cot \frac{1.35}{a}(x-a-b) & \text{for } (a+b) > x > (b-a) \\ 2.679 \tanh\left(\frac{2.679}{a}x\right) & \text{for } (b-a) > |x| \\ -1.35 \cot \frac{1.35}{a}(x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{----(6.12)}$$

for even parity, and

$$U(x) = \frac{\hbar}{ma} \begin{cases} 1.35 \cot \frac{1.35}{a} (x-a-b) & \text{for } (a+b) > x > (b-a) \\ 2.679 \coth(\frac{2.679}{a} x) & \text{for } (b-a) > |x| \\ 1.35 \cot \frac{1.35}{a} (x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{----(6.13)}$$

for odd parity.

Finally, the equation of position coordinate (eqn. (3.38)) has the following form, which represents a stochastic process [53]:

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 1.35 \cot \frac{1.35}{a} (x-a-b).dt + d\xi_+(t) & \text{for } (a+b) > x > (b-a) \\ 2.679 \tanh(\frac{2.679}{a} x).dt + d\xi_+(t) & \text{for } (b-a) > |x| \\ -1.35 \cot \frac{1.35}{a} (x+a+b).dt + d\xi_+(t) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{---(6.14)}$$

for even parity solutions , and :

$$dx(t) = \frac{\hbar}{ma} \begin{cases} 1.35 \cot \frac{1.35}{a} (x-a-b).dt + d\xi_+(t) & \text{for } (a+b) > x > (b-a) \\ 2.679 \coth(\frac{2.679}{a} x).dt + d\xi_+(t) & \text{for } (b-a) > |x| \\ 1.35 \cot \frac{1.35}{a} (x+a+b).dt + d\xi_+(t) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{----(6.15)}$$

for odd parity.

### (6.3) Numerical Simulations:

If one lets  $2 \mathcal{D} dt=1$  (see Ch. 4), eqns. (6.14) and (6.15) become:

$$dx(t) = \frac{1}{a} \begin{cases} 1.35 \cot \frac{1.35}{a} (x-a-b) + N(0,1) & \text{for } (b+a) > x > (b-a) \\ 2.679 \tanh\left(\frac{2.679}{a} x\right) + N(0,1) & \text{for } (b-a) > |x| \\ -1.35 \cot \frac{1.35}{a} (x+a+b) + N(0,1) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{-----}(6.16)$$

for even parity solutions, and

$$dx(t) = \frac{1}{a} \begin{cases} 1.35 \cot \frac{1.35}{a} (x-a-b) + N(0,1) & \text{for } (b+a) > x > (b-a) \\ 2.679 \coth\left(\frac{2.679}{a} x\right) + N(0,1) & \text{for } (b-a) > |x| \\ 1.35 \cot \frac{1.35}{a} (x+a+b) + N(0,1) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{-----}(6.17)$$

for odd parity solutions. In a manner similar to Sec. (4.3), numerical simulations are performed using eqns. (6.16) and (6.17) that represent trajectory equations of the particle in a double well potential for  $\alpha = 3$ . Here, it was found after some numerical tests that the division of the region into 1801 boxes give good results when the time steps are taken as  $5 \times 10^8$ .

As for the problem of a particle in a finite square well, the numerical simulation results obtained here are compared with the probability density  $P(x)$  of conventional quantum mechanics is given by:

(i) for even parity solutions:

$$P(x) = \begin{cases} \tilde{N}_7^2 \sin^2 \frac{\chi}{a} (x-a-b) & \text{for } (a+b) > x > (b-a) \\ \tilde{N}_8^2 \cosh^2 \left( \frac{\eta}{(b-a)} x \right) & \text{for } (b-a) > |x| \\ \tilde{N}_9^2 \sin^2 \frac{\chi}{a} (x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases}$$

and,

(ii) for odd parity solutions:

$$P(x) = \begin{cases} \tilde{N}_{10}^2 \sin^2 \frac{\chi}{a} (x-a-b) & \text{for } (a+b) > x > (b-a) \\ \tilde{N}_{11}^2 \sinh^2 \left( \frac{\eta}{(b-a)} x \right) & \text{for } (b-a) > |x| \\ \tilde{N}_{12}^2 \sin^2 \frac{\chi}{a} (x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases}$$

where  $\tilde{N}_7, \dots, \tilde{N}_{12}$  are normalization constants [75].

For  $\alpha = 3$ ,  $P(x)$  is given by [75]:

$$P(x) = \frac{1}{a} \begin{cases} 0.424 \sin^2 \frac{1.35}{a} (x-a-b) & \text{for } (a+b) > x > (b-a) \\ 0.0014 \cosh^2 \left( \frac{2.679}{a} x \right) & \text{for } (b-a) > |x| \\ 0.424 \sin^2 \frac{1.35}{a} (x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{---- (6.18)}$$

for even parity solutions, and

$$P(x) = \frac{1}{a} \begin{cases} 0.4502 \sin^2 \frac{1.35}{a} (x-a-b) & \text{for } (b+a) > x > (b-a) \\ 0.0015 \sinh^2 \left( \frac{2.679}{a} x \right) & \text{for } (b-a) > |x| \\ 0.4502 \sin^2 \frac{1.35}{a} (x+a+b) & \text{for } -(b-a) > x > -(b+a) \end{cases} \quad \text{--- (6.19)}$$

for odd parity solutions.

Fig. (6.3) shows the results obtained from a first simulation attempt for  $\alpha = 3$  for even and odd parity solutions. This simulation is started from an arbitrary point. It was found through numerical tests that these results can be improved by a thermalization process [53].

Fig. (6.4) shows the results obtained this way for a starting point  $ss = 21$  which gives the best results after many tests for different values of  $ss$ .

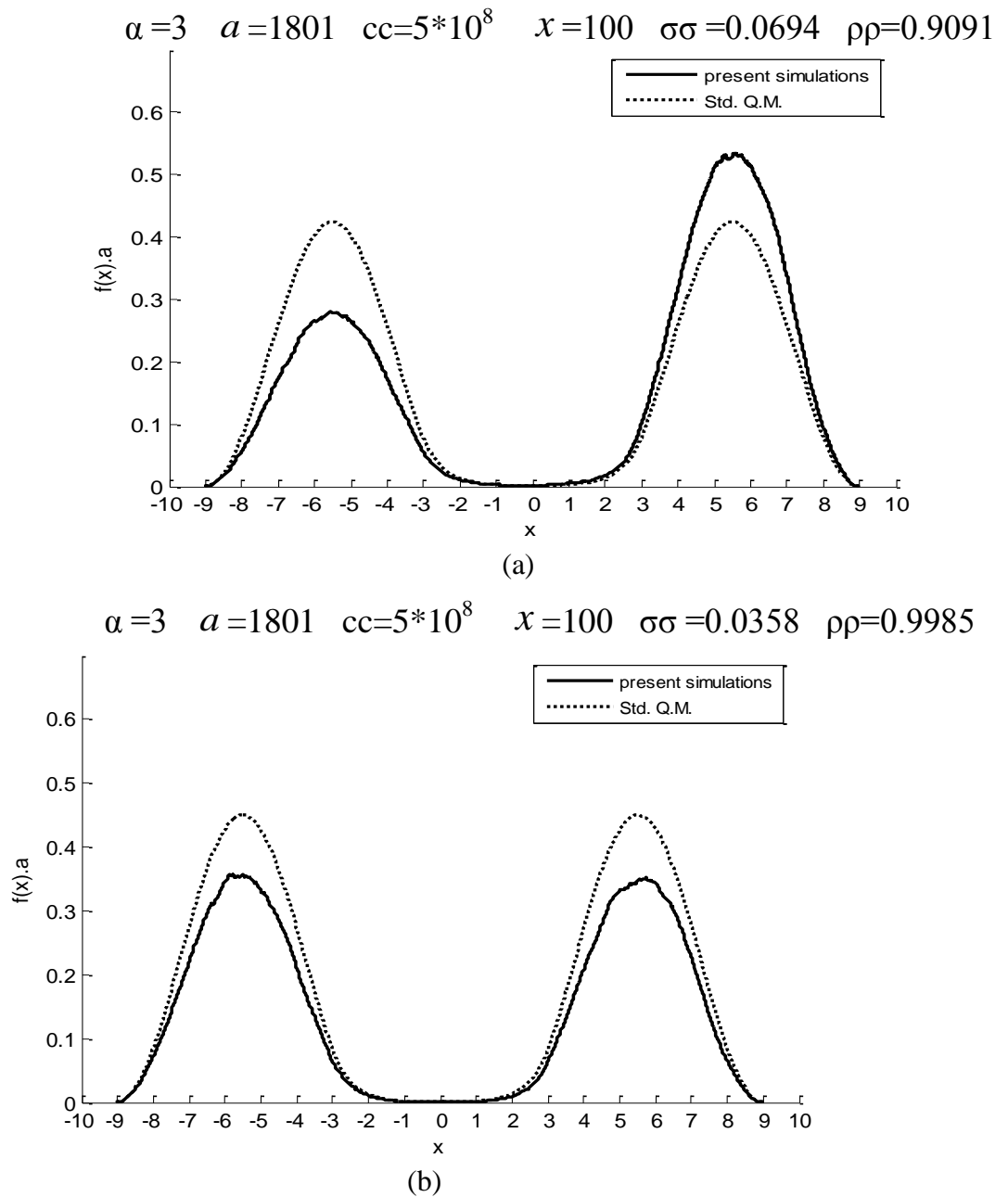
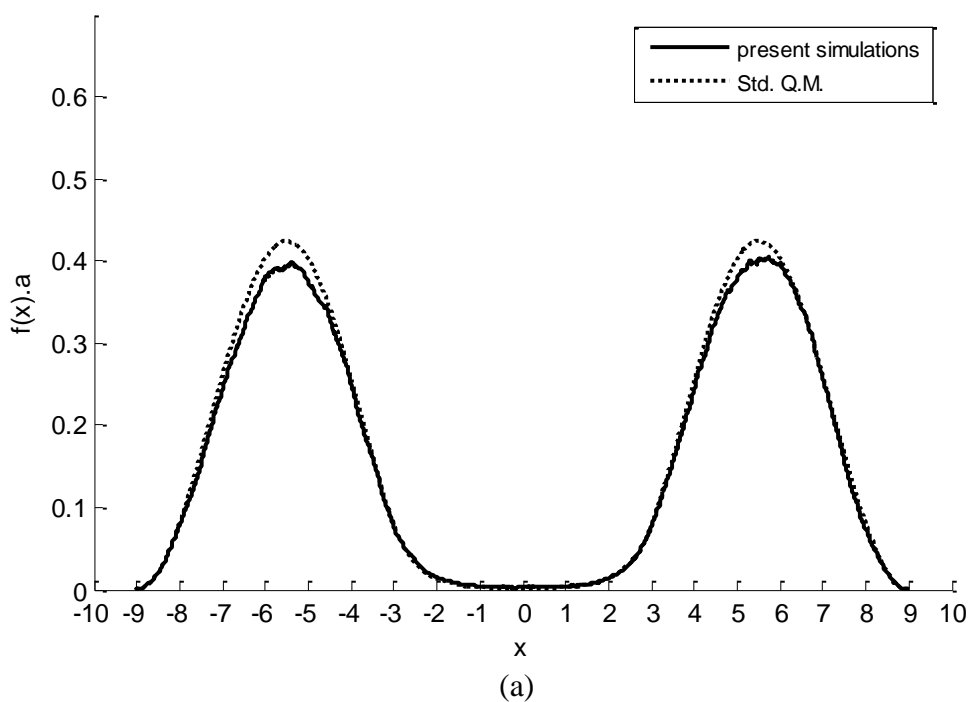


Fig. (6.3) Probability density for  $\alpha = 3$  without thermalization process for (a) even parity solution and (b) odd parity solution.



$\alpha=3$   $a=1801$   $cc=5*10^8$   $ss=21$   $\sigma\sigma=0.0099$   $\rho\rho=0.9994$



$\alpha=3$   $a=1801$   $cc=5*10^8$   $ss=21$   $\sigma\sigma=0.0297$   $\rho\rho=0.9987$

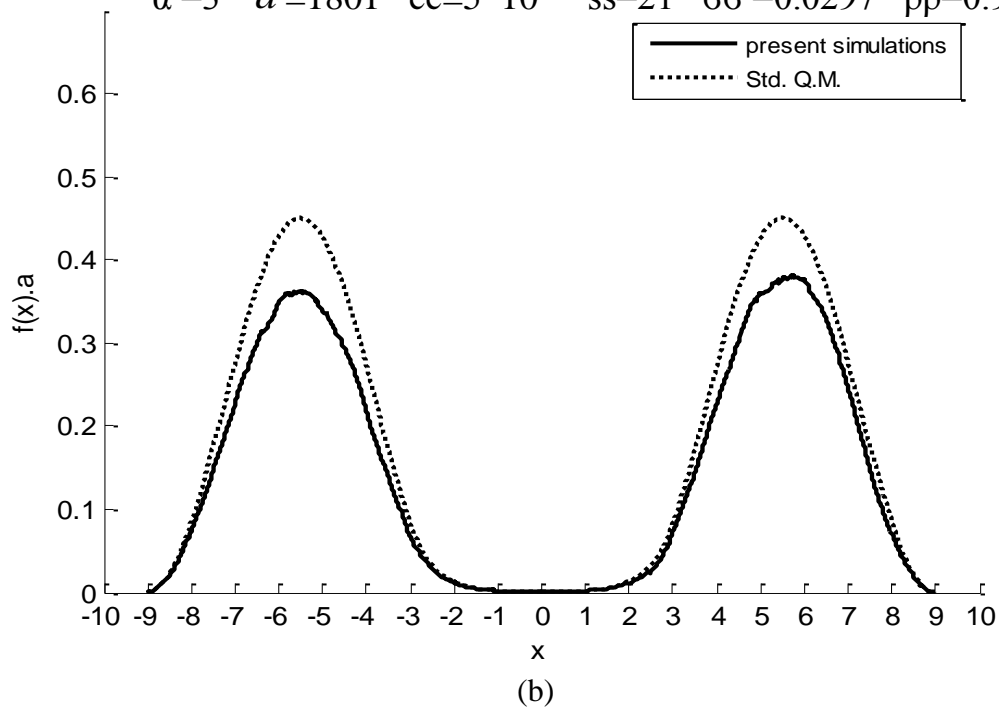


Fig. (6.4) Probability density for  $\alpha = 3$  with thermalization process for (a) even parity solution and (b) odd parity solution.

# **Chapter Seven**

## **Discussion, Conclusions and Suggestions**

### **(7.1) Discussion:**

Quantum mechanics is a well-founded theory as far as the mathematical formulation is concerned [8-15]. Numerical predictions of physical phenomena in the microscopic world based on quantum mechanics are considered to be in very good agreement with experiments so far [8-12]. On the conceptual side, however, quantum mechanics has faced grave difficulties [29-31]. Attempts to overcome these difficulties have followed more than one path. The approach to overcoming the conceptual difficulties of quantum mechanics based on scale relativity (ScR) theory as formulated by Nottale [30-32] is one of them. It's main idea is to give up the differentiability of space-time and, hence, use fractal geometry as a basis to predict the quantum behavior [30-32] .

This approach is usually considered as lying outside main stream physics [76]. However, its reliance on the well-founded mathematics of fractal geometry makes it one of the plausible approaches in this field. Applications of the scale relativistic approach to many fields in quantum physics have been discussed by many authors [30,31,36,38,49]. Also, applications in other fields are available [31,40-44] .

However, in such a situation, direct numerical applications would be of help in explaining the relationship between the concept of fractal space-time, as formulated in ScR, and the quantum behavior. In

particular, it is of interest to see directly through numerical simulations how the quantum behavior arises as a consequence of the fractality of space-time. Preliminary attempts to do so were performed by Hermann [53]. The present work was an attempt to expand on the work of Hermann by performing similar simulations for other quantum-mechanical problems not treated by him or by others [54]. Such a program may seem as a direct extension of Hermann's work. However, as it appears from the work in this thesis, there are many difficulties that were to be overcome to obtain meaningful results that can be compared with conventional quantum mechanical results. On the mathematical side, the discovery of a novel relationship with the well-known Riccati equation has helped in solving some of these difficulties. While, on the numerical side, special attempts to optimize the solution parameters for the problems treated in this thesis were needed to obtain the required results. Such optimization involved using the concept of thermalization, as advocated in this field by Hermann [53], but in a new perspective necessary for the present work.

Looking at the present work in this way, one can see that the aim set up at the beginning has been achieved. More details about the conclusions related to this are given in the next section. However, more work has to be done to understand other aspects related to this work as indicated in Sec. (7.3).

## **(7.2) Conclusions:**

The main conclusions from the present work are as follows:

(i) Hermann [53] has shown that a quantitative correct prediction of the behavior of a quantum particle in an infinite one-dimensional

square well potential can be obtained without explicitly writing the Schrödinger equation nor using any conventional quantum axiom. It can be concluded from the present work that this fact is even correct for other one-dimensional quantum mechanical problems. This leads one to conclude from the present work that ScR is a well-founded theory for deriving quantum mechanics from the concept of fractal space-time.

(ii) Even though many of the aspects of Hermann's work were used in the present work as they are, the application of his approach to the present quantum mechanical problems was not a direct one. Successful applications were not achievable without, among other things, a new adjustment for the time step  $dt$  after some deeper understanding of the underlying particle motion in some problems. It is expected that this understanding is necessary when attempts are made to solve other quantum mechanical problems.

(iii) The appearance of the Riccati equation in connection with ScR theory in the present work, and the use of this equation in conventional quantum mechanics in previous works [57,58] leads one to conclude that this equation is deeply rooted in the quantum mechanical behavior .

(iv) It is also concluded from the attempts made in the present work to improve the numerical simulation results by parameter optimization, that such attempts are successful in improving the results, and further improvement is possible, but requires more computer time.

(v) The computer time taken by the simulations performed for the quantum mechanical problems dealt with in the present work was always found to be much longer than that required for conventional quantum mechanical solutions based on the Schrödinger equation. The last solutions are even, in some problems, analytical and do not require much computer time. This leads to the conclusion that the present approach based on ScR theory is not for solving quantum mechanical problems directly. Rather, its main intention is to expose the relationship between the quantum behavior and the fractality of space-time, which is still a far reaching aim.

### **(7.3) Suggestions for Further Work:**

A number of suggestions for further work can be stated as follows:

(i) Even though the present work has reached the aim as set for it in chapter one, it is felt that similar applications to other quantum-mechanical problems will certainly increase confidence in the conclusions. Of these additional applications one mentions a particle in a double harmonic oscillator potential, a particle in a central potential and the hydrogen atom. Treatment of other problems for which the average classical velocity is not zero (asymmetric potentials), as well as problems in more than one-dimension, would also be helpful in this direction .

(ii) The appearance of the Riccati equation in the present work needs to be further investigated, and the connection with the previous

use of this equation in conventional quantum mechanical problems needs to be explored.

(iii) The success of the direct numerical simulation approach based on ScR theory in the present work in obtaining the quantum mechanical probabilities encourages attempts to investigate the direct quantification of other aspects of quantum mechanics and its axioms based on similar numerical simulations for suitably chosen quantum mechanical setups. In this connection the correspondence, the complementarity and the duality principles may be mentioned as examples which need to be investigated along these lines in any future work. This would establish these principles as a direct consequence of the fractality of space-time in the quantum domain.

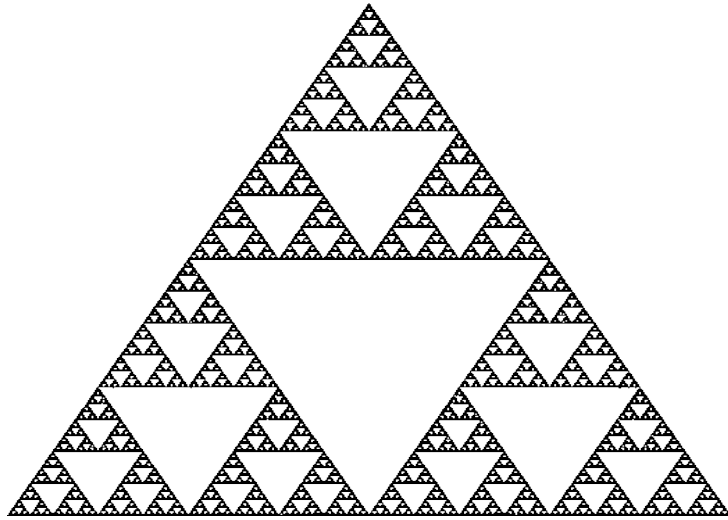
# **Appendix (A)**

## **Fractal Geometry**

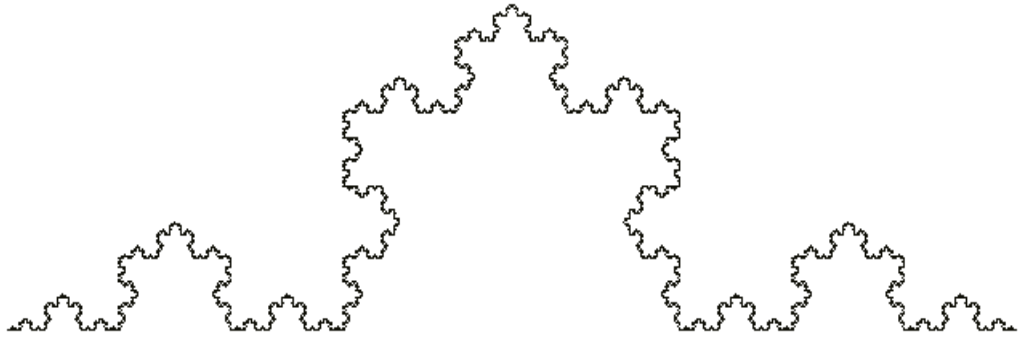
### **(A.1) Definition of a Fractal:**

The roots of fractal geometry go back to the 19<sup>th</sup> century, when mathematicians started to challenge Euclid's principles [77]. Euclidean geometry gives a first approximation to the structure of physical objects. It cannot easily describe non-linear shapes and non-integral systems [78,79]. Then, there is a need to a new geometry to describe these systems. Mandelbrot [78] introduced the term "fractal" to describe objects that are irregular and have many of the seemingly complex shapes [78,80].

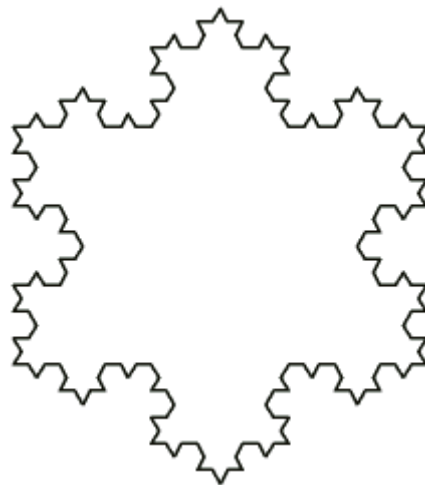
A geometric object whose dimension is fractional is called fractal. Fractals are self-similar or self-affine. For self-similar fractals, any small part of a fractal can be magnified to get the original fractal [78,81]. The common examples of this type of fractals are the Koch curve, the Koch snowflake and the Seirpinski triangle, as show in Fig. (A.1) [78,82]. While, in self-affine fractals, a smaller piece of the whole appears to have undergone different scale reductions in the longitudinal and transverse directions. Examples of this latter type of fractals are shown in Fig. (A.2) [78,81,82].



(a)



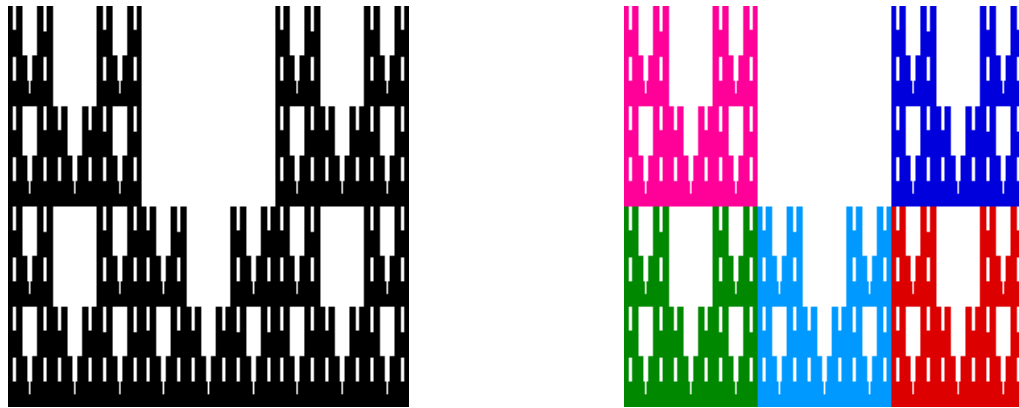
(b)



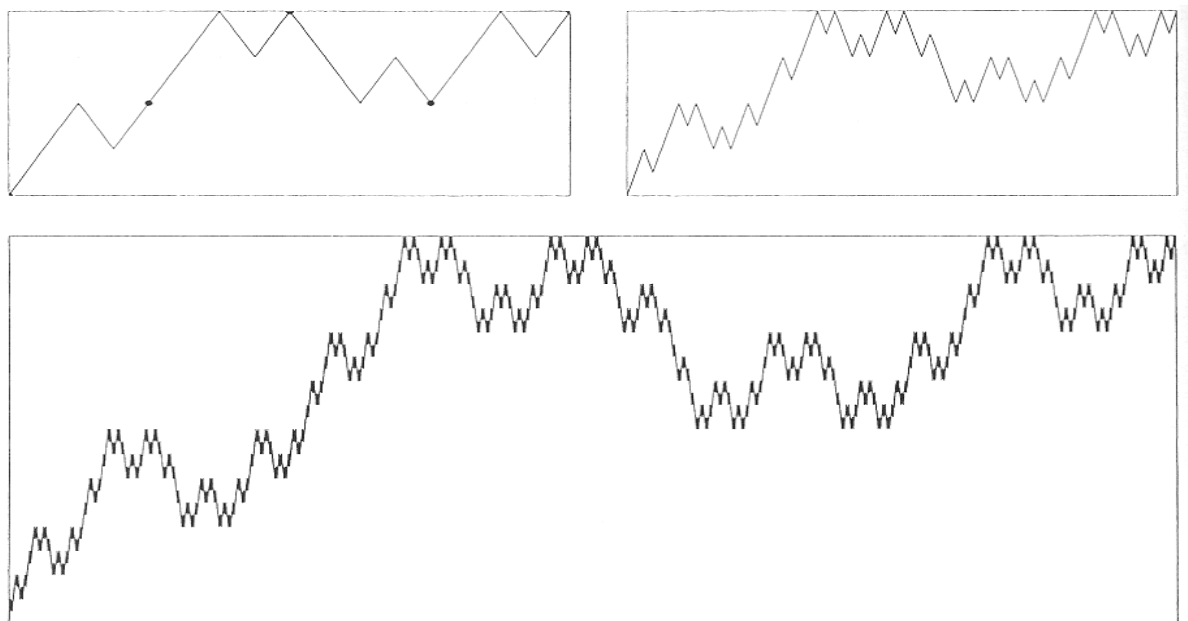
(c)

Fig. (A.1) Common self-similar fractals [78]: (a) Sierpinski triangle, (b) Koch curve and (c).Koch snowflake.





(a) This fractal is **self-affine** instead of self-similar because the pieces are scaled by different amounts in the x- and y-directions. The coloring of the pieces on the right emphasizes this[82].



(b) The Wiener Brownian motion (WBM)[78,81].

**Fig (A.2) Common self-affine fractals.**

## **(A.2) Definitions and Methods of Calculation of Fractal Dimension:**

Mandelbrot [78], Davis [82], Nikora [83], Rosso [84] and Takaysu [85] point out that there are many methods to define and calculate the fractal dimension. Here, the common methods in this field will be explained briefly.

**(A.2.1) Similarity dimension:**

The similarity dimension, which is based on the idea that fractals are usually self-similar objects is sometimes called the fractal dimension [78]. To motivate the definition of similarity dimension, one considers sets which are topologically one, two,...ect dimensional [78]. The following equation can be used to calculate fractal dimension in this case [77]:

$$\mathcal{N} r^d = C \quad \text{----- (A.1)}$$

where  $\mathcal{N}$  is the number of equal parts,  $d$  is the similarity dimension,  $r$  is the side length of each part and  $C$  is a constant. By taking  $C=1$ , the similarity dimension can be defined as[77]:

$$d = \frac{\ln \mathcal{N}}{\ln \frac{1}{r}} \quad \text{----- (A.2)}$$

It is known that  $d_{top.} \leq d_{sim.}$  [77]. For example, a square ( $D_T = 2$ ) can be divided into four squares  $\mathcal{N} = 4$ , then  $r = \frac{1}{2}$ ,  $d_{sim.} = \frac{\ln 4}{\ln 2} \cong 2$  [77] (see Fig. (A.3)).

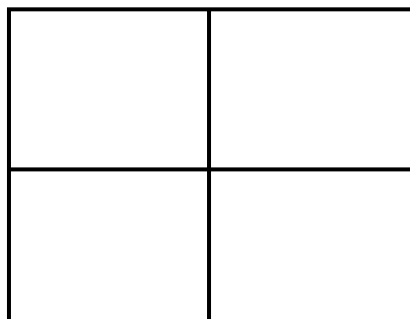


Fig. (A.3) A square divided into 4 squares of side length 1/2 [77].

**(A.2.2) Box dimension:**

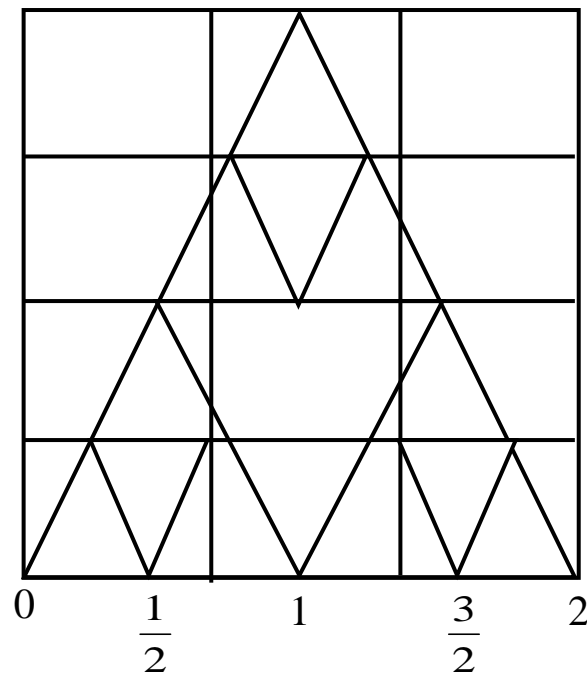
This represents another method for measuring the fractal dimension. This dimension is defined as follows : if X is a bounded subset of the Euclidean space, and  $\varepsilon \geq 0$ , then, let  $\mathcal{N}(X, \varepsilon)$  be the minimal number of boxes in the grid of side length  $\varepsilon$  which are required to cover X . One can say that X has box dimension D if the following limit exists and has value D:

$$\lim_{\varepsilon \rightarrow 0} \frac{\ln(\mathcal{N}(X, \varepsilon))}{\ln \frac{1}{\varepsilon}} \quad \text{----- (A.3)}$$

Consider for example the Seirpinski gasket (see Fig. (A.4)) [82]. One can show that it can be covered by 4 squares of side length 1, 12 squares of side length 1/2, 36 squares of side length 1/4. In general, the minimum number of squares of side length  $1/n$  needed to cover the Seirpinski gasket is  $4 \times 3^n$ .

Hence, the box dimension of the Seirpinski gasket is [77,78]:

$$\lim_{n \rightarrow \infty} \frac{\ln(4 \times 3^n)}{\ln 2^n} = \frac{\ln 3}{\ln 2} \cong 1.585$$



**Fig. (A.4): The box dimension for the Seirpinski gasket [82].**

**(A.2.3) Divider dimension:**

A fractal curve has fractal (or divider) dimension  $D$  if its length  $L$  can be measured with rods that have length  $\ell$  and it is given by [77,78,82]:

$$L = C * \ell^{1-D} \quad \text{----- (A.4)}$$

where  $C$  is a constant that is a certain measure of the apparent length . Eqn. (A.4) must be true for several different values of  $\ell$  . For example, consider the Koch curve [78]. It appears to have length  $L = (4/3)^m$  when measured with rods of length  $\ell = (1/3)^m$  . Hence:

$$\left(\frac{4}{3}\right)^m = C \left(\frac{1}{3}\right)^m (1-D)$$

This implies that:

$$m \ln \frac{4}{3} = \ln(C) + m(1-D) \ln \frac{1}{3}$$

When  $C = 1$ , then  $D = \frac{\ln 4}{\ln 3} \cong 1.2619$  as expected [78,82].

# Appendix (B)

## The Riccati Equation

### (B.1) Definition of the Riccati Equation:

In mathematics, a Riccati equation is any ordinary differential equation that has the form [55]:

$$R' = q_0(x) + q_1(x)R + q_2(x)R^2 \quad \text{----- (B.1)}$$

where  $q_0(x), q_1(x)$  and  $q_2(x)$  are known functions of  $x$  .

### (B.2) Solution of the Riccati Equation:

The Riccati equation is not amenable to elementary techniques in solving differential equations, except as follows. If one can find any solution  $R_1$ , then, the general solution is obtained as [55,56]:

$$R = R_1 + w \quad \text{----- (B.2)}$$

Substituting eqn. (B.2) in the Riccati equation (eqn. (B.1)) yields,

$$R' + w' = q_0 + q_1(R_1 + w) + q_2(R_1 + w)^2 \quad \text{----- (B.3)}$$

and since,

$$\left. \begin{aligned} R' &= q_0 + q_1R + q_2R^2 \\ w' &= q_1w + 2q_2R_1w + q_2w^2 \end{aligned} \right\} \quad \text{----- (B.4)}$$

then,

$$w' = (q_1 + 2q_2R_1)w = q_2w^2 \quad \text{----- (B.5)}$$

which is a Bernoulli equation [55] . The substitution that is needed to solve this Bernoulli equation is [55,56]:

$$Z = u^{1-2} = \frac{1}{u} \quad \text{----- (B.6)}$$

Substituting

$$R = R_1 + \frac{1}{Z} \quad \text{----- (B.7)}$$

directly into the Riccati equation yields the linear equation [55,56]:

$$Z' + (q_1 + 2q_2 R_1)Z = -q_2 \quad \text{----- (B.8)}$$

Then, the general solution to Riccati equation is given by eqn. (B.7) [55,56], where  $Z$  is the general solution to the aforementioned equation [55,56].

The Riccati equation (B.1) can be rewritten in the form [55,56]:

$$\frac{dR}{dx} = \mathcal{S} + r_1 R^2 \quad \text{----- (B.9)}$$

where  $\mathcal{S} = q_0(x) + q_1(x)R$  and  $r_1 = q_2(x)$ . This differential equation may not be solvable analytically. One may write [55]:

$$R = -\frac{u'}{r_1 u} \quad \text{----- (B.10)}$$

where  $u(x)$  is a new dependent variable replacing  $R(x)$ . Then [55]:

$$R' = -\frac{u''}{r_1 u} + \frac{u'^2}{r_1 u^2} + \frac{r_1' u'}{r_1^2 u} \quad \text{----- (B.11)}$$

By substituting eqns. (B.9) and (B.10) into eqn. (B.8), the last equation becomes:

$$r_1 u'' - r_1' u' + \mathcal{S} r_1^2 u = 0 \quad \text{----- (B.12)}$$

This is a linear homogeneous second-order differential equation for  $u(x)$ . It has the general solution [55,56]:

$$u(x) = Wf(x) + Og(x) \quad \text{----- (B.13)}$$

where W and O are integration constants and  $f$  and  $g$  are series [55]. Hence, from eqn. (B.10):

$$R(x) = -\frac{u'}{r_1 u} = -\frac{C_1 f'(x) + g'(x)}{r_1 (C_1 f(x) + g(x))} \quad \text{----- (B.14)}$$

where  $C_1 = W/O$ .

### **(B.3) The Riccati Equation in Quantum Mechanics:**

In quantum mechanics, Price [58] observed that the Schrödinger equation in one-dimension can be reduced to a Riccati form. It can be derived from both the one-dimensional Schrödinger equation [58] and one-space and one-time Klein-Gordon equation [58] in the form:

$$R'(r) + R^2(r) + d_1(r, \mathcal{U}, E) = 0 \quad \text{----- (B.15)}$$

where  $d_1$  is some function of  $r$  (position vector),  $\mathcal{U}$  (potential) and the eigenvalue  $E$  (energy).

The Dirac equation for a combination of scalar potential  $\mathcal{U}$ , four-component vector potential  $\tilde{V}$ , and anomalous magnetic moment term  $\tilde{\mathcal{E}}$ , when all three terms have spherical symmetry, leads to the Riccati equation for a nodeless state [58]:

$$R' - 2KR/r - 2\tilde{\mathcal{E}} + R^2(E - \tilde{V} + m + \mathcal{U}) + (E - \tilde{V} - m + \mathcal{U}) = 0 \quad \text{---- (B.16)}$$

Finally, one can observe that all quantum systems have a Riccati form when one uses the Schrödinger, Klein-Gordon and Dirac equations to solve these systems [58].

# Appendix C

## Cantorian Fractal Space-Time

### (C-1) The Cantor Set:

The Cantor set,  $\varepsilon^{(0)}$ , [78] is a fractal dust which is densely packed into a set of topological dimension zero (a point) as shown in Fig.( C-1). The Hausdorff dimension [78,81] of this fractal set is equal to the golden mean  $\phi = (\sqrt{5} - 1)/2$  [86-89]. Other Cantorian sets,  $\varepsilon^{(i)} (-\infty < i < \infty)$ , are constructed in a similar way [88-89].

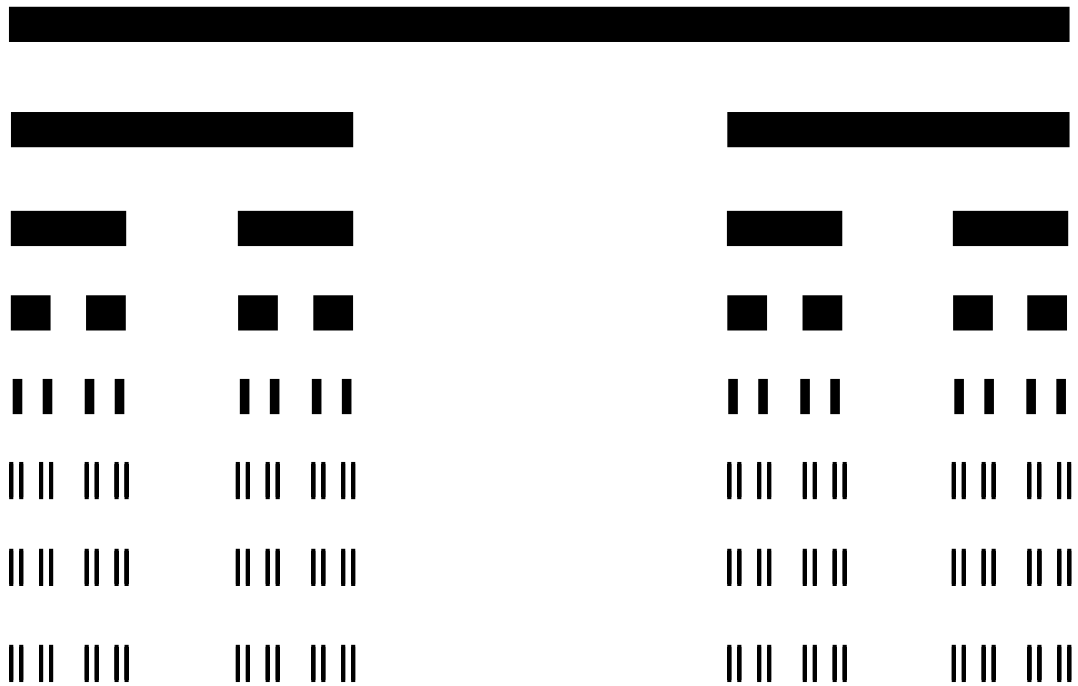


Fig. (C-1) The Cantor Set [78]

### (C-2) $\varepsilon^{(\infty)}$ Theory and Fractal Space-Time:

The construction of the set  $\varepsilon^{(\infty)}$  [65,86-89] contains an infinite number of sets  $\varepsilon^{(i)} (-\infty < i < \infty)$ . The index  $i$  labels the topological



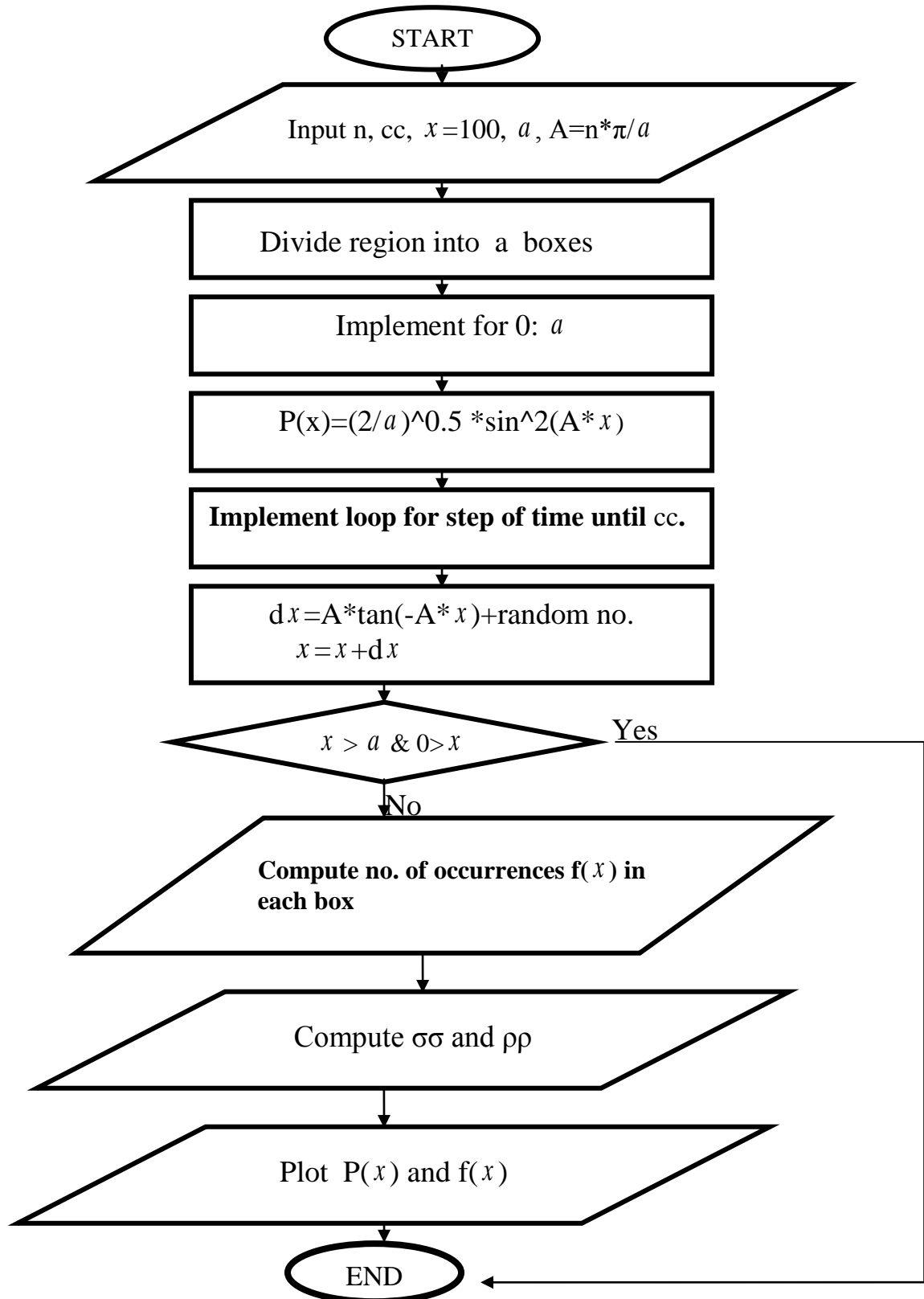
dimension of the smooth space into which the fractal set is densely packed [65,89] .  $\varepsilon^{(\infty)}$  is considered the basis for the construction of fractal space-time by El-Naschie [65,86-88].

The main conceptual idea of El-Naschie's work is a generalization of what Einstein considered the geometry of space-time on the large to be a curved four-dimensional space [1-5]. El-Naschie [65,86-88] in his theory assumes that space-time at quantum scales is far from being smooth, but rather resembles a stormy ocean. The crucial step in  $\varepsilon^{(\infty)}$  theory was to identify the stormy ocean with vacuum fluctuations and in turn to model these fluctuations using the mathematical tools of non-linear dynamics, complexity theory and chaos theory and number theory [86,87,90].

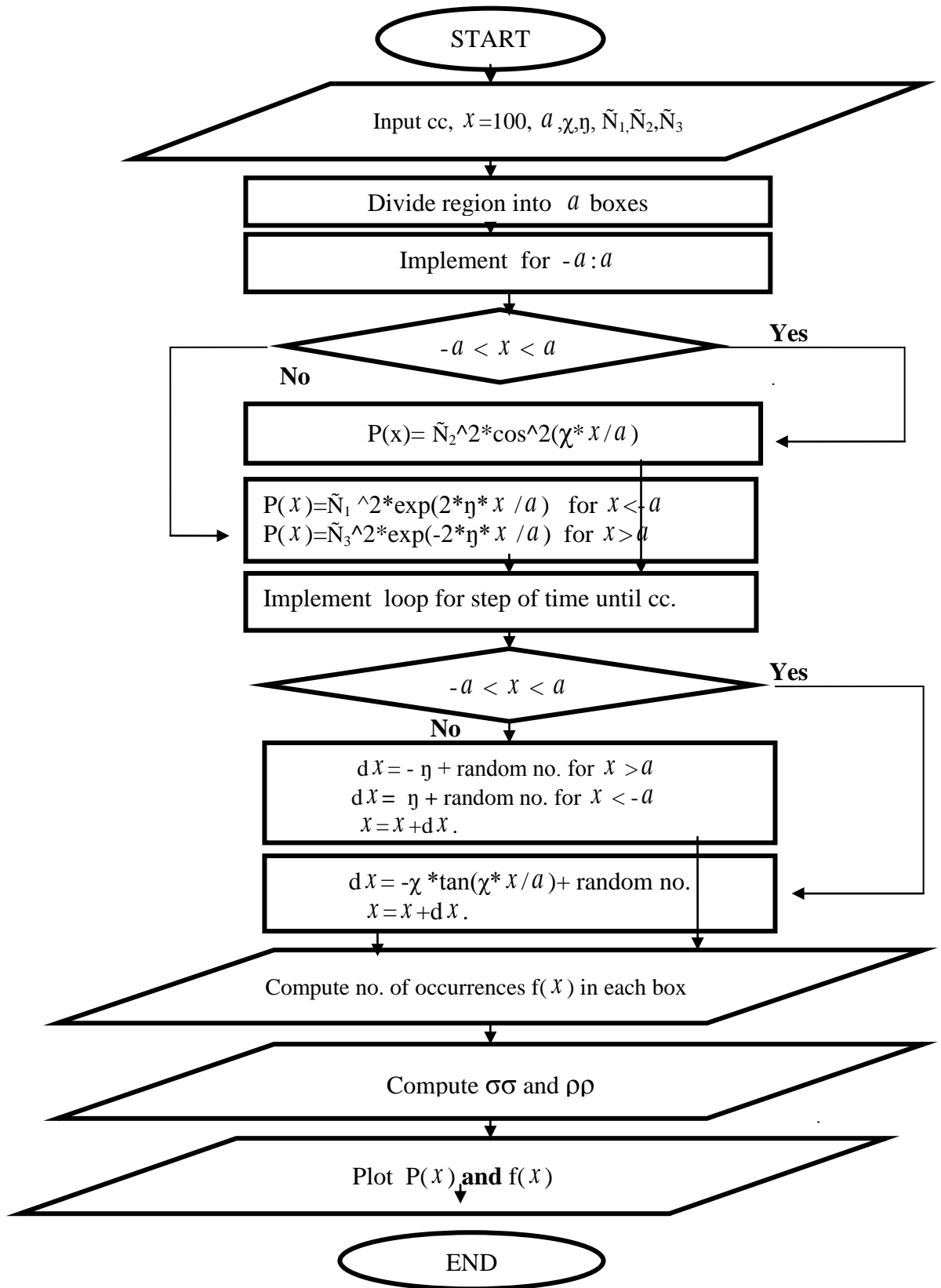
### **(C-3) Relation of $\varepsilon^{(\infty)}$ Theory to ScR Theory:**

There is a strong relation between  $\varepsilon^{(\infty)}$  theory based on Cantorian fractal space-time and the fractal space-time underlying the ScR theory. However, whereas cantorian fractal space-time is a mathematical concept the fractal space-time underlying ScR theory is based on Nottale's generalization of the relativity principle to scales [30-32].

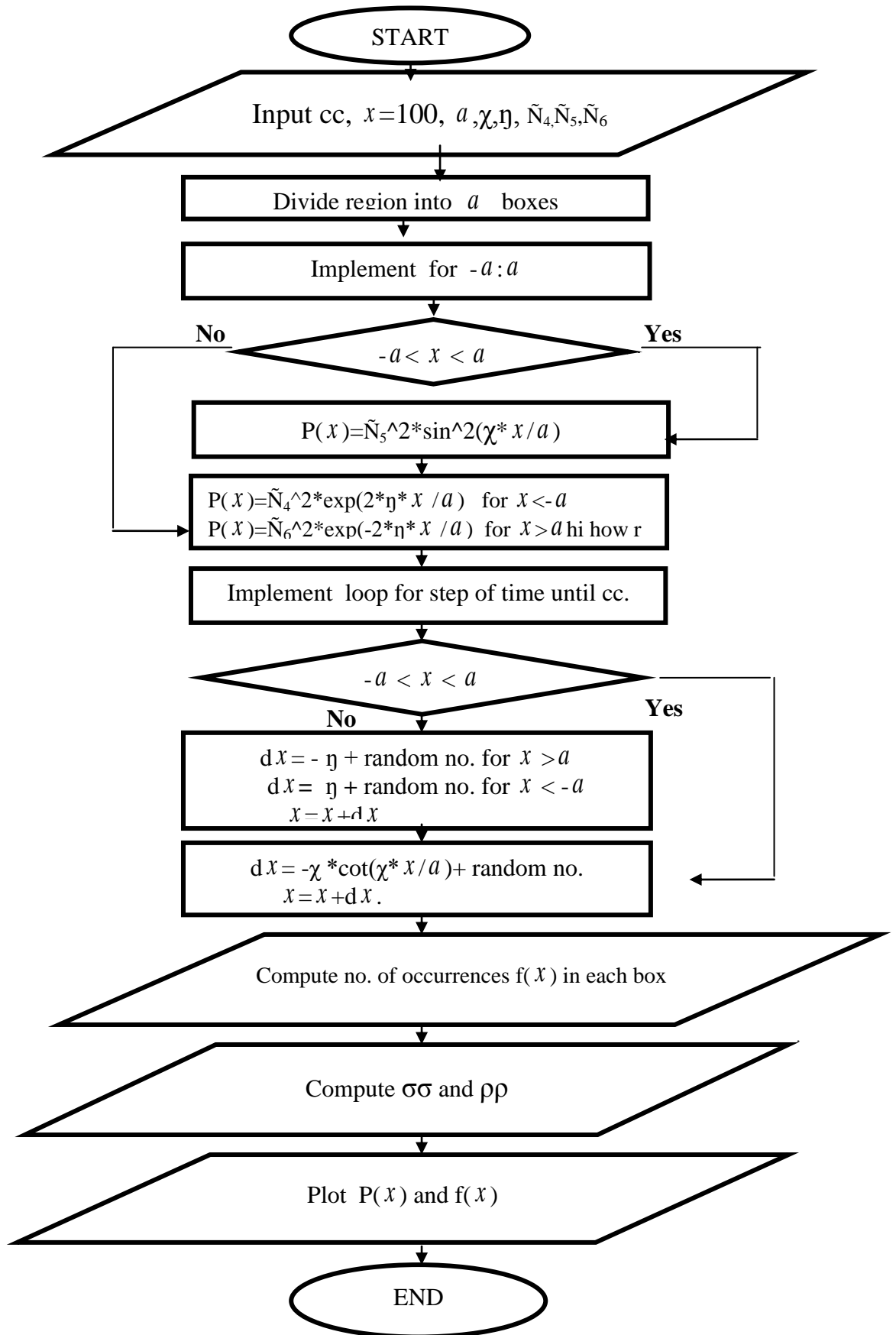
It is expected that El-Naschie's  $\varepsilon^{(\infty)}$  theory [65,86-88] will have far reaching applications in many fields of physics [65,86-90] and not only quantum physics [86,87,90] . Hence, it may furnish a new more accurate look at the laws of nature.



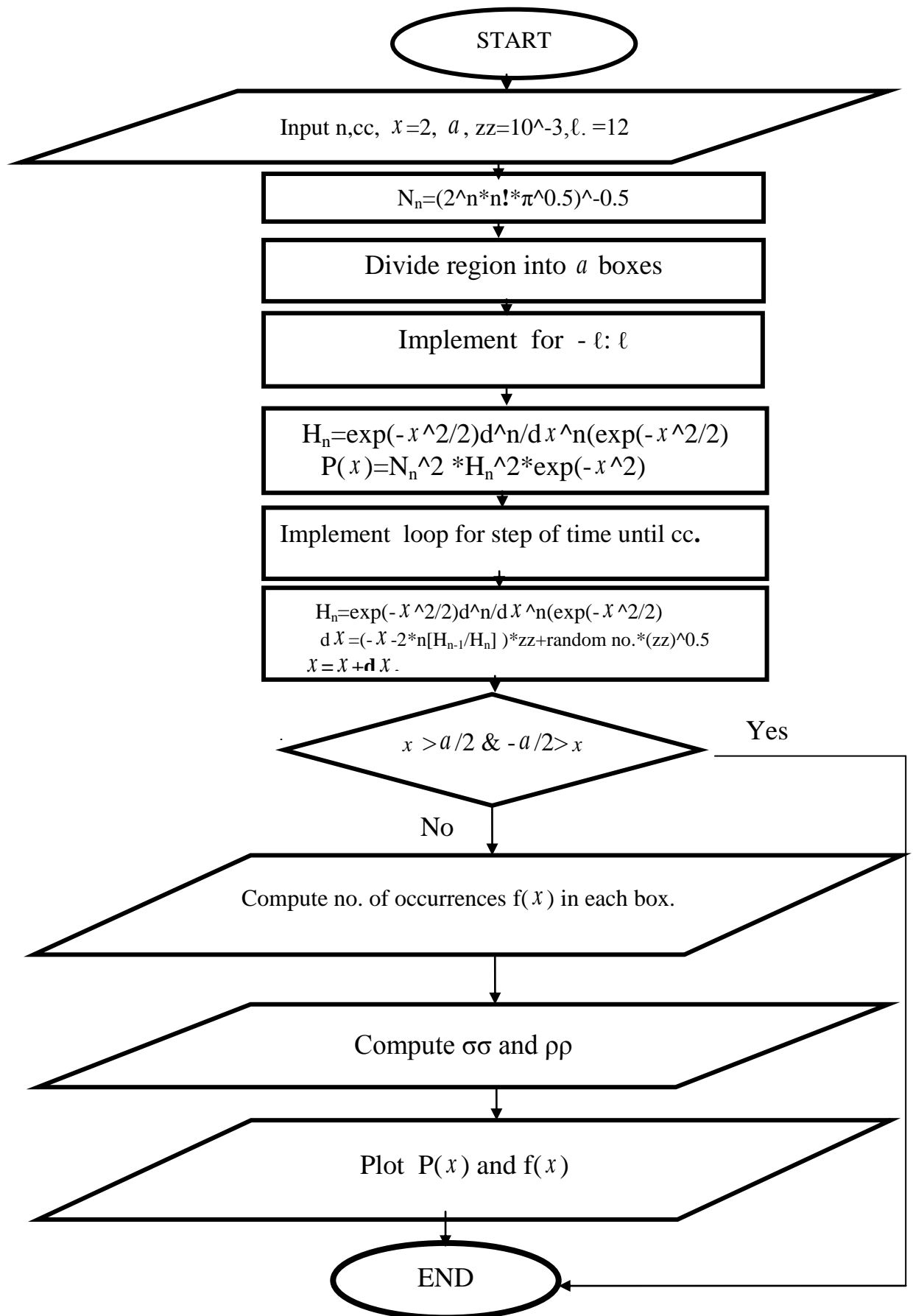
Flowchart (1). A schematic illustration of the different part of the program to calculate probability density of particle in an infinite square well potential.



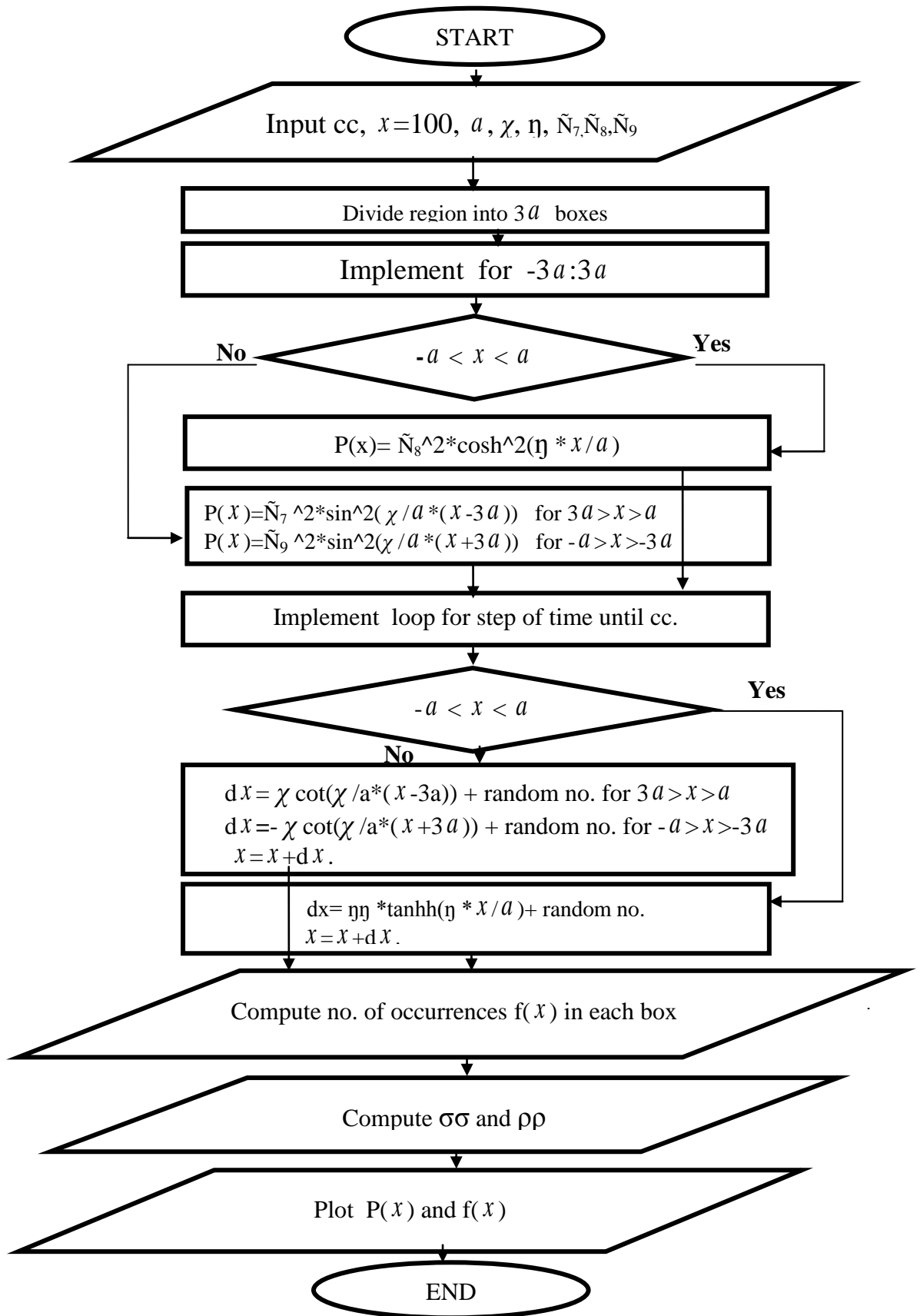
Flowchart (2). A schematic illustration of the different part of the program to calculate probability density of particle in a finite square well potential (even parity).



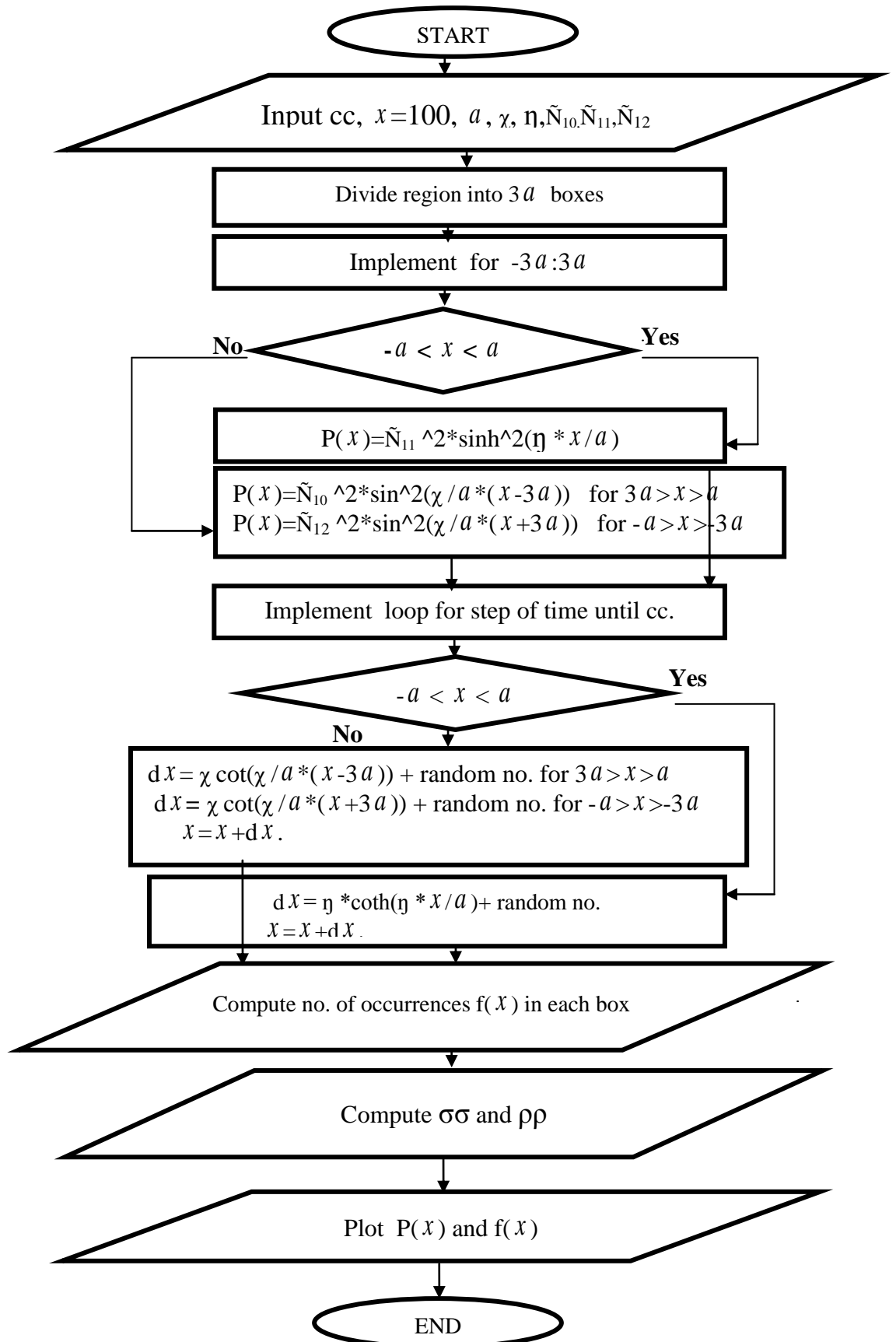
Flowchart (3). A schematic illustration of the different part of the program to calculate probability density of particle in a finite square well potential (odd parity).



Flowchart (4) A schematic illustration of the different part of the program to calculate Probability density of particle in SHO potential.



Flowchart (5). A schematic illustration of the different part of the program to calculate probability density of particle in a double well potential (even parity).



Flowchart (6). A schematic illustration of the different part of the program to calculate probability density of particle in a double well potential (odd parity).

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