J. of Al-Anbar university for pure science . Vol.1. No.3. 2007

ISSN: 1991-8941

NUMERICAL SIMULATIONS OF PARTICLE IN A DOUBLE OSCILLATORS

S. N. T. AL-RASHID

DEPT. OF PHYSICS., COLLEGE OF EDUCATION, AL-ANBAR UNIVERSITY

Received :10/3/2007 *Accepted:4/9/2007*

Abstract

In the present work, we extend the Hermann and Al-Rashid works to the problem of particle in a double oscillators potential. In this problem, one can take a special case when oscillation quantum number (v) is none negative integer. Computer programming is built to make numerical simulations to this problem. The probability density of finding particle in a double oscillators potential is calculated without using Schrödinger equation or any conventional quantum mechanics. This probability is compared with probability of conventional quantum mechanics.

Keywords: Numerical Simulations , Particle in , Double Oscillators

Introduction

Hermann [1] shows quantum behavior of particle in a box [2,3] by a numerical simulation process to fractal position equation of this problem without using Schrödinger equation and any conventional quantum mechanics .This approach is based on Scale Relativity Theory by Nottale [4,5,6,7]. Al-Rashid [8] extended Hermann's work to other quantum systems such as : Finite square well , simple harmonic oscillator and double well potentials. Al-Rashid [8] found that there was a connection between Scale Relativity Theory and Riccati equation [8,9], in addition he showed the quantum behavior of these quantum systems.

The model of double oscillators potential by consideration two masses m_1 and m_2, constrained to move in a straight line and connected with each other by a spring whose force constant is k and whose length at equilibrium is q. The scalar potential of this problem is

$$u = \frac{1}{2} k (|x| - q)^2$$

[10], as shown in fig.(1),where .This example comes from molecular physics . There , one frequently encounters motion in the neighborhood of a state equilibrium configuration, approximated by harmonic potential [10].

In the present work, we will apply Hermann[1] and Al-Rashid [8] approach to solve equation of motion and reveal quantum behavior of double oscillator potential without using Schrödinger equation and any conventional quantum mechanics. The aim of the present work is extending Hermann and Al-Rashid works to another quantum system in one-dimensional by calculation probability density of finding particle in a double oscillator potential so that these results will be compared with the results of conventional quantum mechanics.

Solution of Equation of Motion

Nottale [4,5,7] , in his theory (Scale Relativity), rewrites Newton's fundamental equation of dynamics by complex forms such as:

$$\nabla u = m\frac{\eth}{\mathrm{dt}}V \qquad \text{-----(1)}$$

where u is scalar potential ,V is complex velocity which is define as $V = v - iU$ **where v is classical velocity and U is an imaginary part of complex velocity , and** $\frac{\eth}{dt}$ **is complex derivative operator [4,5,6] which is** $\frac{\partial}{\partial t} + V\ \nabla . - iD\ \Delta$ **where D is diffusion constant ,** $D = \frac{\eta}{2m}$ **.**

As for Hermann [1] and Al-Rashid [7] works , one may start from eqn.(1) to solve equation of motion of double oscillator problem but here replacing $m \to \mu$ **, where** μ **(**$\mu = m_1 m_2/(m_1+m_2)$**) is reducing mass. By using the definition of complex velocity, one can separate eqn.(1) in two real and imaginary parts as[1,7]:**

$$\left.\begin{aligned} -D\Delta U - (U.\nabla)U &= -\nabla u \\ \frac{\partial}{dt}U &= 0 \end{aligned}\right\} \text{---(2)}$$

2nd equation of eqn.(2) shows that the imaginary part of complex velocity depends on position only [1].Eqn.(2) can be written in one-dimensional as:

$$\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}DU(x)+\frac{1}{2}U^2(x)\right)=\frac{1}{\mu}\frac{\partial}{\partial x}u(x) \quad \text{--(3)}$$

then, by integration, one obtains:

$$D\frac{\partial}{\partial x}U(x)+\frac{1}{2}U^2(x)+c_1=\frac{1}{\mu}u(x) \quad \text{----(4)}$$

where c1 is a constant of integration. The constant of integration was defined by Hermann [1] and Al-Rashid [8] as E/μ **where E is the total energy of system. Eqn.(4), then, becomes:**

$$\frac{\partial}{\partial x}U(x)+\frac{1}{2D}U^2(x)+\frac{E}{\mu\ D}=\frac{1}{\mu\ D}u(x) \quad \text{-----(5)}$$

By rearrangement of eqn.(5) and using the definition of $D = \frac{\eta}{2\mu}$ **, eqn.(5) becomes:**

$$\frac{d}{dx}U(x) = -\frac{\mu}{\eta}U^2(x)+\frac{2}{\eta}(u(x)-E) \quad \text{-----(6)}$$

eqn.(6) has the form of Riccati equation [8,9] as Al-Rashid found [7]. Riccati equation can be solved by transforming it into a 2nd order differential equation [8,9] which is:

$$ry''(x)+r^2g(x)y(x)=0 \qquad \text{----(7)}$$

where

$$U(x) = -\frac{1}{r}\frac{y'(x)}{y(x)} \qquad \text{---------(8)}$$

and $y(x)$ **is an arbitrary function of x . From eqn.(6), one can define:**

$$r = -\frac{\mu}{\eta} \quad ; \quad g(x)=\frac{2}{\eta}(u(x)-E) \quad \text{-----(9)}$$

By using eqns. (7),(8) and (9), eqn.(6) becomes:

$$\frac{d^2}{dx^2}y(x)-\frac{2\mu}{\eta^2}(u(x)-E)y(x)=0 \quad \text{--(10)}$$

Now, for the problem of double oscillator potential , the potential is $u(x)=\frac{1}{2}k(|x|-q)^2$ **for** $E < u_o$ **[10] . Then,**

eqn.(10) can be written as:

$$\frac{d^2}{dx^2}y(x)-\frac{2\mu}{\eta^2}(\frac{1}{2}\mu\ \omega^2(|x|-q)^2-E)y(x)=0$$ **--(11)**

where $k=\mu\ \omega^2$ **,** ω **is angular frequency. Here, there are two cases depending on** x **value which are [11]:**

for x **is positive , then, eqn.(11) becomes:**

$$\frac{d^2}{dx^2}y(x)-\frac{\mu^2\omega^2}{\eta^2}(x-q)^2y(x)=\frac{2\mu}{\eta^2}E\ y(x)$$ **--(12)**

Let

$$z=(\frac{2\mu\omega}{\eta})^{\frac{1}{2}}(x-q)\quad ;\quad for\quad x>0\ ,$$

eqn.(12) becomes:

$$\frac{d^2}{dz^2}y(z)-\frac{z^2}{4}y(z)=\frac{1}{\eta\omega}E\ \ y(z)$$ **---- (13)**

Total energy for oscillator is defined as , $E_\nu=\eta\omega(\nu+\frac{1}{2})$ **[10], then, one can write eqn. (13) as:**

$$y''(z)+(\nu+\frac{1}{2}-\frac{1}{4}z^2)y(z)=0$$ **----(14)**

This equation is called Weber differential equation [11] which has even and odd solutions :

for even solutions ,the solution is [11]:

$$y_1(z)=e^{\frac{-z^2}{4}}{}_1F_1(\frac{-\nu}{2};\frac{1}{2};\frac{1}{2}z^2)$$ **---(15)**

from the table [12], the confluent hypergeometric function is :

$${}_1F_1(\frac{-\nu}{2};\frac{1}{2};\frac{1}{2}z^2)=2^{\frac{-1}{2}}\exp(\frac{1}{4}z^2)\ \mathbf{D}_\nu(z)$$ **--(16)**

then, eqn.(16) becomes:

$$y_1(z)=2^{\frac{-1}{2}}\ \mathbf{D}_\nu(z)$$ **----(17)**

where $\mathbf{D}_\nu(z)$ **is parabolic cylinder function [11]. By using eqn.(8) ,one can writte:**

$$U(z)=\frac{\eta}{\mu}(\frac{\mathbf{D}'_\nu(z)}{\mathbf{D}_\nu(z)}dz)$$ **------(18)**

From recurrence relations [11]:

$$\mathbf{D}'_\nu(z)=-\frac{1}{2}z\ \mathbf{D}_\nu(z)+\nu\ \mathbf{D}_{\nu\text{-}1}(z)$$ **---(19)**

then eqn.(18) becomes:

$$U(z)=\frac{\eta}{\mu}(-\frac{1}{2}z+\nu\frac{\mathbf{D}_{\nu-1}(z)}{\mathbf{D}_\nu(z)})dz$$ **-----(20)**

Finally, we can write $U(x)$ **for double oscillator in this case as :**

$$U(x)=(-(x-q)+\sqrt{2}\ \ \nu\frac{\mathbf{D}_{\nu-1}(x)}{\mathbf{D}_\nu(x)})dx$$ **--(21)**

where $\eta=\mu=\omega=1$.

In special cases, one can consider ν **is a nonnegative integer n ,then, can reduce** $\mathbf{D}_n$ **to [11]:**

$$\mathbf{D}_n(z)=2^{\frac{-n}{2}}H_n(\frac{z}{\sqrt{2}})\ e^{\frac{-z^2}{4}}=e^{\frac{-z^2}{4}}\ \ H_{en}(z)$$ **---(22)**

where $H_n(z)$ **is a Hermit polynomial and** $H_{en}(z)$ **is modified Hermit polynomial. Then, eqn.(21) becomes:**

$$U_1(x)=(-(x-q)+2n\frac{H_{n-1}(x-q)}{H_n(x-q)})\quad for\quad x>0$$ **--(23)**

if one compare eqn.(23) with Al-Rashid's work [8] for simple harmonic oscillator, we can see that eqn.(23) goes to simple harmonic when q=0.This is similar to Ψ wave function which goes to simple harmonic when q=0 in conventional quantum mechanics[10].

(ii) the odd solutions for $x > 0$ take a similar way for even solutions, then one can write [11]:

$$y_2(z) = z\ e^{\frac{-z^2}{4}}\ {}_1F_1(\frac{1}{2}-\frac{\nu}{2};\frac{3}{2};\frac{1}{2}z^2)$$

---(24)

and from table[12] , one can find [12]:

$${}_1F_1(\frac{1}{2}-\frac{\nu}{2};\frac{3}{2};\frac{1}{2}z^2) = e^{\frac{z^2}{4}}\ \frac{\mathbf{D}_\nu(z)}{2z}$$

---(25)

This leads to :

$$y_2(z) = \frac{1}{2}\mathbf{D}_\nu(z)$$

------(26)

so:

$$U(z) = \frac{\eta}{\mu}(-\frac{1}{2}z + \nu\ \frac{\mathbf{D}_{\nu-1}(z)}{\mathbf{D}_\nu(z)})dz$$

which is similar to even solutions. Again, for special cases when ν is non-negative integer, one can writ :

$$U_2(x) = (-(x-q) + 2n\frac{H_{n-1}(x-q)}{H_n(x-q)})\quad for\ x>0$$

-(27)

Eqn.(27) , is exactly eqn.(23).

(b) the solutions for $x < 0$ are in similar way for $x > 0$, then, $U(x)$ is:

$$U(x) = (-(x+q) + 2n\frac{H_{n-1}(-(x+q))}{H_n(-(x+q))})\quad for\ x<0$$

--(28)

for even and odd solutions.

Nottale [4,5,6], proves that the position vector X (t) is assimilated into a stochastic process which satisfies the relation, so Hermann [1] and Al-Rashid [7] found that :

$$\left.\begin{aligned} dx(t) &= U_+(x)dt + d\xi_+(t)\quad for dt>0\ (forward)\\ and\\ dx(t) &= U_-(x)dt + d\xi_-(t)\quad for dt<0\ (backward)\end{aligned}\right\}$$

-- (29)

where dξ(t) is a random variable of Gaussian distribution and is of width $\sqrt{2D}\,dt$ [1].By using values of $U(x)$,one can write :

$$dx(t) = ((-(x-q) + 2n\frac{H_{n-1}(x-q)}{H_n(x-q)}))dt + d\xi(t)\quad for\ x>0$$

--(30)

and

$$dx(t) = ((-(x+q) + 2n\frac{H_{n-1}(-(x+q))}{H_n(-(x+q))}))dt + d\xi(t)\quad for\ x<0$$

- (31)

Numerical Simulations

As Hermann [1] and Al-Rashid [8], eqns. (30) and (31) represent a stochastic process. Here, in the problem of double oscillators , it was found that the assumption 2Ddt=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 $\frac{m}{\eta}$ dt=10-3( ) is suitable for the present simulations [8]. It seems that this value of dt is related to the period of the motion in the double oscillators 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, eqns. (30) and (31) become:

$$dx(t) = ((-(x-q) + 2n\frac{H_{n-1}(x-q)}{H_n(x-q)}))\times 10^{-3} + N(0,1)\times\sqrt{10^{-3}}\quad for\ x>0$$

--(32)

and

$$dx(t) = ((-(x+q) + 2n\frac{H_{n-1}(-(x+q))}{H_n(-(x+q))}))\times 10^{-3} + N(0,1)\times\sqrt{10^{-3}}\quad for\ x<0$$

--(33)

where N(0,1) is a normalized random variable [1] and $\eta = \mu = \omega = 1$.

The numerical simulations were performed using eqns. (32) and (33). The output of these simulations give the probability density $f(x)$ of the presence of the particle in the double oscillators potential. These simulations were done by dividing the box of size a into 1200 pieces and counting the number of time steps the particle is in each specific sub box. In 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 [10] which also approximate in this special case($\nu \to n$)

$$\Psi((x-q))=\Phi_n((x-q))=2^{\frac{-n}{2}} H_n((x-q))\, e^{\frac{-(x-q)^2}{2}}$$

and

$$P((x-q))=2^{-n} H_n^2((x-q))\, e^{-(x-q)^2}$$

into ---- (34)

for $x>0$ and

$$\Psi((x+q))=\Phi_n(-(x+q))=2^{\frac{-n}{2}} H_n(-(x+q))\, e^{\frac{-(x+q)^2}{2}}$$

and **--- (35)**

$$P((x+q))=2^{n} H_n^2(-(x+q))\, e^{-(x+q)^2}$$

for $x<0$,where $\eta = \mu = \omega = 1$ and P is probability in conventional quantum mechanics.

This comparison is by calculating the standard deviation σ and the correlation coefficient ρ which are defined as [1]:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N} (P(i) - f(i))^2}{N}} \quad \text{------ (36)}$$

and

$$\rho = \frac{\sum_{i=1}^{N} (P(i) - < P >)(f(i) - < f >)}{\sum_{i=1}^{N} (P(i) - < P >)^2 \sum_{i=1}^{N} (f(i) - < f >)^2} \quad \text{-- (37)}$$

where N is the number of pieces(no. of boxes) , P(i) ≡ P(x) and f(i) ≡ f(x).

In this work, the results of applying a computer program built following the Hermann [1] and Al-Rashid [7] approaches are presented. Fig.(2) shows a first attempt of modeling for n = 0 and 1 when q = 4. Here, the time step(cc) has been chosen as 108. The numerical simulations start with arbitrary point which is x=2 . The continuous curves indicate the results of the present simulations and the dashed curves the results of conventional quantum mechanics. The output of the simulations was normalized by multiplying it with a constant z whose value depends on the number of divisions of the region (here, z=50) In these figures, there is a clear difference between the present results and the results of quantum mechanics, that is measured by σ (approaching zero) and ρ (approaching one).

There are three ways to improve the results suggested [1,7]. They are:

using more steps in time .

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

increasing numbers of pieces (boxes).

Fig. (3) shows the improved results obtained in the present work with n=0 and n=1 when q= 4 for 108 steps by using the thermalization process, starting points(ss) are 25 and 31. The convergence between the simulation results and conventional quantum mechanics is clear by the values of σ and ρ.

Fig. (4) shows the improved numerical results by increasing the number of steps time for n=0 to cc=5*108. 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), where it

appears that there is better agreement between the two results for n=0 when the number of boxes was increased to 2200.

To test our work the numerical results go may back to simple harmonic oscillator results when q=0 [10]. Fig.(6) shows the numerical results for n=0 and 1, which coincide with simple harmonic oscillator results by Al-Rashid [7].

Discussion and Conclusion

The present work was an attempt to expand the works of Hermann [1] and Al-Rashid [8] by performing similar simulations for other quantum-mechanical problems not treated by them or by others. However, as it appears from the work in this paper which is considering a special case for V is non-negative integer, there are many difficulties that should be overcome to obtain meaningful results that can be compared with conventional quantum mechanical results. On the mathematical side, Riccati equation has helped in solving some of these difficulties[7]. While, on the numerical side, special attempts to optimize the solution parameters for the problems treated in this paper were needed to obtain the required results.

In this paper, Quantitative correct prediction of the behavior of a quantum particle in a double oscillators one-dimensional potential can be obtained without explicitly writing the Schrödinger equation nor using any conventional quantum axiom[1,7]. It can be concluded from the present work that this fact is even correct for one-dimensional quantum mechanical problems. This leads one to conclude from the present work that Scale Relativity is a well-founded theory for deriving quantum mechanics from the concept of fractal space-time.

Acknowledgments

I would like to deeply thank Prof. Dr. L. Nottale (Director of Research, CNRS, Paris, France) for clarifying some points regarding his theory of scale relativity and for supplying some literature and Dr. R.. P. Hermann (Dept. of Physics, Univ. de Liege, Belgium) for his suggestions concerning further applications of the theory of Scale Relativity.

References

1. **R. P. Hermann, "Numerical Simulation of a Quantum Patrical in a Box", J. Phys. A; Math. Gen. 30, 1997, pp.3967-3975.**
2. **L. I. Schiff., "Quantum Mechanics", 3rd Ed., Int. Student, McGraw - Hill, 1969.**
3. **S. Gasiorowicz, "Quantum Physics", John Wiley and Sons, Inc., New York, 1974.**
4. **L. Nottale, "The Theory of Scale Relativity". Int. J. of Mod. Phys. A, Vol.7, No.20, 1992, pp. 4899-4936.**
5. **L. Nottale, "Fractal Space-Time and Microphysics:**
6. **Towards of a Theory of Scale Relativity", World Scientific, (First Reprint) 1998.**
7. **L. Nottale, "The Scale Relativity Program", Chaos, Solitons and Fractals, Vol.10, No.2-3, 1994, pp. 459-468.**
8. **Saeed N. T. Al-Rashid "Some Applications of Scale Relativity Theory in Quantum Physics" ,Ph.D. thesis, 2006.**
9. **W. T. Reid, "Riccati Differential Equations". Acade. Press, New York, 1972.**
10. **F. Charlton, "Integrating Factor for First-Order Differential Equations", Classroom Notes, Aston Univ., England, 1998.**
11. **E. Merzbacher ,"Quantum Mechanics",2nd edd., John Wiley & Sons, 1970.**
12. **Whittaker E. T. and Watson G. N. "The parabolic Cylinder Function ",A course in ed. Cambridge University press, 1990.**
13. **Milton Abramowitz and Irene A. Stegun, eds, "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables" , Dover: New York, 1972.**

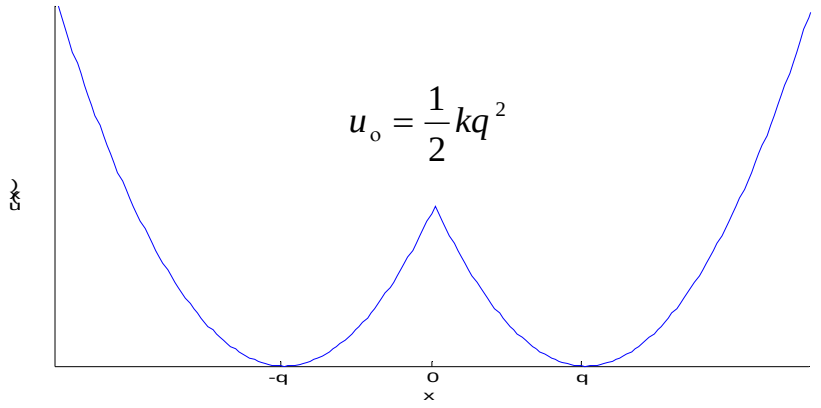
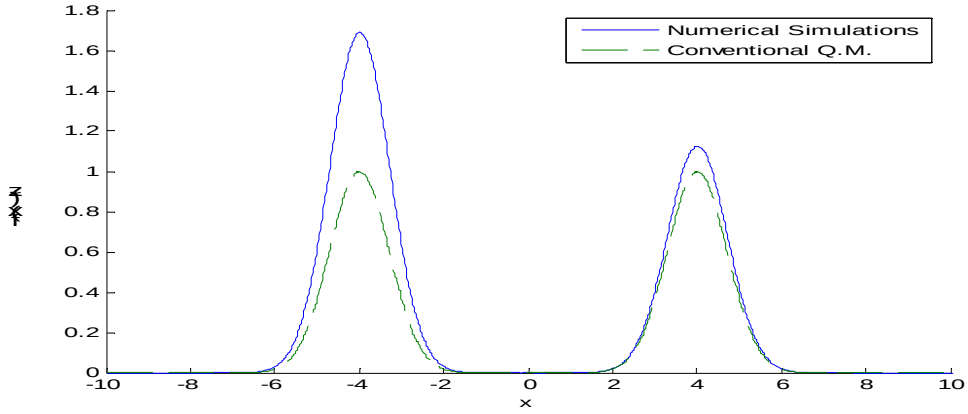


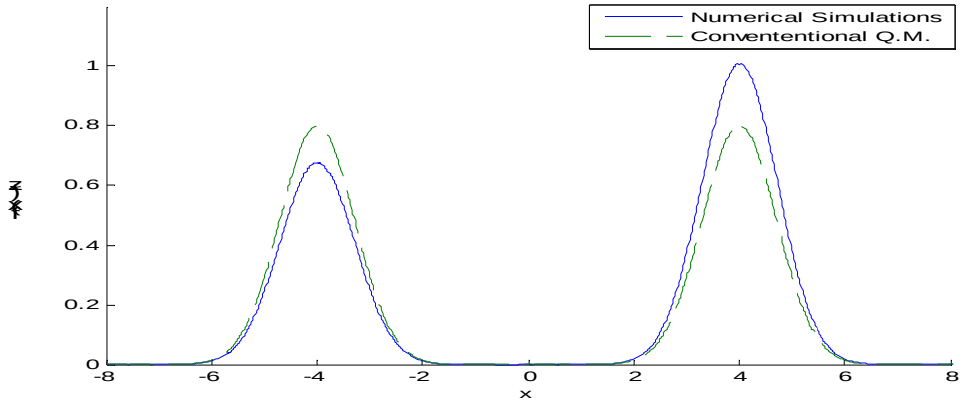
Fig.(1) Potential for a double oscillator [10].

n = 0 a =1200 q=4 cc=10^8 X =2 σ =0.1489 ρ=0.9757



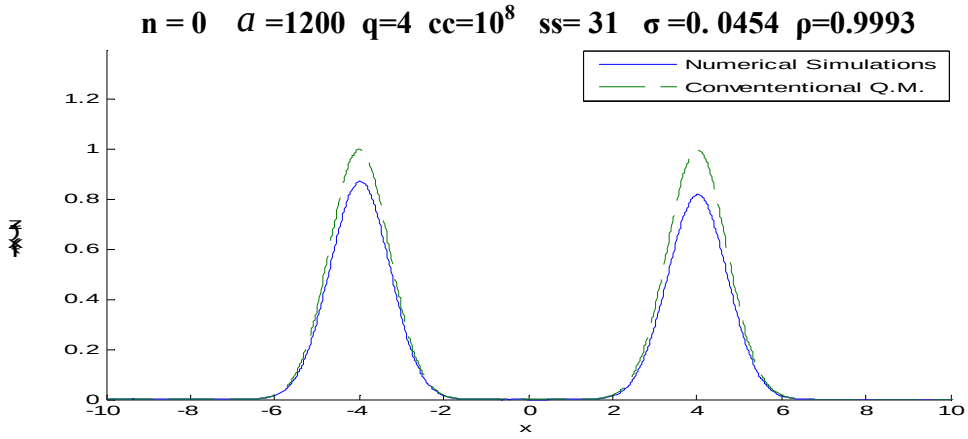
(a)

n = 1 a =1200 q=4 cc=10^8 x= 2 σ =0. 0558 ρ=0.9758

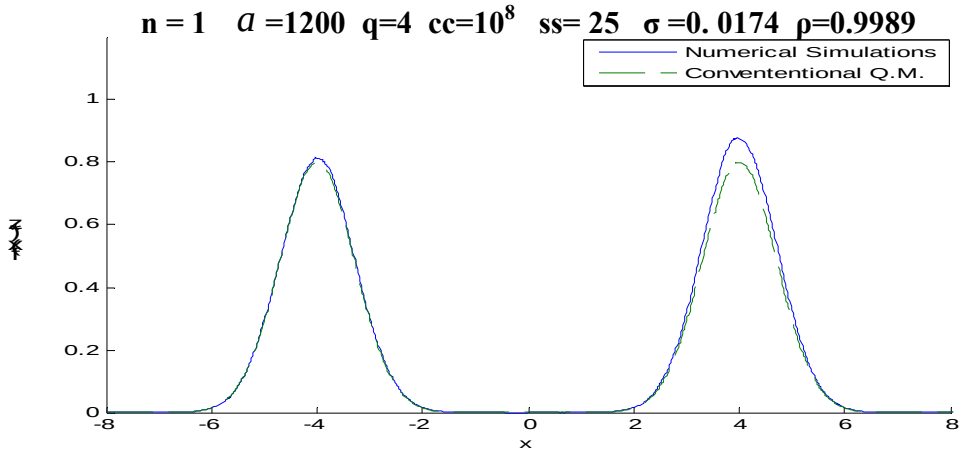


(b)

Fig. (2) Probability density for a particle in a double oscillators potential (a) n= 0 and (b) n= 1, without thermalization process.



(a)



(b)

Fig.(3) Probability density for a particle in a double oscillators potential (a) n=0 and (b) n=1 with thermalization process.

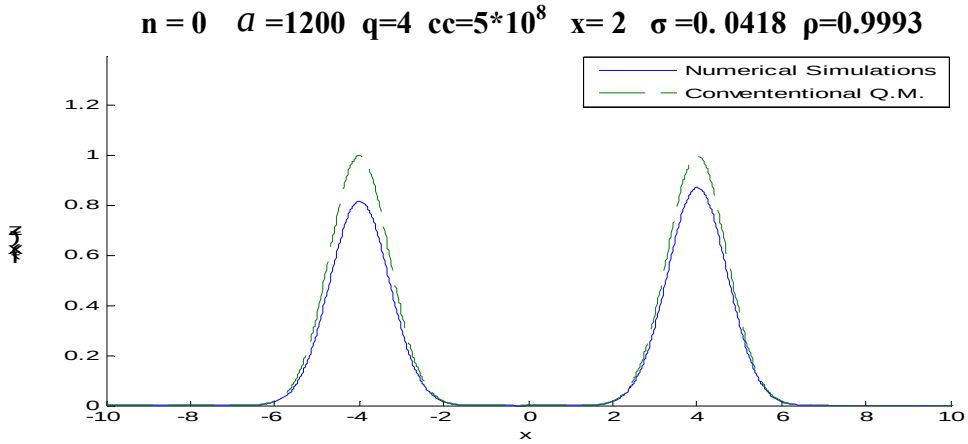


Fig. (4) Probability density for a particle in a double oscillators potential with n=0 for longer time steps ($cc=5\times10^8$).

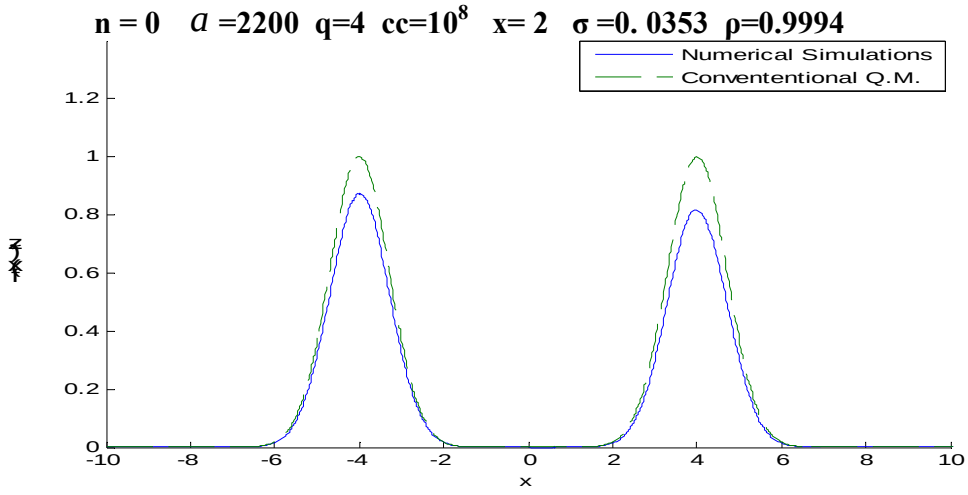


Fig. (5) Probability density for a particle in a double oscillators potential with n=0 after increasing the number of boxes.

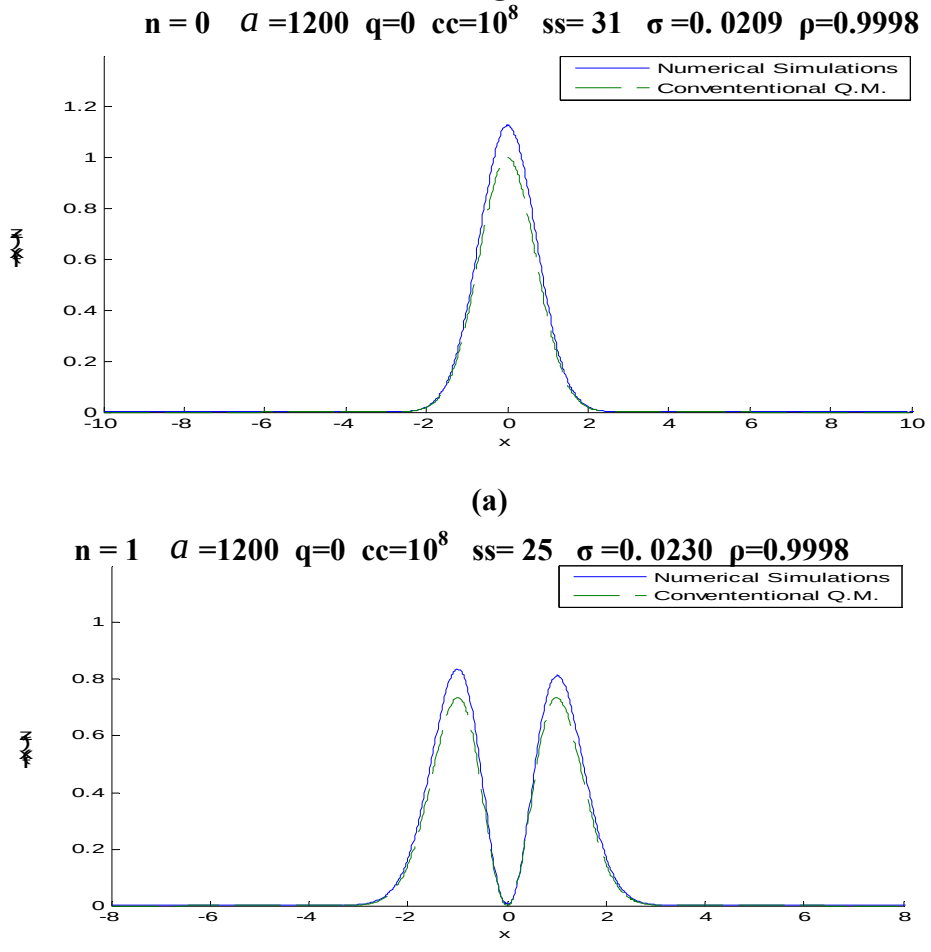


Fig. (6) Probability density for a particle in a double oscillators potential (a) n=0 and (b) n= 0 when q=0.

المحاكاة العددية لحركة جسيم في جهد توافقي ثنائي

سعيد نايف تركي الراشد

قسم الفيزياء – كلية التربية – جامعة الانبار

E-Mail : sntr2006@yahoo.com .

الخلاصة

تـم فـي هذا البحث توسيع عمل هيرمان والراشد لأنظمه كميه أخرى وهو حركة جسيم في جهد توافقي ثنائي ، وفي هذا الـنظام تم اخذ حاله خاصة والتي يكون فيها العدد التذبذبي الكمي (v) عدد صحيح غير سالب. فقد بني برنامج حاسوبي لغرض أجراء عمليه المحاكاة العددية لهذا النظام .كثافة الاحتمالية لهذا الجسيم تم حسابها عن طريق المحاكاة العددية من دون استخدام معادلة شرودينجر أو أي فرضية من فرضيات ميكانيك الكم، وتم مقارنه هذه الاحتمالية مع الاحتمالية التي تم الحصول عليها من ميكانيك الكم.