

“The Study Of Classical Chaos Using Quantum Mechanical Approach ”

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Abstract: The word chaos is the science of surprises of the nonlinear and unpredictable. It teaches us to expect the unexpected. In this chaos theory using mathematical equations we study the behaviour of dynamical system that are highly sensitive to initial condition. To study non linear behaviour of quantum H.H. Oscillator, equation of continuity and Euler equation can be used. The evolution of shanon entropy, density and amplitude correlations and kinetic energy exhibit non linear oscillations. Charge density and velocity potential can be used to study of nonlinear features.

Key words: Chaos theory, H.H. Oscillator, Velocity potential and charge density.

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I. Introduction

Quantum domain behaviour of a classically chaotic system has seen^{12,13,15,16} a great upsurge of interest in recent times. While the transition from regular classical behaviour to corresponding chaotic behaviour is well understood, the quantum mechanical analogue of this transition through a subject matter of research^{2,15} for some time is not quite clear. Coupled non-linear oscillators^{3,39} and kicked rotators^{1,30} are well studied in understanding their chaotic behaviour in the classical domain and of late their quantum domain analogues^{30,31} have been considered to be important. For example, the time dependent Schroedinger equation has been solved numerically for a quantum version of a Henon-Heiles oscillator,^{17-22,30,32-35}. The quantum chaotic behaviour has been characterized in one such study^{8,17} in terms of a correlation function, a phase space volume and an uncertainty product. However, the quantum domain regular or chaotic behaviour could not be correlated with corresponding behaviour in the classical domain. Since Schroedinger’s representation of quantum mechanics is essentially linear because the wave functions ought to obey the superposition principle we explore the possibility of a better vehicle in studying typical non-linear quantum systems. We propose to study the behaviour of a quantum system whose classical counterpart exhibits chaotic dynamics, using Madelung’s representation^{4,5,40} involving two fluid dynamical equations, viz., an equation of continuity and an Euler type equation of motion in terms of charge density $\rho(r,t)$ and current density $j(r,t)$. These equations are non-linear in $\rho(r,t)$ and $j(r,t)$. These two approaches (solution of QFD equations and TDSE) are complementary to each other. While TDSE focuses on properties calculable in terms of the many particle wave function, QFD makes use of $\rho(r, t)$ and $j(r,t)$ for that purpose. Results based on the solution of TDSE of this system are still not very convincing. The quantum domain behaviour of a Henon-Heiles oscillator within a quantum fluid dynamical framework is studied. Note that these equations do not contain additional information in comparison to the original Schroedinger equation but being non-linear may be a better vehicle for studying non-linear phenomenon. We do not intend to explicitly study “quantum chaos” but the quantum domain behaviour of a classically chaotic system which has been considered to be important in recent years^{6, 7, 13, 15, 16, 39}.

II. Quantum Fluid Dynamics of a Henon-Heiles System

Madelung⁴⁰ transformed the time dependent Schroedinger equation(TDSE) for a single particle with unit mass and \hbar scaled to unity, i.e.

$$\left[-\frac{1}{2}\nabla^2 + V \right] \psi = i \frac{\partial \psi}{\partial t} \quad \dots(1)$$

By expressing the wave function in the following polar form

$$\psi(r, t) = \rho^{\frac{1}{2}}(r, t) \exp[iX(r, t)] \quad \dots(2)$$

to two fluid dynamical equations, i.e., a continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad \dots(3a)$$

and an Euler-type equation of motion

$$\rho dv/dt = -\rho \nabla(V + V_{qu}) \quad \dots(3b)$$

In Equation (3), ρ is the charge density, v the velocity (current density, $j=\rho v$, $v = \nabla X$, X is the velocity potential), substantial derivatives $\frac{d}{dt} = \frac{\partial}{\partial t} + (v \cdot \nabla)$ and a quantum potential, $V_{qu} = -1/2\nabla^2 \rho^{1/2}/\rho^{1/2}$. The velocity potential X has been shown⁴⁰ to be related to Berry’s geometrical phase²³. Recently, Wallstrom¹⁴ has discussed some problem associated with the quantum potential that arises in Madelung’s representation. Unless otherwise specified atomic units are used throughout the paper.

Extension of the quantum fluid dynamical approach to many particle system is not straightforward. However, within the Hartree theory⁴¹, Hartree-Fock theory^{36,37} and in terms of natural orbitals²⁴ such an extension has been accomplished. Furthermore the formal equivalence^{25,26} of QFD and time dependent density functional theory (TDDFT) have been established. In , TDDFT any time dependent quantity in principle may be expressed as a function of time dependent charge and current densities.

The QFD equations for a quantum Henon-Heiles system take the following form:

$$\frac{\partial R}{\partial t} = -0.5 R \nabla^2 X - \nabla R \cdot \nabla X; \quad R = \rho^{1/2} \quad \dots \dots (4a)$$

$$\frac{\partial X}{\partial t} = \left(\frac{1}{2}R\right) \nabla^2 R - \frac{1}{2}(\nabla X)^2 - V_{cl} \quad \dots \dots \dots (4b)$$

Where the modified classical potential, V_{cl} is given by:

$$V_{cl}(x, y) = \frac{1}{2}(x^2 + y^2) + \lambda \left[x^2 y - \left(\frac{1}{3}\right) y^3 \right] \quad \dots \dots (4c)$$

The parameter λ introduced in Equation (4c) measures the degree of non-linearity (non-integrability as well) and is equal to unity for classical Henon-Heiles system. The QFD equations can be obtained as Hamilton’s equations of motion^{8,27,42} when the classical Hamiltonian is replaced by a properly chosen energy function of density functional theory (DFT) and one considers ρ and $(-X)$ as the canonically conjugate variables. Following Hamilton’s equations can be used in deriving Equation (4).

$$\frac{\delta H[\rho, X]}{\delta \rho} = \frac{\partial X_1}{\partial t} \quad \dots (5a)$$

and $\frac{\delta H[\rho, X]}{\delta X} = -\frac{\partial \rho}{\partial t} \quad \dots (5b)$

In Equation (5), X_1 is $(-X)$ and the Hamiltonian functional $H[\rho, X]$ is given by

$$H[\rho, X] = 1/2 \int \rho (\nabla X)^2 d\tau + 1/8 \int (\nabla \rho \cdot \nabla \rho) / \rho d\tau + \int V_{cl} \rho d\tau \quad \dots(6)$$

In Equation (6), the first term is the macroscopic kinetic energy (KE), second term refers to the intrinsic KE whose functional form was first suggested by Von Weizsacker⁴³ and the last term is the potential energy. QFD Equation (4) can also be obtained from a least action principle^{27,42}. The variational equation may be written in this case as:

$$\int_{t_1}^{t_2} L[\rho, X] dt = 0 \quad \dots (7a)$$

where the Lagrangian functional is given in terms of the above Hamiltonian functional as:

$$L[\rho, X] = \int \rho \left(\frac{\partial X_1}{\partial t} \right) d\tau - H[\rho, X] \quad \dots \dots (7b)$$

It is expected that important spatial and temporal characteristics of non-linear dynamical systems in quantum domain would be revealed through ρ versus $(-X)$ plots. The classical non-linear systems have been studied^{15,39} successfully with the help of phase-space plots of the trajectories represented in terms of two classical canonically conjugate variables, i.e. coordinate and momentum.

The motivation for using the QFD approach is that QFD equations being non-linear would perhaps turn out to be simpler in obtaining insights into a typical non-linear phenomenon. These equations do not manifest any unphysical non-linear behaviour if the actual dynamics is not non-linear²⁸. Another important aspect of using the QFD approach is its formal similarity with the classical fluid dynamics which may help in visualizing purely quantum phenomenon in terms of classical pictures.

In Equations 4(a) and (b), \hbar has been taken to be unity. However, in the classical limit where dynamical chaos appears, $\hbar \rightarrow 0$. In that case the first term on the right hand side of the equation of motion (EOM) Equation(4b) representing the quantum potential⁴⁴ vanishes and EOM is governed by classical forces only. In most of the studies of quantum domain behaviour of classically chaotic systems^{16,17,32,33} \hbar is scaled to unity. But it has been pointed out¹⁷ that classical domain behaviour is not indicative of regular or chaotic behaviour in a quantum Henon Heiles system. Actually this problem is associated with two dimensionless parameters, i.e., a classical parameter of non-linearity λ and a quantum parameter related to \hbar . Three physical constants, i.e., mass, length and frequency are required in order that Henon-Heiles Hamiltonian represents a complete model of a real non-linear system. So λ no longer represents the degree of non-linear coupling for motions along x and y directions but fixes the length scale because it is inversely proportional¹⁶ to length. Note

that in this case λ can assume any value that cannot be scaled¹⁶ to unity. The important point to mention here is that we can set the length scale $\lambda = 1$ and vary \hbar or we can set $\hbar = 1$ and vary λ to obtain similar results, i.e., lower energy levels approach those of uncoupled harmonic oscillators while higher energy levels in dicte chaos¹⁶.

III. Numerical Solution of QFD Equations

Numerical solution of the QFD equations is important as the number of non-linear partial differential equations solved numerically are much less in comparison to the corresponding number of non-linear ordinary differential equations¹⁰.

Equation (4) have been solved for two different λ values, i.e., $\lambda = 0.0$ (linear) and 0.05. In order to solve the set of Equation (4), mixed boundary conditions (Dirichlet conditions for R and Neumann conditions for X) are used, reflecting the physical fact that the probability density and fluid velocity vanish at the boundaries. An alternating direction implicit (ADI) finite difference scheme³⁸ has been adopted for numerically solving Equation (4). The initial and boundary conditions associated with this problem are as given below:

$$\begin{aligned}
 R(x, y, t = 0) &= 1/\sqrt{\pi} \exp[-0.5[(x - x_0)^2 + (y - y_0)^2]] \\
 x(x, y, t = 0) &= 0, \quad \forall x, y \\
 R(x, \pm\infty) &= 0, \quad \forall t, x \\
 R(\pm\infty, y) &= 0, \quad \forall t, y \\
 \partial X/\partial x(\pm\infty, y) &= 0, \quad \forall t, y \\
 \partial X/\partial y(x, \pm\infty) &= 0, \quad \forall t, x
 \end{aligned} \tag{8}$$

Each ADI cycle comprises four steps, i.e. (i) R is calculated at (n+1)th mesh point in time for all the spatial mesh points by solving the continuity Equation (4a) using R and X at the nth temporal mesh point and by replacing all x derivatives by Crank-Nicolson analogues and y derivatives by explicit scheme; (ii) equation in X at (n+1)th temporal mesh point is obtained using X at the nth mesh point in time, R obtained at the (n+1) temporal mesh point and replacing all the x-derivatives by Crank-Nicolson analogues and y – derivatives by their explicit finite difference forms. (iii) At this stage the terms of finite difference analogues for the directional derivatives are reversed, i.e., all derivatives along x direction are taken explicitly while derivatives along y axis are replaced by Crank-Nicolson analogues. In this step we obtained and solve the X equation to obtain X at the (n+2)th mesh point in time using R and X values at the (n+1)th temporal mesh point (iv). Finally R at the (n+2) th mesh point in time is obtained using values of R and X obtained at the (n+1) th and (n+2) th temporal mesh points respectively, with the finite difference analogues of the partial derivatives evaluated as in the step (iii). For each of these four steps of the ADI cycle discussed above we solve a set of finite difference equations. Let us consider the first step in the ADI cycle. At this step we obtain the following set of finite difference equations for any mesh point in time t and for a particular mesh point along y axis is

$$c_i R_{i-1,j}^{n+1} + a_i R_{i,j}^{n+1} + b_i R_{i+1,j}^{n+1} = d_i \tag{9}$$

where $i=1, \dots, x_{max}$ and $j = 1, \dots, y_{max}$, c, a and b are the coefficients with $c_1 = b_{x_{max}} = 0$ and x_{max} and y_{max} are the number of mesh points along x and y directions respectively.

Various coefficients at this step are as follows:

$$a_i = 1/\Delta t \tag{10a}$$

$$b_i = \frac{1}{2} \Delta x \left[\frac{\partial X}{\partial x} \right]^n \tag{10b}$$

$$c_i = -\frac{1}{2} \Delta x \left[\frac{\partial X}{\partial x} \right]^n \tag{10c}$$

$$d_i = \frac{R_{i,j}^n}{\Delta t} - \frac{1}{2} R_{i,j}^n \left[\left(\frac{\partial^2 X}{\partial x^2} \right)^n + \left(\frac{\partial^2 X}{\partial y^2} \right)^n \right] = - \left[\frac{\partial X}{\partial x} \right]^n \cdot \left[\frac{\partial R}{\partial y} \right]^n \tag{10d}$$

where the following central difference explicit FD analogues for different derivatives are used:

$$\left[\frac{\partial X}{\partial x} \right]^n = [X_{i+1,j}^n - X_{i-1,j}^n]/2\Delta x \tag{11a}$$

$$\left[\frac{\partial X}{\partial y} \right]^n = [X_{i,j+1}^n - X_{i,j-1}^n]/2\Delta y \tag{11b}$$

$$\left[\frac{\partial R}{\partial y} \right]^n = [R_{i,j+1}^n - R_{i,j-1}^n]/2\Delta y \tag{11c}$$

$$\left[\frac{\partial^2 X}{\partial x^2} \right]^n = [X_{i+1,j}^n - 2X_{i,j}^n + X_{i-1,j}^n]/(\Delta x)^2 \tag{11d}$$

$$\left[\frac{\partial^2 X}{\partial y^2} \right]^n = [X_{i,j+1}^n - 2X_{i,j}^n + X_{i,j-1}^n]/(\Delta y)^2 \tag{11e}$$

In Equatis (10) and (11), $\Delta x, \Delta y$ and Δt are the spatial (along x and y directions) and temporal mesh sizes respectively. The mesh sizes adopted are $\Delta x = \Delta y = 0.2$ au and $\Delta t = 0.0065$ au ensuring stability of the forward-time-central-space type numerical scheme adopted here.

Numerical stability and accuracy of the scheme used here have been checked through conservation of norm and energy as well as reproduction of the wave packet by propagating it up to the end of the simulation followed by its back evolution.

In order to understand the temporal evolution of a quantum Henon-Heiles oscillator we calculate different macroscopic quantities defined as follows;

- (a) Shanon entropy: The Shanon entropy is given by

$$S = -k \int \rho \ln(\rho) d\tau$$

where k is the Boltzman constant.

- (b) Density coerrelation: The density correlation is given by

$$C_d = 2\pi \int \rho(0)\rho(t)d\tau$$

- (c) Amplitude correlation: The amplitude correlation is given by

$$C_a = \int \rho^{\frac{1}{2}}(0)\rho^{\frac{1}{2}}(t)d\tau$$

and

- (d) Average kinetic energy: The average kinetic energy is given by

$$T = \frac{1}{2} \int \rho (\nabla X)^2 d\tau$$

The average KE defined above is different from the intrinsic KE of the system. Once we obtain the charge density and the velocity potential through the numerical solution of Equation (4) at different time steps, the time dependence of above quantities can be followed easily. The kinetic energy T defined here is the macroscopic kinetic energy arising out of the motion of the probability fluid. This motion takes place as a resultant of the quantum potential and the classical potential acting on the system. The zero average kinetic energy corresponds to the static stationary state²⁹.

IV. Results and Discussion

It is important to note that irrespective of the nature of V_{cl} (for zero or non-zero λ value), an initial zero velocity condition will start giving non-zero X in course of time.

In the linear case ($\lambda = 0.0$), barring the boundary regions almost all the contour lines are closed about the origin and exhibit reflection symmetry about both the axes as well as rotational symmetry. A reduction in symmetry is easily discernible as we move to the contous plots for the non-zero λ value. They reveal a definite loss of reflection symmetry about the $x - axis$ although this symmetry about the $y - axis$ although this symmetry about the $y - axis$ and the rotational tours in the case are open. As the quantum fluid velocity is expressed as $v = \nabla x$, qualitative idea of velocity field can be obtained from these contour plots. For the non-zero λ value, the contour plots of $(-X)$ exhibit different curvatures (both inward and outward with respect to the origin) and hence expected to generate irregular velocity patterns unlike in the linear case where always outward contours are obtained.

For the λ values considered here S does not exceed the initial value. However, it has been shown¹¹ that Shanon entropy becomes more than its initial value if λ is very high. It is observed that the S evolves in a periodic manner with a time period of approximately 240 time steps. At $\lambda = 0.05$ the nature of Shanon entropy curve changes. In place of the single amplitude oscillation there arises an oscillation with two different amplitudes. On comparison, it is found that in place of two time periods along the t axis for $\lambda = 0.0$ we now have three periods. Although the upper bound to Shanon entropy remains same [$k(1 + 1n\pi)$ in either case, its minimum value (S_{min}) increases for non-zero λ ($S_{min})(\lambda = 0.0) = 2.134526 k, \lambda = (S_{min})(\lambda = 0.05) = 2.134501 k$]. Since Shanon entropy measures the global randomness present, this indicates an increase in disorder with the introduction of non-linearity.

A slightly different correlation function²² defined as $|\langle \psi(0)\psi(t) \rangle|^2$ has shown¹⁷ temporal decay when the classical energy of the system has been increased. The average kinetic energy in the linear case has an oscillatory behaviour with a period of approximately 120 time steps. For the non-zero λ value is very conspicuous. For the non-zero λ value a clear transition from period two to period three behaviour is observed. The average kinetic energy (KE) T , studied here is the macroscopic KE of the probability fluid. The macroscopic KE arises from the resultant of the classical electrostatic force acting on the probability fluid of density $\rho(r, t)$ and the force originating from the quantum potential²⁹. In QFD framework the quantum mechanical KE appears in the form of a potential energy. When these two forces are exactly balanced, the macroscopic KE becomes zero since there is no fluid motion in that state. The system is then said to be in a

static stationary state ($v = 0, \partial\rho/\partial t = 0, \partial v/\partial t = 0$) in contrast to a dynamic stationary state, ($v \neq 0, \frac{\partial\rho}{\partial t} = 0, \frac{\partial v}{\partial t} = 0$).

The iterative one dimensional maps of probability density and velocity potential both measured at the origin are also studied. The velocity potential map does not exhibit any closed loop like structure and forms a straight line for the values of the non-linearity parameter λ used.

However a transition from period two to period three behaviour associated with non-zero λ value has been observed, i.e., in temporal evolutions of entropy, density and amplitude correlations and kinetic energy as well as in $\rho^n(0,0)$ versus $-x^n(0,0)$ plot, a global maximum (minimum) is replaced by a local minimum (maximum), almost around the same abscissa value, separated by two local maxima (minima).

V. Conclusion

The salient features of the results obtained from the present study of quantum fluid dynamics of Henon-Heiles oscillator may be summarized as follows:

(i) To our knowledge, QFD equations for this system have been solved here for the first time and the spatio-temporal behaviour of various quantities calculated here has not been considered before in this context. The numerical algorithm used here is new in the sense that the order of various explicit-implicit schemes and quasi-linearization of non-linearities in derivatives are tested here for the first time. The numerical scheme used here is stable and accurate because it conserves the norm and the energy and an initial wave packet is reproduced once propagated through 600 time steps and then back evolved.

(ii) The time dependent probability density ρ does not reveal any significant difference between linear and non-linear cases.

(iii) The negative of velocity potential ($-X$) shows prominent differences between the linear and non-linear cases. The presence of saddle points in the ($-X$) surfaces is indicative of possible unsteady flow of the probability current.

(iv) The variation of probability density ρ with the negative velocity potential ($-X$) shows a spread of the probability density over a range of $-X$ with the introduction of non-linearity to the system. It implies that more states are accessible to the system as we introduce non-linearity. To our knowledge, the consideration of ρ and ($-X$) as canonically conjugate variables and the study of their behaviour in this context has not been done before.

(v) Temporal behaviour of global quantities like Shannon entropy, amplitude correlation and density correlation functions and kinetic energy provides clear signs of the non-linearity for the non-zero λ value. The shift from period two to period three behaviour can be regarded as a signature of quasi periodicity with an increase in the non-linear perturbation.

(vi) A transition from period two to a period three behaviour is observed in ρ versus ($-X$) both measured at the origin at different times, when non-linearity is introduced in the system.

It is hoped⁹ that the quantum domain behaviour of a typical classical non-linear system like Henon-Heiles oscillator may be better understood within the purview of a quantum fluid dynamical framework as developed in the present study. It may lend important and hitherto unknown insights into “ the signatures of classical chaos in the quantum world” as has been discussed very recently by Jensen¹².

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