# Chapter 1

## Introduction

In this thesis the quantum dynamics of nonintegrable systems is studied using the quantum fluid dynamics (QFD)[1] and the quantum theory of motion QTM [2] as developed by de Broglie and Bohm in their causal interpretation of quantum mechanics.

This introductory chapter comprises five sections.Since the behaviour of nonintegrable systems in the quantum domain is intimately connected with the corresponding classical domain dynamics, we begin with the section dealing with the classical dynamics of integrable and nonintegrable systems.This is followed by the section reviewing certain important approaches to the study of chaos in quantum mechanical systems.The quantum fluid dynamics or the hydrodynamic formulation of quantum mechanics constitutes the third section, following which the quantum theory of motion or the causal interpretation of quantum mechanics is introduced.The fifth and final section discusses the principal motivation and objective of the present work.This section also summarizes the contents of the thesis.

### 1.1 Classical dynamics of integrable and nonintegrable systems

The exactly solvable systems in classical mechanics,usually referred to as "integrable" systems display motion which in a certain sense is well ordered and regular.The phase space trajectories of such systems are confined to certain well defined regions of phase space displaying certain symmetries and little or no change in behaviour with "small" changes in initial conditions.However,it has been found that introduction of a small but suitably chosen perturbation term to the original Hamiltonian of certain systems can make significant changes in their dynamic behaviour.While some measure of original regular motion may remain,there appears a regime of highly "irregular" motion where the trajectories become extremely sensitive to small changes in initial conditions and can move "erratically" over a large part of the dynamically (energetically) accessible

phase space.The dynamics is then regarded as chaotic and the system is considered to exhibit chaos.It should be noted that whereas chaotic dynamics may appear random without any obvious correlation between successive states of such a system,the dynamics nevertheless is strictly deterministic obeying the fundamental equations of classical mechanics.

The presence of chaos plays a very important role in different areas of physics and chemistry such as celestial motion or astronomy [3], accelerator physics [4],plasma physics [5], theories of chemical kinetics [6,7] and in a host of other related [8-13] disciplines.The study of nonintegrable and chaotic dynamics also has important implications in quantum mechanics [14].

In this section certain fundamental concepts of classical dynamics essential for the study of integrable and nonintegrable Hamiltonian systems are briefly introduced followed by short discussions on certain computational techniques employed to investigate integrable and nonintegrable systems.

### 1.1.1 Invariant tori and onset of chaos

A conservative Hamiltonian system of N degrees of freedom is considered for which $H(\mathbf{p},\mathbf{q})=E$.The state of the Hamiltonian system is described by N generalised momenta $\mathbf{p}=(p_1,....p_N)$ and the corresponding canonically conjugate coordinates $\mathbf{q}=(q_1,....q_N)$.The time evolution of the phase space coordinates $(\mathbf{p},\mathbf{q})$ is then determined by the equations of motion,

$$\dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} H(\boldsymbol{p},\boldsymbol{q}) \qquad (1.1.1a)$$

$$\dot{\boldsymbol{q}} = \nabla_{\boldsymbol{p}} H(\boldsymbol{p},\boldsymbol{q}) \qquad (1.1.1b)$$

If then the system has N single-valued analytic functions of $\mathbf{p}$ and $\mathbf{q}$, $f_i(\mathbf{p},\mathbf{q})$ such that the

Poisson bracket for any pair

$$\{f_i, f_j\}=0 \qquad i,j=1,....N \qquad (1.1.2)$$

then the system is exactly integrable [15,16] and the phase space trajectories can be shown to lie on manifolds with N-dimensional toroidal topology.

Introducing canonical coordinates referred to as the action-angle variables $(\mathbf{I},\theta)$ [17] if the Hamiltonian can be expressed in terms of N action coordinates $\mathbf{I}$ only, $\theta$ being the coordinate vector, then the Hamiltonian has the form

$$H=H(\boldsymbol{I}) \qquad \boldsymbol{I}=I_1,....I_N \qquad (1.1.3)$$

with the Hamilton's equations of motion as

$$\dot{\boldsymbol{I}}=-\nabla_{\theta}H(\boldsymbol{I})=o \qquad (1.1.4a)$$

$$\dot{\boldsymbol{\theta}}=\nabla_{I}H(\boldsymbol{I})=\boldsymbol{\omega}(\boldsymbol{I}) \qquad (1.1.4b)$$

where $\boldsymbol{\omega}(\mathbf{I})$ is the frequency vector $\boldsymbol{\omega}=[\omega_1....\omega_N]$. The preceding equations can be trivially integrated to obtain

$$I = constant \tag{1.1.5a}$$

$$\theta = \omega(I)t + \delta \tag{1.1.5b}$$

where $\delta$ is a set of arbitrary phases.Each element of the action vector specifies the position of an N-dimensional torus in the phase space and the conjugate vector of angle $\theta$ specifies the position of a trajectory on it.

Thus the problem of solving the original equations of motion (1.1.1) can be accomplished once a transformation to the action-angle variables can be found.This transformation can be generally obtained using the canonical perturbation theory [18,19] where essentially each of the generalised coordinates and momenta $q_1....q_N,p_1....p_N$ are expressed as a power series in all the new variables $I_1....I_N,\theta_1....\theta_N$.The unknown coefficients in the series are then obtained by substituting the series in $H(\mathbf{p},\mathbf{q})$ and the equations of motion (1.1.1).Equating those expressions to the equations(1.1.4) up to the lowest order terms in $\mathbf{I},\theta$ the lowest order coefficients can be found.The process is repeated again to find the higher order coefficients to obtain a series.A system is then regarded as integrable if this series is convergent.Such series were examined in detail by Birkoff [20,21] who studied the conditions for their existence and are referred to as the Birkoff series.

For integrable systems defined by equations (1.1.5) the angle variables are seen to be periodic in $2\pi$ because of the toroidal topology of the manifold on which such trajectories lie.Accordingly the motion can be expressed in terms of a finite Fourier series as follows

$$q(t)=\sum_{n} a_n(I)\exp(in.\Theta(t))=\sum_{n} a_n(I)\exp(in.(\omega t+\delta)) \qquad (1.1.6a)$$

$$p(t)=\sum_{n} b_n(I)\exp(in.\Theta(t))=\sum_{n} b_n(I)\exp(in.(\omega t+\delta)) \qquad (1.1.6b)$$

where $\mathbf{a_n(I)}$,$\mathbf{b_n(I)}$ are N-dimensional vectors of Fourier coefficients each component being labelled by an N-dimensional vector **n** of indices.The dynamics in such cases are referred to as quasiperiodic.The motion of a particle on an invariant torus characterized by the action **I**=constant and the frequency vector $\omega(\mathbf{I})$ is defined uniquely when the components of the frequency vector are functionally independent.The system is then considered to be a nondegenerate one with the nondegeneracy condition being given as follows

$$\det\left|\frac{\partial\omega_i(I)}{\partial I_i}\right|=\det\left|\frac{\partial^2 H(I)}{\partial I_i I_j}\right|\neq 0 \qquad (1.1.7)$$

In general the set of frequencies $\{\omega_i\}$ i=1....N are incommensurate and the trajectory covers the entire torus and is open in that it can never close on itself.However, it may so happen that the frequency components loose their functional independence so that the following relation holds

$$\sum_{i=1}^{N} m_i\omega_i=0 \qquad (1.1.8)$$

for a certain set of integers $\{m_i\}$ i=1....N.Under such condition the trajectory is said to be in resonance and the system is considered to be degenerate.It has been shown by Walker and Ford [22] that the existence of two or more resonant frequencies corresponding to

more than one pair of degenerate trajectories on the invariant torus can give rise to a divergent Birkoff series [18] with the introduction of an external perturbing Hamiltonian.Under this condition the system loses its integrability and the invariant torus with the resonant trajectories is broken up in the sense that there are no longer any well defined action vectors determining the torus.The phase trajectories of such destroyed tori contains elliptic and hyperbolic fixed points in their neighbourhood.The elliptic fixed points correspond to stable periodic (closed) orbits and is surrounded by smooth curves corresponding to "higher" order tori which may be intact.The hyperbolic fixed points correspond to unstable periodic (closed) orbits and the neighbouring phase space becomes dense with the so called homoclinic points [3,16,23]. The phase space trajectories near homoclinic points are extremely complicated and takes on an apparently random character signifying chaos.In such regions of the phase space any infinitesimal change in initial conditions of a trajectory can give rise to completely different motion uncorrelated to its original dynamics.It has been observed that in such cases effects of the order 1 may result from initial changes of the order $10^{-16}$ in a short time [24,25].

It has been shown by Seigel [26] that for randomly chosen analytic Hamiltonians with $N \geq 2$ the nonintegrable Hamiltonians are densely distributed among all analytic Hamiltonians.Further it has been observed [27 ] that the integrable Hamiltonians are not similarly dense everywhere, so that the dynamics of an integrable system perturbed with a small nonintegrable term in the Hamiltonian assumes great significance in the study of transition from integrable to nonintegrable dynamics.The theorem of Kolmogorov,Arnold and Moser [15-16,28-29] is of vital importance for such perturbed integrable Hamiltonian systems.Essentially the theorem states that for extremely small strength of the nonintegrable perturbations the erstwhile smooth invariant tori corresponding to the integrable system undergoes certain distortion but retains its toroidal structure, so that the phase space trajectories of the perturbed system are still constrained to lie on the tori albeit distorted now termed as the KAM tori.This implies that the transition from integrability to nonintegrability is not a sharply defined process in the sense that for sufficiently small values of perturbation, the trajectories do retain certain "integrable"

characteristics .However, for sufficiently strong perturbation the KAM tori break up and the trajectories are free to wander over the accessible phase space,the latter being now covered with the homoclinic points giving rise to extreme sensitivity to initial condition signifying chaos.

### 1.1.2 Techniques for studying nonintegrable dynamics

A. Surface of sections and return maps

The concept of surface of section was first introduced by Poincaré to study the essential characteristics of a phase space trajectory in a convenient form.For conservative Hamiltonian systems with two degrees of freedom the energy is a conserved quantity and the Hamiltonian is then an isolating integral of motion and can be written as

$$H(p_1,p_2,q_1,q_2)=E \tag{1.1.9}$$

where the energy E is constant and restricts the trajectories to lie on a three dimensional surface within the four dimensional phase space.Equivalently one of the generalised momenta components can be expressed as

$$p_2=p_2(p_1,q_1,q_2,E) \quad . \tag{1.1.10}$$

If now the system possesses another integral of motion

$$I_2(p_1,p_2,q_1,q_2)=C_2 \tag{1.1.11}$$

where $C_2$ is a constant then it too defines a three dimensional surface.Since for specific initial conditions E and $C_2$ are fixed the phase space trajectory will be constrained to move on the two dimensional surface of intersection of the two constant surfaces which is the toroidal surface.Combining equations (1.1.10) and (1.1.11) $\mathbf{p}_1$ can be written as

$$p_1 = p_1(q_1, q_2, E, C_2) \quad . \tag{1.1.12}$$

If now the intersection of this two dimensional surface is considered with the surface, say $q_2=0$ a one dimensional curve is obtained which is nothing but a mapping of the phase space trajectory on the surface $q_2=0$.This is a method of obtaining a two dimensional mapping of a four dimensional phase space trajectory is referred to as the Poincaré mapping or the method of Poincaré surface of section.This method is applied to determine whether a Hamiltonian system has any integral of motion.The Hamilton's equations are solved numerically for specific energy values and a pair of coordinates $(p_2,q_2)$ may be plotted for $q_1=0$ and $p_1>0$ to have a surface of section mapping of the trajectory.For nondegenerate integrable systems, because the trajectories lie on the toroidal surface,the plot so obtained is a one dimensional curve while for a trajectory with commensurate frequencies the mapping displays a number of fixed points which are always mapped unto themselves.The situation is significantly changed in absence of integral of motion.For systems having a small amount of nonintegrability obeying the KAM theorem the curves obtained are conspicuously distorted reflecting the KAM tori.However,for higher values of energy of such systems with the increasing nonintegrability the KAM tori are broken and instead of smooth curves the surface of section displays a random scatter of points heralding the onset of chaos.

While the surface of section of Poincaré requires the solution of the relevant Hamilton's equation be obtained,the essence of the dynamics behind an evolving system can be studied from the time series of a single dynamical variable as well [31].If z(t) be the time dependent variable sampled at a time interval $\tau$ we have the following time series

$$z_0 = z(0), z_1 = z(\tau), \ldots z_n = z(n\tau) \tag{1.1.13}$$

and a certain sequence of n dimensional vectors can be formed as follows,

$$\begin{matrix}(z(0),z(T)....z(nT))\\(z(\tau),z(\tau+T)....z(\tau+nT))\\.\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\\(z(k\tau),z(k\tau+T)....z(k\tau+nT))\end{matrix} \qquad (1.1.14)$$

where T represents a time delay which is chosen to be an integral multiple of τ.Such a sequence of vectors may be plotted conveniently for n=2 or n=3 to give a phase plot of the dynamics.This procedure would be strictly valid for systems with two or three degrees of freedom whereas for systems with higher degrees of freedom a projected plot will be obtained.This construction is referred to as the return map for obvious reasons.

B. Spectral properties

For a Hamiltonian system with quasiperiodic trajectories, the Fourier transform reveals a finite number of discrete lines.The trajectories with incommensurate frequencies also display a finite spectrum [32].However. in chaotic systems the Fourier transform of trajectories reveals a dramatic difference with a very "grassy" and almost continuous spectrum [33].But the spectral analysis of trajectories have a limitation in that both deterministic chaos and random signals produce the similar continuous spectra making a distinction between them difficult.

C. Lyapunov exponent and Kolmogorov-Sinai entropy

Trajectories in the chaotic region of the phase space for a nonintegrable system are extremely sensitive to initial conditions.Trajectories which are infinitesimally close to one another separate rapidly and proceed in a completely independent manner.For chaotic systems there exist certain directions along which such trajectory separation evolves exponentially in time.

If the continuous motion of a dynamical system is discretized and if the motion can be obtained as a mapping $\hat{T}$ of the state vector **z** defining a phase point then we have

$$z_{n+1}=\hat{T}z_n \qquad (1.1.15)$$

where n is the discrete time index.The Jacobian matrix M of the mapping T is defined as

$$M_{ij,n}=\frac{\partial x_{i,n+1}}{\partial x_{j,n}} \qquad (i,j=1....N) \tag{1.1.16}$$

where N is the degrees of freedom for the Hamiltonian system considered. For a Hamiltonian system phase volume of the system is a conserved quantity so that $|M|=1$ at all times. Diagonalization of the matrix M yields a vector of 2N eigenvalues $\sigma$ which are in general complex valued.Arranged in ascending order of absolute values

$$|\sigma_1| \le |\sigma_2| \le .... \le |\sigma_k| \le .... \le |\sigma_{2N}|$$

where all eigenvalues up to and including the kth one have absolute values less than unity.Then there are 2N-k number of eigenvalues with absolute values greater than or equal to unity and correspondingly there are 2N-k eigenvectors defining 2N-k directions along which the state vector z is stretched in length.Therefore along these directions an element of phase volume undergoes expansion and consequently there are contractions of the volume element along the remaining k directions.The Lyapunov exponent [34-37] is defined as

$$\lambda_i = \ln|\sigma_i| \quad . \tag{1.1.17}$$

After n mappings a state vector will be stretched in a particular direction as

$$z_i(n) - z_i(0)\exp(\lambda_i n\,\tau) \qquad (1.1.18)$$

$\tau$ being the time step.If $|d|$ be the initial infinitesimal separation (Euclidean norm) between two trajectories and $|d_i|$ be the subsequent separation then it has been shown [37 ] that the largest Lyapunov exponent may be obtained as

$$\lambda_{max} - \lim_{n\to\infty}\sum_{i=1}^{n} \ln\frac{|d_i|}{|d|} \quad . \qquad (1.1.19)$$

The computation of Lyapunov exponent is one of the easiest ways of identifying both qualitatively and quantitatively the nature of dynamics of a classical system with positive values signifying an extreme sensitivity to initial conditions thus identifying the presence of chaos.

The existence of positive Lyapunov numbers for a dynamical system has significant effect on an element of phase volume $\Delta\Gamma(t)$ of a system.In such cases because of the exponential separation of trajectories, the phase volume element soon acquires a very complicated tangled structure.If the dynamically accessible phase space of the system is considered to be permeated with a phase fluid then such a fluid may be considered to have undergone a thorough mixing with the empty phase space.However, since in Hamiltonian systems the phase volume is conserved a concept of a coarse phase volume $\Delta\Gamma'(t)$ is introduced which gives the effective volume of the phase element.This coarse phase volume may now include the empty phase space within it as cavities so that we have $\Delta\Gamma'(t) > \Delta\Gamma(t)$ because of the mixing of the phase volume element as a consequence to the chaotic dynamics of the system.The Kolmogorov-Sinai entropy is then calculated as

$$h = \ln \Delta\Gamma'(t) \quad , \tag{1.1.20}$$

The Kolmogorov-Sinai entropy is related [39] to the positive Lyapunov exponents as

$$h = \sum_{\lambda>0} \lambda \quad . \tag{1.1.21}$$

## 1.2. Nonintegrability and chaos in quantum systems

The role of nonintegrability and chaos in quantum systems has gained importance in recent years.Since the concept of integrability and the whole edifice of dynamics in general is firmly grounded in classical mechanics, the study of quantum chaos has refocussed attention on to the classical correspondence of quantum mechanics.Therefore in the study of nonintegrability and chaos in quantum systems the semiclassical quantization of classical systems holds a significant position.So this discussion on chaos in quantum systems begins with the method of semiclassical quantization.

### 1.2.1 Semiclassical quantization rules

It was Neils Bohr who first proposed certain quantization rules to modify the classical mechanics to arrive at an expression for obtaining the energy levels of the Hydrogen atom.This was superseded by the wave mechanics.Prior to that, the Bohr quantizaton rules were generalized by Sommerfeld and others for application to other systems like the helium atom.However, this approach was unsuccessful for such complex systems.

It was pointed out by Einstein [40] that only classical systems with invariant phase space tori could possibly be quantized by the Bohr-Sommerfeld quantization rules.According to him systems without well defined phase space tori could not be quantized using those rules.

The best known semiclassical approximation for the eigenvalues of a quantum system within the ambit of Schrödinger wave mechanics have been provided by Wentzel-

Kramers-Brillouin (WKB) method [41].The basic idea is to solve Schrödinger's equation by substituting an ansatz for the wavefunction in the form

$$\psi(q)=A(q)\exp(iS(q)/\hbar) \tag{1.2.1}$$

where terms $o(\hbar^2)$ in S(q) are ignored and $\psi$ is required to decay exponentially in classically forbidden regions.Near the classical turning points in q the ansatz is to be replaced by the actual expression of the wavefunction.Asymptotic expansion of the exact wavefunction then enables connection between classically allowed and forbidden regions.The result for all turning points are combined to finally obtain a quantization condition ,

$$\frac{1}{2\pi}\oint p(H,q)dq=(n+\frac{1}{2})\hbar \quad . \tag{1.2.2}$$

For completely integrable motion the canonical coordinates can be transformed to action-angles variables so that for a given value of the action vector $\mathbf{I}=(I_1,.....I_N)$ the components defined as

$$I_i=\frac{1}{2\pi}\oint_{C_i} p dq \qquad\qquad i=1....N \tag{1.2.3}$$

where $C_i$ are the N topologically independent contours on the N-dimensional torus associated with **I**.The Einstein-Brillouin-Keller quantization rule [42 ] allows a bound state to be associated in the semiclassical limit with the torus whose action then satisfy the quantization rule

$$I_m=(m+\frac{\alpha}{4}) \qquad (1.2.4)$$

where **m** is the vector of quantum numbers and $\alpha$ represents the vector of Maslov indices [ 43 ].These refer to the number of classical turning points along the paths $C_i$.The energy of the nth state is then obtained as

$$E_m=H(I_m) \qquad (1.2.5)$$

for an integrable Hamiltonian.

The salient feature of Keller's treatment of wavefunctions obtained from the invariant tori is that it allows one to draw parallels with classical mechanics and proceed on to weakly chaotic situations where the classical KAM theorem allows the presence of distorted KAM tori.The KAM theorem ensures that the transition from integrable to chaotic regime is in general a continuous process with a close coexistence of invariant tori and chaotic regions being the prominent feature in this transition region.So using Kellers's idea quantum mechanics can be considered to retain its classical correspondence into such weakly nonintegrable systems.

This idea of classical correspondence for weakly nonintegrable systems has been successfully used by Delos and Swimm [44] relying on the fundamental work done by Gustavson [45] and Birkoff [46].The basic philosophy is to examine the motion of a dynamical system in the neighbourhood of a point of stable equilibrium.The Hamiltonian is expanded in the momentum and position coordinates about the point so that the kinetic energy is quadratic in momenta and the potential energy term is expanded in powers of position coordinates about the point of equilibrium.The lowest term then has a quadratic form in position coordinates.The Hamiltonian is diagonalized by appropriate linear orthogonal transformation and with the additional transformations $p=p/\sqrt{(m\omega)}$ and $q=q\sqrt{(m\omega)}$ the original Hamiltonian is obtained as a series

$$H=\sum_{k=1}^{n}\frac{\omega_k}{2}(p_k^2+q_k^2)+H^{(3)}(p,q)\ .....\qquad (1.2.6)$$

where $H^{(i)}$ (i=1..r ) is a homogeneous polynomial of ith degree in p and q.The aim is to express $H^{(i)}$ as a function of the variables $\rho_k=(p_k^2+q_k^2)/2$ ,thus reducing the partial Hamiltonians $H^{(i)}$ to its normal form.The above procedure is equivalent to finding n new approximate constants of motion in suitably transformed coordinates.Finally transforming back to original coordinates a number of integrals of motion equal to the number of degrees of freedom are found.As in general the normalization procedure does not necessarily converge the series given by equation (1.2.6) has to be truncated.Swimm and Delos [47] carried out this procedure for Hamiltonians of Hénon-Heiles type [30 ] and a truncation at the eighth order was regarded sufficient.

The quantization of the Henon-Heiles system worked out by Swimm and Delos [47 ] with the EBK rules [42] then require that

$$\rho_k=(p_k^2+q_k^2)/2=(n_k+\frac{1}{2})\hbar\qquad (1.2.7)$$

where $n_k\geq 0$, the 1/2 corresponds to a Maslov index [43] of value 2 for each degree of freedom.

The energy level spectrum is then obtained as

$$E(n_1,n_2..)=H'((n_1+\frac{1}{2})\hbar,(n_1+\frac{1}{2})\hbar,....)\qquad (1.2.8)$$

where H' is the Hamiltonian after transformation to the normal form and truncation at a suitable term.It has been observed [47 ] that for the third order perturbating potential term

$$H^{(3)}=\lambda q_2(q_1^2+\eta q_2^2) \qquad (1.2.9)$$

where $\lambda$= -0.1,$\eta$=0.1 and incommensurate frequencies $\omega_1$=1.3 and $\omega_2$=0.7 the maximum error when compared with results obtained from exact quantum mechanical approach do not exceed 0.5% for the 82 bound level states out of the 83 levels computed from solving the Schrödinger's equation.

An alternative way of applying the EBK rules is to use the multiperiodic behaviour of the classical trajectories.Since according to equation (1.1.6) the coordinates of a classical trajectory can be expanded in a Fourier series with the number of component frequencies equalling the number of degrees of freedom,the classical quantization rules can be applied to these frequencies without the necessity of identifying the supporting invariant tori.This idea has been applied by Marcus and his co-workers [33,48,49] and a few examples were treated numerically [50 ].The principle feature in this approach is the evaluation of the approximations to the energy levels of a conservative Hamiltonian system from the frequency spectrum of the integrable trajectories of that system.By numerical trials a function $E(\omega_1,....\omega_n)$ is obtained giving the energy of the classical trajectories whose frequencies are $\omega_1,....\omega_n$.To obtain the Hamiltonian $H(I_1,....I_n)$ as a function of the action integrals it is noted that H(**I**) is not uniquely determined by the function $E(\omega)$.For each component vector in the frequency ($\omega$) space the values of the corresponding actions have to be obtained independently.Marcus and his co-workers tackled this problem by selecting initial conditions for the perturbed system which satisfy the EBK conditions for action integrals in the integrable (unperturbed) system.The action integrals then become fixed uniquely allowing the energy levels to be computed by the discrete values of $H((n_1+1/2)\hbar,(n_2+1/2)\hbar,....)$ in terms of the quantum numbers

$(n_1,n_2)$. The energy levels calculated for the Hénon-Heiles system in equation (1.2.9) are found to be in excellent agreement with that in the exact quantum calculations.

### 1.2.2 Energy level statistics and quantum chaos

The energy level statistics was first introduced by Wigner [ 51 ] to formulate a general theory that could describe the features of nuclear energy levels following certain ideas of Dyson [ 52 ] regarding the nature of the matrix elements of the Hamiltonians of complex nuclei. According to Wigner the matrix elements are not analyzable in detail and a statistical approach was called for.

If the level spacing distribution P(s) is defined so that P(s)ds is the probability of finding the spacing between any two neighbouring energy levels in the interval s and s+ds then the Wigner distribution of energy level spacings in terms of the average spacings is obtained as

$$P_W(s)=\frac{\pi s}{2D^2}\exp^{-(\pi s^2/4D^2)} \quad . \qquad (1.2.10)$$

The energy levels for a random Hamiltonian matrix are correlated exhibiting level repulsion. However, for a random distribution of energy levels it is found that the level spacing distribution has the form of a Poisson distribution

$$P_P(s)=\frac{1}{D}\exp^{-(s/D)} \qquad (1.2.11)$$

where once again D is the average energy level spacing.

The fundamental problem of the random matrix theory [53 ] is then the setting up of a normalized probability distribution on the elements of the Hamiltonian matrix which should retain its norm under similarity transformations. Based on the nature of the Hamiltonian under consideration viz., real symmetric, hermitian and real quaternion the

probability distributions represent Gaussian Orthogonal Ensembles (GOE ) or the Wigner distribution,Gaussian Unitary Ensembles (GUE ) and the Gaussian Symplectic Ensemble (GSE ) respectively.

It has been suggested [14] that in the semiclassical limit as in the classical mechanics an integrable system undergoing a transition to chaotic regime loses the constants of motion accordingly in the quantum domain analogue the quantum numbers defining the quantum dynamics lose their significance.Under this condition, the level spacing statistics could be applied to study the transition to chaos in the quantum domain.The level spacing statistics first applied by Berry and Tabor [54] for studying integrable systems in the quantum domain was observed to exhibit a Poisson-like distribution.

The first direct evidence of manifestation of chaos through spectral properties of energy levels was obtained by McDonald and Kaufman [55] in their studies on integrable and nonintegrable billiards.It was found that an integrable billiard displayed maximum probability of small spacings while a nonintegrable billiard exhibited a certain evidence of level repulsion signifying a presence of correlation between energy levels.This observation essentially mirrors the Poisson distribution and the Wigner distribution of energy levels in the integrable and nonintegrable chaotic domains respectively.This fact has been further confirmed for the nonintegrable Sinai billiard [56] which exhibits [57] a $\Delta_3$-statistics [58] close to that of the GOE (Wigner distribution), while an integrable billiard was found to display a level spacing statistics following the Poisson distribution [59,60].However,a rectangular incommensurate billiard which is classically integrable was found to have large fluctuations away from Poisson distribution for small level spacings [59]. This was shown to be specific [61] for square well potentials.

Corresponding to the transition from regular integrable to chaotic motion in classical dynamics the spectral statistics of the energy levels show a shift from the poisson statistics to the Gaussian Ensemble statistics.Rigorous analyses have been carried out by Pechukas [62 ], Yukawa [63 ] and Nakamura with his coworkers [64 ].A set of 'equations

of motion' for a nonintegrability parameter λ has been obtained from Schrödinger eigenvalue problem [64].The equations of motion so derived has been shown to be equivalent to those of a completely integrable N-particle Calogero-Moser system with an internal complex vector space.

Numerical computations of the transition of spectral statistics have been carried out by Seligman and co-workers [65] who have made a detailed study of a system with the Hamiltonian

$$H=1/2(p_1^2+p_2^2)+V_1(x_1)+V_2(x_2)+V_{12}(x_1-x_2) \qquad (1.2.12)$$

where $V_i(x)=V_i(\alpha_i x^2+\beta_i x^4+\gamma_i x^6)$ i=1,2,12 with the system being integrable for $V_{12}=0$.This model has been studied in regular as well as chaotic regime.The spectral levels were found to change from Poisson to Wigner distribution (GOE) reflecting the change in the corresponding classical dynamics.A coupled Morse oscillator in integrable and chaotic regimes has been found [66] to display a similar transition in the energy level statistics.In this case the nearest neighbour level spacing histograms were fitted to a Brody distribution [67] which is a single parameter function obtained by interpolation between Poisson and Wigner distributions.

Recently highly excited Hydrogen and Hydrogen-like atoms (which are effectively single electron systems) subjected to external electric and magnetic fields,have provided excellent case studies for understanding different aspects of quantum chaos.With the advent of tunable lasers such atoms can be excited to Rydberg states [68 ] making the conditions for investigating chaos in such systems experimentally feasible.A large number of experimental and theoretical investigations have been carried out [68-74].A Hydrogenic Rydberg state atom subjected to an oscillating electric field has been studied [69] revealing transition from regular to chaotic behaviour depending on the field strength and frequency.The quadratic Zeeman effect for a Rydberg state atom has been investigated [74 ]experimentally and theoretically [68,70,71,75 ].It has been found that for

such systems the electron motion is regular for weak magnetic fields, the corresponding energy spectrum following the Poisson distribution for level statistics.With increasing magnetic field strengths a smooth transition to chaotic motion is reflected by a shift to the GOE statistics exhibited by the energy level spacings.For the transition regime corresponding to intermediate field strengths the level spacing statistics follow a statistics that is intermediate to the Poisson and Wigner (GOE ) distributions.

A related model for the study of quantum chaos is a Hydrogen atom in a van Waals interaction potential.The interaction is expressed [72,76 ] by the Hamiltonian

$$H=\frac{p^2}{2}-\frac{1}{\gamma_i}(x^2+y^2+2z^2) \qquad (1.2.13)$$

where $\gamma_i = 1/(16d^3)$,d being the separation distance between two atomic dipoles whose interaction gives rise to the van der Waals (induced dipole-dipole ) interaction.This system has been generalized [77 ] to obtain a generalized Van der Waals interaction Hamiltonian

$$H=\frac{p^2}{2}-\frac{i}{\gamma}+\gamma(x^2+y^2+\beta^2z^2) \qquad (1.2.14)$$

which covers different systems for appropriate choices of adjustable parameters [78] $\gamma$ and $\beta$.Such a system has been treated as two coupled anharmonic oscillators .The system displays [79 ] successive chaos-order-transitions for increasing values of $\beta$ parameter for arbitrary $\gamma$.The corresponding quantum system has been treated [80 ] to obtain the energy level spacings which displays a sequence of level spacing statistics [81] with increasing $\beta$ values mirroring the classical dynamics.

### 1.2.3 Semiclassical path integral quantization

Feynman derived an expression for the quantal propagator as an integral over classical paths, of terms involving functions of classical actions [82].As the classical

propagator theory involves eigenfunctions and density of classical states , a connection between classical paths and quantum eigenvalues was expected to be existent.This idea was first pursued by Gutzwiller [83-86] and Balian and Bloch [87-90].Various aspects of the path integral approach as applied to integrable systems have been discussed by Voros [91] and Berry and Tabor [54,92].

To arrive at the semiclassical approximation to the propagator , the Feynman propagator is expressed as an eigenfunction expansion.If $\hat{H}$ be the Hamiltonian, $E_n$ be the energy eigenvalues and $\Phi_n$ be the corresponding eigenfunctions the propagator $K(\mathbf{q}',\mathbf{q},t)$ is given by

$$K(q',q,t)=\sum_n \exp^{-iE_n t/\hbar}\phi_n^*(q')\phi_n(q) \qquad (1.2.15)$$

The Laplace transform to the energy domain is then the energy Green's function

$$G(q',q,E)=\frac{1}{\pi\hbar}\int_0^\infty \exp(iEt/\hbar)K(q',q,t)dt \qquad (1.2.16)$$

which is defined for Im(E) >0 and has the final form

$$G(q',q,E)=\frac{i}{\pi}\sum_n \frac{\phi_n^*(q')\phi_n(q')}{E-E_n} \quad . \qquad (1.2.17)$$

Applying the identity

$$\lim_{\varepsilon\to 0}\left(\frac{1}{E-E_0+i\varepsilon}\right)=P\left(\frac{1}{E-E_0}\right)-i\pi\delta(E-E_0) \qquad (1.2.18)$$

where P stands for Cauchy's principal value,the Green's function can be expressed as

$$Re\, G(q',q,E)=\sum_n \phi_n^*(q')\phi_n(q)\delta(E-E_n) \quad . \tag{1.2.19}$$

The density of energy states ρ(E) is obtained by equating **q'**=**q** and integrating over **q** to yield

$$\rho(E)=\sum_n \delta(E-E_n) \tag{1.2.20}$$

for a system with Hamiltonian $\hat{H}$.In the propagator formalism ρ(E) is expressed as

$$\rho(E)=Re\frac{2}{\pi\hbar}\int_0^{\infty} dt\, \exp(iEt/\hbar)\int d^N q K(q,q,t) \quad . \tag{1.2.21}$$

The Feynman representation of the propagator is

$$K(q',q,t)=\int D[q]\exp\left(\frac{iS(q',q)t}{\hbar}\right) \tag{1.2.22}$$

where **S(q',q,t)** is the classical action along a path **q**(τ),**p**(τ) satisfying the boundary conditions **q**(0)=**q** and D[**q**] indicates integration over all such classical paths satisfying the boundary conditions.A stationary phase approximation of equations (1.2.22) then yields the semiclassical approximation to the Feynman propagator, with the second variation of S introducing the determinantal Jacobian amplitude

$$D(q',q,t)=\det\left(\frac{-\partial^2 S}{\partial q'\partial q}\right) \quad . \tag{1.2.23}$$

The semiclassical approximation then has the following general form

$$K_{sc}(q',q,t)=\frac{1}{(2i\pi\hbar)^{N/2}}\sum_{n}|D_n|^{\frac{1}{2}}\exp\, i\left(\frac{S_n}{\hbar}-\frac{\alpha_n\pi}{2}\right) \qquad (1.2.24)$$

where n indexes all the classical paths Equations 1.2.21 and 1.2.24 essentially constitute the semiclassical path integral quantization.For integrable Hamiltonians further simplification using action angle variables has been carried out [92] and it has been shown [92] that the EBK quantization rule [3] can also yield the same result confirming the exactness of the semiclassical path integral quantization.The semiclassical path energy Green's function is obtained by applying a Laplace transform to the semiclassical Feynman propagator and has been applied [93] to derive the spectral rigidity ($\Delta_3$) statistics [58] for an integrable billiard.

For chaotic systems with isolated periodic orbits Gutzwiller [94] has computed the density of energy states through a different approach.Because in the corresponding classical system the particle trajectories are no longer restricted to the invariant tori the trace of the energy Green's function cannot be obtained in an explicit manner.A stationary state approximation was employed to express the energy Green's function in terms of a sum over all classical stable and unstable periodic trajectories.The Gutzwiller trace formula [11,94] has been successfully applied to compute the energy eigenvalues of a completely chaotic system such as the anisotropic Kepler system.

The experimentally observed spectra [95,96] for the quadratic Zeeman effect on a Rydberg state atom have been found to be in good agreement with the theoretical results obtained from the trace formula [11,94].The photon absorption peaks for Rydberg state Hydrogen atoms subject to strong magnetic field has been related by Du and Delos [97] with the unstable periodic orbits in the underlying classically chaotic system.The periodic orbits in the classical domain for the diamagnetic Hydrogen have been classified by Eckhardt and Wintgen [98].The phenomena of "quantum scars" observed by Heller [99] in numerical studies of wavefunction evolution has been related to the unstable periodic orbits of the classical analogue using the semiclassical path integral methods [100] thus

highlighting the role of semiclassical path integral methods in the wavefunction aspect of the quantum mechanics as well.

### 1.2.4 Wavefunctions in nonintegrable and chaotic systems

For a quantum system the complex wavefunction $\psi(\mathbf{q},t)$ defines its state at any time completely and uniquely.Therefore it is expected that the symptoms of chaos will be present in the time dependence of $\psi(\mathbf{q},t)$ for systems exhibiting chaos in the classical domain.Since the eigenfunctions of the related time independent Schrödinger equation for any specific energy exhibit analytic behaviour being expandable in a convergent power series of the coordinate, a straightforward signature of chaos through the study of wavefunctions is not available at present.Due to this problem various approaches have been tried out to glean evidence of nonintegrability and chaos through the wavefunction of a system.

A. Nodal patterns and scars

As the Hamiltonian operator H is linear and real valued in the absence of magnetic field the eigenfunctions can always be transformed into real valued functions.Accordingly Pechukas [101] first proposed that the study of the wavefunctions might reveal some information regarding the integrability of a quantum system.

For a separable integrable system with n degrees of freedom there will be n families of roughly parallel (n-1) dimensional nodal surfaces with the quantum numbers uniquely defining the numbers of such nodal surfaces in each family.In the nonintegrable regime there exists no quantum numbers so that this nodal pattern is lost with the destruction of nodal lines separating the positive and negative regions producing very complicated looping patterns.A thorough investigation [102 ] of the nodal pattern for a certain variant of the Contopoulos Hamiltonian [103] has been carried out leading to classification of eigenstates into classes referred to as regular, uncertain and ergodic by inspection.Such assignments were then checked out with physical variables like electric

dipole moment which gave evidence of chaotic nature of the system.Similar analysis was carried out on the stadium, a Hamiltonian system proved [104,105] to be strongly chaotic by McDonald and Kaufman [55] and calculations were found to show a very impressive albeit qualitative picture of the chaotic dynamics of the system.

To obtain a more detailed picture of the eigenstates for the stadium, further computations with a very large set of eigenstates were made [106] revealing certain conspicuous intensity patterns displayed by the probability function.These patterns have been termed 'scars' [107] and have been shown to be related to the classical domain unstable periodic orbits [100].

A related feature of classically chaotic systems is the phenomenon of 'localization'.It has been observed [108] that in a periodically kicked rotator exhibiting chaos for irrational period of kicks ,exhibit a certain bounded fluctuation of energy in time whereas the classical analogue shows an increase in energy with time.This has been related [109] to the Anderson localization [110] in solid state physics and the effect is explained as due to the localization of the wavefunction due to interference.

B. Wigner function

The Wigner function [111] provides a quantal analogue to the classical phase distribution function of Boltzmann.It is defined as

$$W(p,q)=\frac{1}{(\pi\hbar)^N}\int dx\, e^{-2ip\cdot x/\hbar}\,\psi(q+x)\psi^*(q-x) \quad . \tag{1.2.25}$$

If $\phi(\mathbf{p})$ be the Fourier transform of the wave function $\psi(\mathbf{q})$ defined as

$$\phi(p)=(2\pi\hbar)^{-N/2}\int d^N q\;\psi(q)e^{-ip\cdot q/\hbar} \tag{1.2.26}$$

where N is the degree of freedom ,then

$$\int dq\; W(p,q)=|\phi(p)|^2 \tag{1.2.27}$$

$$\int dp\; W(p,q)=|\psi(q)|^2 \tag{1.2.28}$$

So that $W(\mathbf{p},\mathbf{q})$ can be interpreted as a probability distribution in the phase space in that, it yields the correct projections into the position and momentum space.Examination of $W(\mathbf{p},\mathbf{q})$ in a particular phase plane $(p_i,q_i)$ provides a quantal analogue to the Poincare surface of section [112 ].For regular integrable systems the semiclassical form of the wavefunction $\psi_n(\mathbf{q})$ can be used to evaluate the associated Wigner function.It has been shown [112 ] that in the classical limit $\hbar\to 0$ the Wigner function reduces to the following form

$$W_m(p,q)=\frac{1}{2\pi^N}\delta(I(p,q)-I_m) \quad . \tag{1.2.29}$$

Therefore the Wigner distribution collapses onto a delta function on the classical invariant torus characterized by the action vector $\mathbf{I}_m$ corresponding to the mth eigenstate.In the semiclassical limit of finite $\hbar$ the projection of the Wigner function $W_m(\mathbf{p},\mathbf{q})$ onto the coordinate plane yields the appropriate oscillatory form of $|\psi_m(\mathbf{p},\mathbf{q})|^2$.The surface of section of the Wigner function for a Hénon-Heiles system [30] in a regular integrable

regime has been studied [113 ].It has been observed that the Wigner function has smooth concentric patterns of phase density reflecting the corresponding integrable dynamics of the system in classical regime.

For the strongly chaotic systems , an irregular state is associated with a large part of the corresponding energy shell.In this situation the Wigner function has the suggested form [91,114,115 ] of a microcanonical distribution as follows,

$$W(p,q)=\frac{\delta(E-H(p,q))}{\int dp \int dq\,\delta(E-H(p,q))} \qquad (1.2.30)$$

with the surface of section of W(**p**,**q**) for the quantum domain (finite $\hbar$ ) displaying behaviour analogous to that of the classically chaotic systems.It has been pointed out [115] that for systems with two or more degrees of freedom $|\psi(\mathbf{q})|^2$ vanishes at the classical boundaries for chaotic systems displaying what has been termed 'anticaustics' by Berry [115 ], in marked contrast to the caustic structure found for regular integrable states.

C. Wave packet dynamics for nonintegrable systems

Since the nearest approximation to the point particlesof classical mechanics are the coherent wavepackets [116 ], the dynamics of a quantum system is sought to be studied through the time evolution of such wavepackets.For the most general wavepacket defined [117] the equation of motion has been derived [118] using semiclassical arguments.It is found that the center of the wavepacket moves along the classical path with the packet width depending on the stability of the classical path, the width remaining constant for quadratic potentials like the harmonic oscillator potential.It has been shown [119] that the Gaussian wavepackets centered on unstable orbits disperses much faster assuming a very complicated tendril like structure around the hyperbolic fixed points compared to those wavepackets centered on stable orbits.

The dynamics of wavepacket evolution has been mostly studied through the survival probability defined as

$$P(t) = |\langle \psi(t) | \psi(0) \rangle|^2 \quad . \tag{1.2.31}$$

Numerical computations have shown [120,121] that for a Hénon-Heiles system [30] there is a significant difference in behaviour of the Survival probability P(t) for wavepackets located in the classically chaotic and regular regions of the phase space. While for the classically integrable regions the wavepacket exhibits a certain recurrence, for nonintegrable regions P(t) decays rapidly and oscillate irregularly with small amplitude.Similar investigations have also been carried out by Bixon and Jortner [122], Weissman and Jortner [123] revealing more or less similar features.Feit and Fleck [124] have used the idea of phase volume and its evolution in time has been studied [124] to get an idea about the degree of chaos in the system concerned.

Another important technique in understanding chaotic behaviour of quantum systems is through the study of the respective quantum fluid dynamics which we present in the next section.

## 1.3 Quantum fluid dynamics

The hydrodynamic interpretation of quantum mechanics was first introduced by Madelung [125] soon after the introduction of Schrödinger's wave equation.In this formalism the Scrödinger's time dependent wave equation for a single particle is transformed into two fluid dynamical equations: an equation of continuity, and an Euler type equation of motion.In this formalism the probability density defined by $|\psi|^2$ is interpreted as the charge density , $\rho = |\psi|^2$ and the velocity v of this charge fluid is obtained from the phase of the complex-valued wavefunction.The introduction of the concept of a fluid with associated density and velocity for studying time evolution of a quantum system provides a "classical" approach in describing quantum phenomena.

However, it was through the works of Bohm [126,127], de Broglie [128,129] and Takabayashi [130,131] that the hydrodynamic interpretation has gained acceptance and has seen wide use in different areas of physics and chemistry.

### 1.3.1 Basic aspects of quantum fluid dynamics

To obtain the quantum fluid dynamical equations, the time dependent single-particle wavefunction is expressed as an ansatz

$$\psi(r,t)=\rho^{\frac{1}{2}}(r,t)\exp\frac{iS(r,t)}{\hbar} \tag{1.3.1}$$

where $\rho=|\psi|^2 = R^2$ ; R and S being real functions of position and time.Substituting this ansatz in the single particle time dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=i\hbar\frac{\partial\psi}{\partial t} \tag{1.3.2}$$

and separating the real and imaginary parts ,the two quantum fluid dynamical equations are obtained as follows,the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla.(\rho v)=0 \tag{1.3.3a}$$

and the equation of motion;

$$m\rho\frac{dv}{dt}=-\rho\nabla(V+V_{qu}) \tag{1.3.3b}$$

where

$$v=\frac{1}{m}\nabla S \tag{1.3.4a}$$

$$\frac{dv}{dt}=\frac{\partial v}{\partial t}+(v.\nabla)v \tag{1.3.4b}$$

and

$$V_{qu} = -\frac{\hbar^2}{2m}\nabla^2\rho^{\frac{1}{2}}/\rho^{\frac{1}{2}} \quad . \tag{1.3.4c}$$

Like the time dependent Schrödinger wave equation from which they are derived , the fluid dynamical equations essentially constitute an initial value problem.Since the Schrödinger wavefunction $\psi$ is a single valued function of position, the associated fluid dynamical variables R or equivalently $\rho^{1/2}$ and S need to satisfy certain conditions.The single valuedness of $\psi$ requires that R be single-valued as well, while the phase function S is not so constrained.In fact due to the polar form of the ansatz equation 1.3.1 used, S can be multivalued so that any two S functions differing by an integral multiple of $2\pi\hbar$ may give rise to the same $\psi$. Alternatively for any circuit along a closed curve C where $\psi \neq 0$ we have

$$\oint_C dS = \int \nabla S.dr = nh \tag{1.3.5}$$

where n is an integer. A nonzero value of n would then imply a discontinuity in the phase function. Since $\psi$ is an analytic function differentiable everywhere a discontinuity in S can arise only when the closed loop encompasses a node of the wavefunction where $\psi=0$.In a nodal region the phase function is not well defined and may undergo a discontinuous jump.It has been pointed out by Wallstrom [132,133] that this condition on the multivalued S function has to be introduced properly in the solution of quantum fluid dynamical equations so as to obtain solutions consistent with the wavefunction solution of the Schrödinger equation.In fact it has been shown [132] that unless this condition on S is imposed for regions separated by nodes where $\psi=0$ an infinite number of different solutions to the fluid dynamical equations may arise.

As seen in equations 1.3.3b, the fluid dynamical equation of motion contains two potential terms, viz.The classical potential V and a quantum potential or the so called Bohm potential [126,134] $V_{qu}$. So unlike classical hydrodynamics the quantum fluid is subjected to an additional potential which is of purely quantum origin, so that the dynamics of local fluid dynamical quantities are dependent on this quantum potential

[135] However, the global behaviour of physically observable entities of the quantum systems are found to be unaffected by this quantum potential [135], as the expectation values of position and momentum coordinates for a particle are dependent only on the externally applied classical potential V.In this regard the basic characters of the fundamental fluid dynamical variables, viz, charge density ρ and the fluid velocity **v** requires some attention.While the charge density is a physical observable,the local velocity field **v** cannot be so regarded.It has been shown explicitly by Kan and Griffin [136] that the current density **j**=ρ**v** being a physical observable the fluid velocity **v** cannot be represented by a linear hermitian operator so that it cannot be a bonafide physical observable.

### 1.3.2 Quantum trajectories and vortices

As discussed, the quantum fluid velocity field **v** is not a physical observable. However, it offers the very significant advantage in carrying over the common classical pictures into the quantum domain to "classically" explain certain quantum processes.The quantum trajectories [2] introduced in the de Broglie-Bohm causal interpretation of quantum mechanics plays a key role.The quantum trajectories are obtained from the equation 1.3.4a by solving

$$\boldsymbol{v} = \frac{d\boldsymbol{r}}{dt} = \frac{1}{m}\nabla S \tag{1.3.6}$$

to obtain the function **r**(t).It should be noted that the fluid velocity **v**=∇S/m is related to the complex momentum **p** as

$$\boldsymbol{p} = m\boldsymbol{v} + \frac{\hbar}{i}\nabla \ln \rho^{1/2} \quad . \tag{1.3.7}$$

and the individual trajectories computed from equation 1.3.6 for different initial positions do not represent the actual single particle quantum system.The quantum trajectories have been computed by Hirschfelder et al [137] for a Debye-Picht [138,139] wavepacket

incident on a two dimensional square potential barrier and other [140,141] dynamical systems As discussed the single-valuedness of the wavefunction $\psi$, implies in the Madelung transcription a similar single valuedness on the probability amplitude R and a quantization condition on the gradient of the phase function S.Since the fluid velocity is expressed as $\mathbf{v}=\nabla S/m$ , then this condition can be expressed as

$$\oint_C \mathbf{v}.d\mathbf{r} = \frac{nh}{m} \tag{1.3.8}$$

where n=0,±1,±2,....Using Stoke's theorem this can be related to a surface integral over the area bounded by C as

$$\int_A (\nabla \times \mathbf{v}).d\mathbf{A} = \frac{nh}{m} \tag{1.3.9}$$

where as before n=0,±1,±2,.....But the quantity $(\nabla \times \mathbf{v})$ is the well known hydrodynamical vorticity $\omega$ allowing the equation 1.3.9 to be recast as

$$\int_A \boldsymbol{\omega} \times d\mathbf{A} = \frac{nh}{m} \tag{1.3.10}$$

with the quantization condition ,n=0,±1,±2,....For an area containing a node of the wavefunction $\psi$, $n \neq 0$ implies a nonzero value of the vorticity $\omega$.Since $\omega$ satisfies the quantization condition as given by equation 1.3.9, the vorticity around wavefunction nodes are quantized, as first discovered by Dirac [142,143].Furthermore it has been pointed out that [144] since the wavefunction can be generally divided into a real and an imaginary component, a wavefunction node requires that both the components are simultaneously equal to zero .

In their study of a Hydrogen atom colliding with a collinear Hydrogen molecule McCullough and Wyatt [145] have reported occurrence of a vortex in the probability current plot, which have been termed by them as "the quantum whirlpool effect".This has

been further confirmed by studies of Kuppermann and coworkers [146 ].A detailed study of nodal topology of wavefunctions giving rise to such vortices has been carried out by Reiss [147-150] and Heller et al [151 ].

### 1.3.3 Wavefunction eigenstates in quantum fluid dynamics

In the conventional quantum mechanics, an eigenstate of a system is obtained from the solution of the corresponding time independent Schrödinger equation.In this case the time dependent wavefunction is expressed as

$$\psi(r,t) - \rho^{1/2}(r)\exp\frac{iEt}{\hbar} \quad . \tag{1.3.11}$$

In the quantum fluid dynamical formalism the stationary state is defined by the solution of the time independent solution of the fluid dynamical equations.In this case the fluid density $\rho$ and $\mathbf{v}$ are constant in time.Accordingly the stationary states have been defined [152] in terms of body motion of the quantum fluid.A stationary state where the velocity field $\mathbf{v}=0$ is referred to as the static stationary state where the phase function S is independent of position and can be expressed as S=Et.While a state with $\mathbf{v}\neq 0$ corresponds to a dynamic stationary state.In the static stationary state the total energy E of the system can be expressed as

$$[V+V_{qu}]=E \tag{1.3.12a}$$

so that

$$\nabla[V+V_{qu}]=0 \tag{1.3.12b}$$

which means that for static stationary state the resultant force acting on the quantum fluid is zero, with the forces of classical and quantum potential nullifying each other.This has been applied [153] to interpret the stability of the ground state of the Hydrogen atom.Due to the apparent contradiction of a zero velocity field with the nonzero angular momentum of a ground state Hydrogen atom objections have been raised [154,155] against the

hydrodynamical approach to quantum mechanics.However, this is resolved by noting that following equation (1.3.7) the momentum field mv=∇S is only the real component of the linear momentum operator **p**.

### 1.3.4 Generalization of quantum fluid dynamics

The quantum fluid dynamical equations for a single particle has been extended to situations where there is a magnetic field along with the scaler field.If **E** and **B** be the electric field and the magnetic field respectively then the fluid dynamical equations have been obtained [156] as

$$\frac{\partial \rho}{\partial t}+\nabla.(\rho \boldsymbol{v})=0 \qquad (1.3.13a)$$

$$m\rho\frac{d\boldsymbol{v}}{dt}=\rho(e\boldsymbol{E}+\frac{e}{c}\boldsymbol{v}\times\boldsymbol{B})-\rho\nabla(V+V_{qu}) \qquad (1.3.13b)$$

where the fluid velocity is expressed as

$$\boldsymbol{v}=\frac{1}{m}(\nabla S-\frac{e}{c}\boldsymbol{A}) \quad . \qquad (1.3.13c)$$

The spin-magnetic interaction term has been included [151] and the modified fluid dynamical interactions have been obtained.The electron spin has been incorporated more rigorously using the Pauli spin and the relevant equations [131,157,158] have been derived, while the quantum fluid dynamical equations for the relativistic case have been obtained [159].

As in the case of single particle systems, the Schrödinger equation can be transformed into a continuity equation and an Euler-type equation of motion for many particle systems as well.For an N-particle system these equations have the general form

$$\frac{\partial \rho}{\partial t}+\sum_{i=1}^{N}\nabla_i(\rho v_i)=0 \qquad (1.3.14a)$$

$$\frac{\partial v_i}{\partial t}+\sum_{i=1}^{N}(v_i.\nabla_i)v_i=-\nabla_i\{V_{cl}(r_1,\ldots,r_N)+V_{qu}\} \qquad (1.3.14b)$$

where i denotes the ith particle of the N-particle system.However, the fluid-dynamical quantities like the density and velocity field correspond to a fluid in the 3N dimensional configuration space, which do not have direct physical significance for N>1.In this case the interpretation of the essentially fluid dynamical features like vortices and streamlines are no longer germane and the power of visualization so unique to the single particle quantum fluid dynamics appears to be lost.Attempts to directly project the fluid dynamical equations for such many particle systems onto the 3D Euclidean space have not seen much success [160], except within some approximate single body theories like the Hartree and the Hartree-Fock theories.While Takabayashi [130] formulated the quantum fluid dynamical equation for a many-particle system using Hartree theory,Wong and coworkers [161,162] have applied the time dependent Hartree-Fock theory for the N-body quantum fluid system.Using the concept of natural orbital theory [163],a many-electron system subject to electric and magnetic fields has been treated within 3D quantum fluid dynamics [164].

The formulation of density functional theory (DFT) [165,166] for many particle systems has been very successful in explaining the electronic structure, bonding and properties of atoms and molecules for time independent situations and for ground states in terms of single-particle density $\rho(r,t)$ as the fundamental variable.The essence of the density functional theory is that the electron density contains all information about the ground state of a many-electron system and the true charge density distribution minimizes the related energy functional [165].The density functional theory has been further extended to a time dependent situation [167,168].To treat the dynamical problem for many electron systems the quantum fluid dynamics (QFD) [169,170] and the time dependent

density functional theory (TDDFT) have been combined to obtain the quantum fluid density functional theory (QFDFT) [171-179].In the quantum fluid density functional theory an N-electron system is mapped onto a system of N noninteracting particles moving under the influence of an effective potential $V_{eff}(\mathbf{r},t)$ to obtain a generalised nonlinear Schrödinger equation which is solved to yield the time dependent single "orbital" $\phi(\mathbf{r},t)$ for the many electron system considered.The quantum fluid dynamical quantities of this system viz. $\rho(\mathbf{r},t)$ and the current density $\mathbf{j}(\mathbf{r},t)$ or the velocity is obtained as

$$\rho = |\phi|^2 \tag{1.3.15a}$$

$$\boldsymbol{j} = \rho \nabla \chi \tag{1.3.15b}$$

where

$$\phi(\boldsymbol{r},t) = \rho^{1/2} \exp(i\chi) \quad . \tag{1.3.15c}$$

Recently QFDFT has been successfully applied in solving the ion-atom collision problems [173-177] and atom-field interaction problems [178,179].

The quantum fluid dynamics of nonlinear oscillators have been investigated [180-182] to study the signatures of nonintegrability through the hydrodynamic formalism.Certain distinctive features characteristic to nonlinear systems have been manifested through the various fluid dynamical and related quantities.The nonlinear features in processes involving many particle systems such as an ion colliding with a many electron atom [183] have been studied using the quantum fluid density functional theory in order to understand the associated charge transfer process and related electronic structure principles.

## 1.4 Quantum theory of motion

There are certain aspects of the conventional interpretation of quantum mechanics which have been open to serious criticism right from its inception. For instance, the

concept of completeness of wavefunction $\psi$ in describing the state of a system has been criticized by Einstein [184-187].To illustrate his ideas further Einstein considered a version of the celebrated cat problem of Schrödinger [188].He felt that the quantum theory fails to describe a reality independent of the act of observation.

Another very controversial issue for conventional interpretation of quantum mechanics has been the problem of measurement in the quantum domain. Since unlike measurement as perceived in classical physics, in quantum mechanics the experimental apparatus plays an interactive and intrusive role it is very difficult to talk about a quantum system separated from the experimental equipments. This arises partly due to the specific properties of the Schrödinger equation, especially its linearity which generates irreducible couplings between objects observed and the apparatus. As these interactions transform the observed system the ideas of observable and measurement have been strongly criticized [189]. Furthermore conventional quantum mechanics fails to explain the assignment of particular eigenvalues to an observed state entailed by the act of observation. To explain this von Neumann [190] proposed his theory of measurement of quantum mechanical state, where Schrödinger's evolution equation no longer holds and what actually occurs in nature is proposed by the hypothesis of wavefunction collapse. In this hypothesis it is proposed that a quantum mechanical state collapses to the observed value due to the intervention of the observer. A detailed discussion may be obtained in articles by Wigner [191,192] and Redhead [193] among others.

Even if the collapse of the system wavefunction can be accounted for by a suitable modification of Schrödinger's wave equation, the definite observed state so obtained will be a wavefunction and the assignment of definite variables to the indicator of the measuring device goes beyond conventional quantum mechanics. If it is argued that classical objects can always be defined by classical variables (regardless of its coupling with a observed quantum state) then the impossibility of strictly defining the micro and macro levels necessitates assignment of such variables to quantum (micro) level as well. This is the basic tenet of de Broglie-Bohm theory [194-204].

### 1.4.1 Basic concept of causal theory of de Broglie and Bohm.

Counter to the conventional quantum mechanics, de Broglie [195-199] introduced the idea that the wavefunction should instead of replacing the concept of material point be in coexistence with the point particle thus extending the classical concepts into quantum domain. It was suggested that in the nonrelativistic situation the Schrödinger wavefunction can be associated with an ensemble of identical particles differing in positions and distributed according to the conventional interpretation of $|\psi|^2$ proposed by Born.Essentially de Broglie assigned a dual role to be played by the Schrödinger wavefunction $\psi$ in that along with the conventional interpretation regarding likely location of a particle it also influences causally the trajectory of the ensemble elements. The wave function $\psi$ is now considered to behave as pilot-wave guiding ensemble element.de Broglie applied the guidance principle to compute the orbits for Hydrogen atom stationary states [128,134].

In principle de Broglie's approach is closer to Einstein's view regarding the conventional Copenhagen interpretation of quantum mechanics. Einstein's interpretation advocated Born's statistical state in the sense that $\psi$ refers to an ensemble of systems and not a single physical system. In this view $\psi$ is considered as an incomplete representation of actual physical state and plays a role similar to that of the distribution function in classical statistical mechanics.Einstein's interpretation has been developed into the statistical approach to quantum mechanics [205,206] but does not seem to offer any greater insight into the nature of quantum phenomena as compared to the conventional Copenhagen view .It is regarding the role of the wavefunction $\psi$ that the de Broglie approach stands out as in this view the wavefunction becomes a physical entity associated with individual ensemble element.

de Broglie's causal interpretation was further developed by Bohm [200,201] who set up a consistent counterexample to prove that the assumption of completeness of the wavefunction in describing a physical system was not a logical necessity.

### 1.4.2 Mathematical formulation

As already discussed the fundamental concept of the de Broglie-Bohm theory is

the idea of an ensemble of systems each of which evolve under the influence of the wavefunction $\psi$ obeying Schrodinger's wave equation.Furthermore it is postulated that the quantity $|\psi|^2 d\mathbf{r}$ now gives probability of an ensemble element to lie in the region of space between $\mathbf{r}$ and $\mathbf{r}+d\mathbf{r}$.

The concept of ensemble of particles (elements) allows us to introduce the idea of individual dynamics of these elements using the following line of reasoning.The time dependent Schrödinger wave equation is written as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \qquad (1.4.1)$$

where m is the mass of the particle and V= V($\mathbf{r}$,t) is the potential energy due to an externally applied classical field.The following polar form of the wavefunction is substituted in the Schrödinger wave equation

$$\psi(r,t) = R\exp(iS/\hbar) \qquad (1.4.2)$$

where R($\mathbf{r}$,t) and S($\mathbf{r}$,t) are the two real valued functions representing the amplitude and phase factors of the wavefunction respectively.Then equating real and imaginary parts of the eqn. 1.4.1 the following field equations are obtained,

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + V = 0 \qquad (1.4.3)$$

$$\frac{\partial R^2}{\partial t} + \nabla.\left(\frac{R^2\nabla S}{m}\right) = 0 \quad . \qquad (1.4.4)$$

with the condition of single-valuedness of $\psi$ requiring that R($\mathbf{r}$,t) be single-valued and the phase function S obey the condition

$$\oint_C dS = \oint_C \nabla S.dr = nh \qquad (1.4.5)$$

where n is an integer.It is then seen that eqn. 1.4.3 has the form of the classical Hamilton-Jacobi equation apart from the term

$$V_{qu}(r,t) = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} \quad . \qquad (1.4.6)$$

The function $V_{qu}(\mathbf{r},t)$ is referred to as the quantum potential discussed in the previous section.The eqn. 1.4.4 then expresses the conservation of the probability current.Eq. 1.4.3 finally takes the following form

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V_{qu} + V = 0 \quad . \qquad (1.4.7)$$

Then following arguments along the line of classical mechanics a vector field $\mathbf{v}=\nabla S/m$ can be constructed and it is assumed that the field defines at each point of space the tangent to a possible particle trajectory through that point. Thus the concept of an ensemble of particle arises quite naturally and the trajectories are orthogonal to the surface S=constant and is obtained from the equation of motion

$$\begin{aligned} \dot{r} &= v(r,t)\big|_{r=r(t)} \\ &= \frac{1}{m}\nabla S(r,t)\big|_{r=r(t)} \end{aligned} \qquad (1.4.8)$$

where the initial particle position $\mathbf{r}(0)=\mathbf{r}_0$ has to be specified. It is further seen that the velocity field $\mathbf{v}(\mathbf{r},t)$ is related to the probability current density defined as

$$j = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) \qquad (1.4.9)$$

and we have

$$j(r,t) = R^2\left(\frac{\nabla S}{m}\right) = R^2 v(r,t) \quad , \tag{1.4.10}$$

a form already introduced in the last section. Hence the trajectories r(t) can be identified with the direction of flow of the probability current density. Since VS is a single valued function of position there exists a unique tangent vector associated with ∇S and consequently there can be a single trajectory through a space point, which signifies that trajectories of the ensemble elements do not intersect one another.

The set of equations from 1.4.6 to 1.4.10 may be considered to form the mathematical basis of the de Broglie-Bohm causal interpretation of quantum mechanics hereafter referred to as the quantum theory of motion.

### 1.4.3 Classical limit of the causal theory

For an appreciation of the causal quantum theoretic approach to the classical limit, a brief discussion regarding classical limit version of conventional quantum mechanics is in order. In conventional quantum mechanics one of the most widely used criteria for the classical limit is the condition $\hbar \to 0$ when compared to with quantities of the same dimension pertinent to the system under consideration. Even there the Schrödinger wavefunction has to satisfy equations containing $\hbar$ and may contain $\hbar$ parameters. The fundamental problem here is the concept of quantum state $\psi$ which after all does not have a classical analogue. The common procedure of identifying the classical limit through such aspects of quantum mechanics as energy levels and large quantum numbers may not be correct in the sense that the underlying process remains in the quantum domain without any classical law of motion being manifested. Similar arguments may be raised in case of identifying classical like behaviour of quantum systems as the classical limit behaviour of the system.

The quantum theory of motion, however, seems to be free from the ambiguity inherent in classical limit studies of conventional quantum mechanics. Since it starts with a definition of quantum state that admits an objective physical system like a point particle with definite position, along with the Schrödinger wave function, one can always look for

entities that approach the classical limit. In this approach classical dynamics theory or at least the classical limit is sought to be deduced from the causal theory [207,208].

In the quantum theory of motion the classical domain is considered to be the state where the wave component of matter exerts no influence on the particle behaviour [2]. Mathematically this is implied by the condition $V_{qu} \to 0$ in eqn.(1.4.9) so that the Hamilton-Jacobi equation in its classical form is recovered along with the continuity equation as

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = 0 \qquad (1.4.11)$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left( \frac{R^2 \nabla S}{m} \right) = 0 \quad . \qquad (1.4.12)$$

Under such conditions the classical limit of the quantum mechanical one-body pure state problem is a particular classical statistical mechanics of a single body in the Hamilton-Jacobi formalism [2].

### 1.4.4 Application of quantum theory of motion

The mathematical formulation of the quantum theory of motion effectively draws from the Schrödinger's equation and as such all the experimentally observed facts supporting the conventional formulation is reproduced in the quantum theory of motion. It is, however, in the possibility of identifying causal agents of the observed effects that the quantum theory of motion has met with great success.

The historically important matter wave interference effects [29]were studied experimentally for electrons [209-211] and neutrons [212]. All the cases confirm the predictions of quantum mechanics. Such observations have been theoretically interpreted by Philippidis et al [213,214] who computed the quantum trajectories of individual ensemble elements for the double slit interferometer. A causal version of the neutron interferometer [212] has been investigated [215] where the interferometer mirrors have been represented by square potential barriers and the neutron beam is represented by a Gaussian distribution of the initial particle (ensemble element) positions.The penetration

and scattering phenomena for different potentials have also been studied in causal interpretation [216,217] and the various experimentally observed effects have been explained in terms of the quantum theory of motion.

The Aharonov-Bohm effect [218] is supposed to imply [39] that the role played by the potentials in quantum mechanics transcends their role in classical mechanics. The issues raised in this regard [219] are still to be resolved completely.

A consistent causal interpretation of this phenomenon has been obtained [214] by the local action of the vector potential **A** on the particle by means of the force derived from the quantum potential.

Recently the causal interpretation has seen applications in development of useful concepts where the conventional quantum mechanical predictions are not clearly defined. One such area of confusion is the concept of time in conventional quantum mechanics. This difficulty in defining time spent by a particle to traverse a certain region is highlighted in the case of a particle tunneling through a potential barrier. Various definitions of `mean times' involving expressions derived from the Schrödinger wavefunction has been proposed [220]. From the causal interpretation point of view, the fundamental difficulty in obtaining a general definition through the wavefunction concept alone ,lies with the fact that there is no feature in the conventional theory that relates to the individual tunneling process. The causal interpretation introducing the concept of particle (ensemble element) trajectory is, however, equipped with handling this problem. Various investigators [221-224] have applied the quantum theory of motion (de Broglie-Bohm theory) to provide clear definition of transit time in different physical situations.

The introduction of trajectory concepts and the associated deterministic evolution of the ensemble elements have provided a new avenue to study chaos in quantum systems.Very recently the Lyapunov exponent and Kolmogorov-Sinai entropy have been generalised to treat quantum systems through the quantum theory of motion.Such generic cases as the kicked rotor and the quantum Weigert map for a charge localized in a unit square has been successfully treated [225,226]. Parmenter et al [227] have claimed to have found certain class of systems which exhibit deterministic chaos in the quantum domain as per the causal approach but behaves regularly in the classical domain.Sengupta

and Chatiaraj [228] have studied the quantum Hénon-Heiles oscillator by applying the quantum theory of motion and has extended their studies into a general class of anisotropic oscillators [229a] and the Rydberg atom[229b].The results obtained point to a very close relation between deterministic chaos in classical and quantum regimes when studied using the causal approach.

### 1.5 Motivation for the present work and the contents of the thesis

The quantum fluid dynamics and the quantum theory of motion offer a unique opportunity of investigating the problem of chaos in quantum systems from a 'classical' viewpoint.The hydrodynamical equations provide us with the classical concepts of velocity field ,vorticity and charge flow for both single particle systems as well as for many particle systems (combined with density functional theory) and the equations are nonlinear.

The conventional quantum mechanics cannot treat chaos in the same footing as the classical chaos since the concepts of individual trajectories is not present in the quantum domain.As is obvious from previous discussions , chaos in the quantum domain is treated indirectly through the study of mean value of quantum operators and spectral structure of energy eigenvalues.Defining a quantum analogue of the sensitive dependence on initial conditions and measure of irregularity in a quantum system remains a problem [230].

However, the quantum theory of motion allows a simultaneous existence of particles and waves so that one can assign trajectories to quantum particles.In that case, all the concepts used for studying classical chaos like the sensitive dependence on initial conditions, entropies etc. can be applied to quantum systems that exhibit chaos in the classical domain.

Chapter 1 is now concluded by providing an outline of the contents of the thesis.The thesis consists of seven chapters.Chapter 1 reviews various studies on quantum domain dynamics of classical nonlinear systems exhibiting chaos.The quantum fluid dynamics and the quantum theory of motion are introduced and the motivation for the present work is explained.Chapter 2 discusses the quantum fluid dynamical studies on a Hénon-Heiles oscillator.In Chapter 3 the quantum domain behaviour of a Hénon-Heiles

oscillator is studied in terms of the quantum theory of motion.In Chapter 4 we investigate the chaotic dynamics of some quantum anharmonic oscillators using the quantum theory of motion.Application of the quantum theory of motion in understanding the dynamics of an electronically excited Hydrogen atom in presence of an intense electric field constitutes the subject matter of Chapter 5.Chapter 6 deals with the causal interpretation of the quantum dynamics of a Rydberg atom colliding with a proton.Chapter 7 highlights the dynamical variants of some electronic structure principles within a quantum fluid density functional framework.This Chapter attempts to broaden the scope of quantum fluid dynamics in tackling quantum dynamics of many-particle systems.We conclude with the bibliography containing all the references followed by a brief summary of the present work.