NUMERICAL INVESTIGATIONS OF QUANTUM EFFECTS OF CHAOS

DISSERTATION

Presented to the Graduate Council of the
University of North Texas in Partial
Fulfillment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

Miroslaw Latka, M.Sc.
Denton, Texas
August, 1993
NUMERICAL INVESTIGATIONS OF QUANTUM EFFECTS OF CHAOS

DISSERTATION

Presented to the Graduate Council of the
University of North Texas in Partial
Fulfillment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

Miroslaw Latka, M.Sc.
Denton, Texas
August, 1993
The quantum dynamics of minimum uncertainty wave packets in a system described by the surface-state-electron (SSE) Hamiltonian are studied herein. The quantum evolution is found to be strongly dependent upon the orbit structure in the classical phase space. A Gaussian wave packet, initially centered on the part of the phase space incased by KAM tori remains localized, while the packets located in the chaotic region spread rapidly, filling the available phase space. To quantify the observed spreading quantum uncertainty is introduced as a dynamical variable, its time development is determined by the ballistic growth of the position uncertainty and the erratic oscillations of the momentum uncertainty. Further, the classical concept of diffusion previously used in this context is shown to be inappropriate. The quantum evolution is analyzed within the framework of the Floquet formalism. The Floquet spectrum of the stable packet is shown to be dominated by a few quasienergy states with the corresponding Husimi distribution embedded in the classical stability island. Finally, it is demonstrated that the prominent nonlinear resonance (KAM island) persists in the quantum phase space as the dynamical barrier which hinders the wave packet from exploring the classically inaccessible region.
ACKNOWLEDGMENTS

I am very grateful to my advisor Professor B.J. West for suggesting this project and for his continued guidance, constructive criticism and support. I am also indebted to Professor P. Grigollini for the help I received during the course of my work and many valuable discussions.

This work has greatly benefited from the stimulating interaction with M. Bianucci, L. Bonci, X. Fang, M. Molina, G. Tréfan, R. Roncaglia and D. Vitali. It is pleasure to thank them for their friendships who made my staying at the University of North Texas much more enjoyable.

I appreciate the interest and advice of Professor J.M. Kowalski and Professor S. Ward.

I am deeply grateful to my wife Maria and my children Agnieszka and Andrzej who patiently awaited for my return home.

Finally, I am very obliged to my parents for their constant support and encouragement especially during a troublesome period. This work could not have been completed without their generous assistance and it is dedicated to them.

I acknowledge the partial support of this research by the Texas Advanced Research Program (Project No. 0035494-038) and thank the National Science Foundation for support of the numerical calculations performed on the CRAY Y-MP at the Pittsburgh Supercomputing Center (Grant PHY920023P).
TABLE OF CONTENTS

LIST OF TABLES ........................................................................................................ vi

LIST OF FIGURES ...................................................................................................... vii

Chapter

I. INTRODUCTION ........................................................................................................ 1

1.1 "Quantum Chaos" problem .................................................................................. 1
1.2 Outline of the Thesis .............................................................................................. 7

II. HARMONICALLY DRIVEN SURFACE STATE ELECTRON MODEL ................ 9

2.1 Model ....................................................................................................................... 9
2.2 Classical Properties ............................................................................................... 12
2.3 Quantum Properties .............................................................................................. 16

III. DISTRIBUTION FUNCTIONS IN QUANTUM MECHANICS ...................... 27

3.1 Introduction ............................................................................................................ 27
3.2 Weyl transformation .............................................................................................. 29
3.3 Wigner distribution function ................................................................................ 37
3.4 Husimi distribution function ................................................................................ 42
3.5 General distribution function ............................................................................... 50
3.6 Wigner and Husimi distributions in the SSE Model ............................................. 60
IV. NUMERICAL RESULTS FOR THE DRIVEN SSE MODEL ...............67

4.1 Quantum Dynamics .................................................................67
4.2 Floquet Analysis .....................................................................74
4.3 KAM Quantum Dynamical Barriers .........................................78
4.4 Conclusions and Proposed Future Work .................................82

APPENDIX

A1 Surface State Electron Hamiltonian in Action-Angle Variables ....86
A2 Solution of Eigenvalue Problem for the SSE Hamiltonian ..........89
A3 Derivation of the Weyl Transform of the Product of Two Operators.92
A4 Derivation of Formula (3.2.39). ..................................................95
A5 Derivation of Formula (3.4.24) ....................................................98
A6 Derivation of Identity (3.5.39) ....................................................100

FIGURES ..........................................................................................103

REFERENCES ..................................................................................162
<table>
<thead>
<tr>
<th>TABLE</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Properties of Quantum Distributions</td>
<td>58</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Classical orbits of the SSE Hamiltonian</td>
</tr>
<tr>
<td>2</td>
<td>Eigenfunctions $\Psi_n(p)$ of the SSE Hamiltonian</td>
</tr>
<tr>
<td>3</td>
<td>Eigenfunctions $\Psi_n(x)$ of the SSE Hamiltonian</td>
</tr>
<tr>
<td>4</td>
<td>Relations between the Wigner and Husimi distribution functions $\rho_W$ and $\rho_H$ and their classical counterparts $\rho_C$ and $\rho_{CG}$</td>
</tr>
<tr>
<td>5</td>
<td>Wigner distribution of the eigenfunction $</td>
</tr>
<tr>
<td>6</td>
<td>Husimi distribution of the eigenfunction $</td>
</tr>
<tr>
<td>7</td>
<td>Comparison of the Wigner and Husimi distribution functions corresponding to the eigenfunction $</td>
</tr>
<tr>
<td>8</td>
<td>Husimi distributions of the eigenfunction $</td>
</tr>
<tr>
<td>9</td>
<td>Comparison of the contour plots of the Husimi distributions from Fig. 8 with the probability densities for the eigenfunction $</td>
</tr>
<tr>
<td>10</td>
<td>(a) Poincaré surface of section for $\Omega = 1 / (66)^3$ a.u. and $F = 0.01 / (66)^4$ a.u., (b) magnified central part of the Fig. 10(a)</td>
</tr>
<tr>
<td>11</td>
<td>(a) Poincaré surface of section for $\Omega = 1 / (66)^3$ a.u. and $F = 0.03 / (66)^4$ a.u. (b) The regular part of the classical phase space is enlarged to reveal the structure of nonlinear resonances</td>
</tr>
<tr>
<td>12</td>
<td>Husimi function of the packet $P_1$ at $t = 0$</td>
</tr>
<tr>
<td>13</td>
<td>The projection of three minimum uncertainty wave packets on the basis states</td>
</tr>
</tbody>
</table>
of the SSE Hamiltonian ..................................................................................116
14 Time evolution of the wave packet $P_1$ initially localized at the regular part of the classical phase space ..........................................................................................117
15 Time evolution of the wave packet $P_2$ initially overlapping the regular part of the classical phase space ..........................................................................................121
16 Time evolution of the wave packet $P_3$ initially localized in the chaotic region of the classical phase space .................................................................................................125
17 Survival probability for (a) wave packet $P_1$, (b) wave packet $P_2$, and (c) wave packet $P_3$ ..........................................................................................................................129
18 Husimi function of (a) the wave packet $P_1$ at $t = 3T$, (b) the wave packet $P_2$ at $t = 2T$ .................................................................................................................................130
19 Time evolution of (a) quantum mechanical uncertainty, (b) position uncertainty, (c) momentum uncertainty for the wave packets $P_1$, $P_2$, and $P_3$ ........................132
20 Time evolution of (a) quantum mechanical uncertainty, (b) position uncertainty, (c) momentum uncertainty in the numerical experiment with $|\Phi_{80}\rangle$ ......................133
21 (a) Husimi function of $|\Phi_{80}\rangle$, (b) Husimi function at $t = 30T$ in the numerical experiment with $|\Phi_{80}\rangle$ ........................................................................................................134
22 Time evolution of (a) quantum uncertainty, (b) position uncertainty, (c) momentum uncertainty in the numerical experiment with $|\Phi_{64}\rangle$, $|\Phi_{72}\rangle$, and $|\Phi_{79}\rangle$ ..................................................................................................................136
23 Time evolution of the survival probability in the numerical experiments with (a) $|\Phi_{64}\rangle$, (b) $|\Phi_{72}\rangle$, (c) $|\Phi_{79}\rangle$ ..................................................................................................................137
24 Time development of the Husimi function in the experiment with $|\Phi_{64}\rangle$ ...138
25 Time reversal” experiment for the wave packet $P_3$: (a) time evolution of position uncertainty, (b) time evolution of survival probability .............................................142
26 Floquet spectra corresponding to the wave packets (a) $P_1$, (b) $P_2$, (c) $P_3$. .143
27 Husimi representation of two quasienergy states significantly overlapping the packet $P_1$ .................................................................144
28 Husimi representation of the quasienergy state significantly overlapping the packet $P_2$ .........................................................................................146
29 Husimi representation of two quasienergy states significantly overlapping the packet $P_3$ .........................................................................................147
30 Basis expansion of selected Floquet states......................................................149
31 Floquet spectrum of the wave packet $P_4$ ..........................................................150
32 Time evolution of the survival probability for the wave packet $P_4$ ...............150
33 Time evolution of (a) quantum uncertainty, (b) position uncertainty, (c) momentum uncertainty for the wave packet $P_4$ ..........................................................151
34 Time evolution of the Husimi distribution of wave packet $P_4$ ......................152
35 Husimi representation of the quasienergy states significantly overlapping the packet $P_4$ .........................................................................................157
CHAPTER 1

INTRODUCTION

1.1 "Quantum Chaos" problem

The quantum dynamics of Hamiltonian systems whose classical analogs are nonintegrable has recently been the subject of great scientific interest [1]. However, this problem is almost as old as quantum mechanics itself. In order to explain the energy spectrum of the hydrogen atom Bohr postulated that the conserved angular momentum be equal to a multiple of Planck's constant (throughout this thesis Planck's constant is denoted by $\bar{\hbar}$). The spectacular success of this approach, which could be fully understood only after the advent of wave mechanics, has led to the generalization of Bohr's original concept. Among the most famous contributors were Sommerfeld, Einstein and Kramers. The extended quantization rules assigned a multiple of $\hbar$ to every conserved action integral. This technique worked well for a few simple, integrable systems (systems that have as many constants of motions as they have degrees of freedom) but completely failed when applied to the problem of the ground state of the hydrogen molecule ion or the helium atom. As early as 1917 Einstein [2] turned the problem around and asked what classical systems may be the subject of these quantization rules. He correctly pointed out that the absence of invariant tori (using modern terminology) in the case of nonintegrable systems prevents the direct application of quantization rules. He also realized that nonintegrable systems are the most commonly encountered in nature. Einstein's original paper was essentially ignored until 1973 when Percival pointed out that in the light of much deeper understanding of classical mechanics of nonintegrable systems provided by the Kolmogorov-Arnold-Moser (KAM) theory, the problem recognized by Einstein should be revisited [3]. Percival conjectured [4]
that in the semiclassical limit $\hbar \to 0$ the bound-state quantum energy levels corresponding to the irregular or chaotic regions of the classical phase space form an irregular spectrum with properties significantly different from a regular spectrum associated with the portions of the phase space occupied by KAM tori. He suggested that these two kinds of spectra, regular and irregular, may be distinguished by the system's response to external perturbation.

This problem is now a part of a much broader, rapidly expanding research field whose primary goal is to explore the modification introduced into quantum mechanics by the properties of classically chaotic systems. This field is also known as "quantum chaos". This intriguing term has been the source of great controversy. The following anecdote attributed to P.W. Milloni [5] gives the flavor of the emotions associated with the concept of quantum chaos. A very distinguished physicist asked by Milloni about his thoughts on quantum chaos replied "so many otherwise intelligent people have said such foolish things about the subject that I've decided to stay away from it".

The controversy concerning the combination of words "quantum" and "chaos" has its origin in the profound differences between classical and quantum mechanics [6]. For example the hallmark of chaos is the sensitive dependence on the initial conditions. A bundle of trajectories originating from a small cloud in phase space diverges exponentially, i.e. the distance between any two initially close trajectories grows exponentially in time, the growth rate being the so-called Lyapunov exponent. On the other hand, for regular motion the corresponding distance between trajectories may increase as a power of time but never exponentially. In this latter case the Lyapunov exponent vanishes. However, the limits imposed by the uncertainty principle on the simultaneous measurement of position and momentum prevents the direct implementation of the concept of phase space in quantum mechanics. This property of quantum systems may be partially circumvented with the help of quasiprobability distribution functions such as the
Wigner function or the Husimi function which are discussed in more detail in Chapter 3. The notion of "initially close trajectories" also loses its meaning when turning from classical to quantum mechanics. Due to the unitarity of quantum dynamics the overlap of two wavefunctions remains time independent,

\[ |\langle \Phi(t) | \Psi(t) \rangle|^2 = |\langle \Phi(0) | \Psi(0) \rangle|^2, \]

provided the time evolution of \( \Phi(t) \) and \( \Psi(t) \) is governed by the same Hamiltonian.

Thus one may ask whether there exists a quantum mechanical property which unambiguously indicates the integrability of the overarching classical mechanics. It is now well established [6] that the statistics of energy level spacings (or quasi-energy levels for periodically driven systems) provides this kind of information. Generic classically integrable systems have levels that tend to cluster and may cross each other when a Hamiltonian parameter is varied. In this case the level spacing distribution is Poissonian

\[ P_p(s) = \frac{1}{D} e^{-s/D}, \]  

where \( s \) is the energy level spacing and \( D \) is a constant. On the other hand, classically nonintegrable systems exhibit level repulsion, i.e. the levels are correlated in such a way that the crossings are strongly avoided. There are three universality classes of level repulsion: linear, quadratic and quartic \( (P(s) \sim s^\beta, \beta = 1, 2, 4, \ s \to 0) \). The character of the level repulsion is determined by the symmetry of the system. For the linear repulsion the corresponding level spacing statistics is described by the Wigner distribution

\[ P_W(s) = \frac{\pi s}{2D^2} e^{-\pi s^2/(4D^2)}. \]

The first evidence that the manifestations of chaos might appear in the spectral statistics was provided by the numerical experiments performed by McDonald and Kaufman [7] on billiards. They used a "stadium" billiard consisting of two
semincicles connected by straight line segments. If the length of the segments goes to zero the stadium reduces to a circle. The classical dynamics of a particle moving inside a circle billiard table is integrable. Any deviation of the shape from the circle yields chaotic dynamics. McDonald and Kaufman solved the time-independent Schrödinger equation (which in this particular case is just the Helmholtz equation with the boundary conditions $\Psi = 0$ at the walls of the billiard table) and found that an integrable billiard problem had a high probability of small level spacings while a nonintegrable one showed clear energy level repulsion. Billiards may be either integrable or nonintegrable but the discontinuity of their Hamiltonians at the walls distinguish them from the more common soft Hamiltonians. The latter systems exhibit rather gradual transition from the predominantly regular to predominantly chaotic dynamics as the value of the nonlinear coupling or the strength of the external perturbation is varied. This transition is manifested by the change in the level statistics from Poissonian-like to Wigner-like.

McDonald and Kaufman also calculated the eigenstates of the stadium billiard and graphed their nodal structure. They found the nodal lines to form intricate, disordered patterns in sharp contrast with the regular structure of eigenfunctions of the classically integrable circle billiard table. These results were in agreement with the predictions of the "semiclassical eigenfunction hypothesis" put forward by Berry and Voros [8-10]: each semiclassical eigenstate has a Wigner function concentrated on the region explored by a typical orbit over infinite time. This hypothesis implies that as $\hbar \to 0$ wavefunctions may be classified into two universality classes associated with regular and irregular classical motion. In the regular case $\Psi$, associated with tori, have distinctive anisotropic interference oscillations and the probability density $|\Psi|^2$ peaks on caustics. Irregular wavefunctions have random patterns of oscillation (which becomes isotropic for ergodic systems) and $|\Psi|^2$ vanishes at the classical boundaries in sharp contrast to the caustic structure found for regular states. It should be emphasized that this classification holds true
only for $\hbar \to 0$. Far away from the semiclassical limit it is often difficult to unambiguously assign an eigenstate to either the regular or irregular class. The further studies of eigenfunctions of the stadium, performed by Heller [11] provided new, totally unexpected results. Many eigenfunctions (but not all of them) have strong enhancement of probability amplitude along the classical unstable periodic orbits. This phenomenon has been dubbed *scarring*.

However, the importance of periodic orbits goes far beyond their influence on the structure of eigenstates. We mentioned earlier that the most difficult problem in the semiclassical approximation of quantum mechanics is the treatment of non-integrable systems. Recently, (see Gutzwiller [1] and references therein) it was shown that using the Feynman path integral formalism it is possible to express the trace of the semiclassical Green's function as a sum over all periodic orbits of the corresponding classical Hamiltonian. Gutzwiller successfully applied this method (now known as Gutzwiller's trace formula) to determine the energy levels of a donor impurity in silicon. It should be stressed that the corresponding classical dynamics is completely chaotic. The convincing confirmation of the role of the periodic orbits was provided by experiments with the hydrogen atoms in strong magnetic fields [12]. Using the Gutzwiller trace formula Du and Delos [13-15] were able to relate experimentally observed photon absorption peaks obtained near the ionization threshold of the hydrogen atoms to unstable periodic orbits in the corresponding classical chaotic system. It should be emphasized that the application of the Gutzwiller periodic-orbit theory is by no means simple and it still gives rise to several problems. Among them is the question of the convergence of the sum over the periodic orbits. The applicability of the theory is strongly limited by the fact that the effort for the resolution of single energy levels grows exponentially (due to exponential proliferation of the periodic orbits) when one considers higher energy levels. Nevertheless, semiclassical methods based on the periodic-orbit theory are experiencing a renaissance. The most remarkable demonstration
of their capabilities is the evaluation of the helium atom spectrum by Wintgen et al [16]. This solves the long-standing problem which daunted the old quantum theory and served as midwife to the birth of modern quantum mechanics.

In this thesis we investigate differences between quantum dynamics in the classically regular and classically chaotic regions of phase space for a model Hamiltonian system. This problem was recently studied by, among others Lin and Ballentine [17,18] and Plata and Llorente [19] for a monochromatically driven double-well potential. It was found that a Gaussian wave packet may undergo coherent or incoherent motion depending upon whether the initial position of the wave packet is in the regular or irregular part of the phase space. The Poincaré surface of section of this system has a small regular island in each well immersed in a chaotic sea which extends over both wells. It is shown numerically by Lin and Ballentine [17,18] that a wave packet initially centered on one stability island tunnels to the other one. The tunneling between the classical phase space structures retains its coherent, oscillatory nature despite the fact that the wave packet is not completely embedded in the KAM island. The driven tunneling phenomenon has a rate $10^4$ faster than that for the undriven case and is determined by the energy splitting of a pair of Floquet states localized on two stability regions. Symmetric and antisymmetric combinations of these states yield packets initially localized in each well which in the course of time oscillate between the stability regions. On the other hand if a wave packet is launched from the classically chaotic portion of the phase space it rapidly spreads and covers the entire chaotic sea.

Lin and Ballentine [18] suggest that while localized quasienergy states (in the case of periodically perturbed systems) are associated with regular islands in the classical phase space, the extended states correspond to the chaotic sea. Consequently, if the wave packet is initially located in the regular island its time evolution will be determined by a small number of very well localized quasienergy states. Therefore the time development of the dynamical variables should appear
regular. On the other hand, a packet launched from the chaotic part of the phase space is a superposition of a great number of the extended quasienergy states and produces an erratic time evolution of the dynamical variables. In the present paper we test whether this type of behavior holds for a system described by a driven surface-state-electron (SSE) Hamiltonian and may therefore be generic. The dynamics of the SSE system is quite different from that in the double well potential mentioned above, being very complicated in both the classical and quantum domains.

The driven SSE model has been used to describe the ionization of highly excited hydrogenic atoms. Jensen et al [20] present a quantum mechanism for the suppression of chaotic ionization that, they argue, explains the existence of anomalously stable states observed in the microwave ionization experiments of Koch et al [21]. The mechanism is the peaking of the wave function in the region of the phase space containing unstable periodic orbits, these are Heller’s “scars”. The scarred wavefunction inhibits ionization, since it remains localized in regions of phase space where the classical dynamical orbits are unstable and chaotic. They do point out, however, that we do not have a detailed understanding of the physical mechanisms that cause scarred wave functions. Herein we show that the scarred wave functions noted above may in fact be implicit in the general picture suggested by Lin and Ballentine.

1.2 Outline of the thesis

The thesis is organized as follows. In Chapter 2 we review the essential classical and quantum properties of the driven-SSE model. We describe the methods used to integrate the classical equations of motion and time-dependent Schrödinger equation. We briefly discuss the Floquet formalism which provides deep insight into non-perturbative quantum dynamics of periodically driven systems. We also introduce quantum uncertainty as a dynamical variable. The growth
of quantum uncertainty supersedes the "diffusive" energy increase as a diagnostic
of the system dynamics.

The notion of quantum quasiprobability distribution function and quantum
phase space are the subject of Chapter 3. We examine the properties of the Wigner
and Husimi distribution functions. We also discuss the concept of the quantum
characteristic function which is used to define a general class of quasiprobability
distributions comprising the Wigner, Husimi, and Glauber functions. Using this
approach it is possible to express these three distribution functions in terms of cre-
ation and annihilation operators and establish the connection with the formalism
commonly used in quantum optics.

In Chapter 4 we carefully investigate the influence of the structure of the classi-
cal phase space of the driven SSE model on its quantum dynamics. We present the
results of numerical, quantum calculations for four minimum uncertainty wave
packets launched from the different portions of the phase space. Temporal evolu-
tion of the wavefunctions is visualized with the help of the Husimi distribution
function. The conclusions drawn from the main numerical data are verified by the
supplementary computations performed with the different initial wavefunctions
and/or different values of the model parameters. Quantum dynamics is analyzed
within the Floquet formalism. We display the Husimi representation of the
quasienergy states which play the dominant role in the evolution of the wave pack-
ets under investigation. This Chapter is concluded with the outline of proposed fu-
ture research work.
CHAPTER TWO

HARMONICALLY DRIVEN SURFACE STATE ELECTRON (SSE) MODEL

2.1 Model

Much of our understanding of the quantum dynamics of classically chaotic systems has been initially derived from the extensive investigations of the quantized standard map [22] and references therein. However, the unexpected discovery of the microwave ionization of highly excited hydrogen atoms, in the experiment performed by Bayfield and Koch [23], provided a unique opportunity for direct testing of many intriguing concepts of quantum chaos. It is interesting that after almost twenty years this phenomenon is still the subject of intensive experimental, numerical and theoretical work.

In their original experiment Bayfield and Koch measured the ionization rate of a beam of hydrogen atoms with high principal quantum numbers \( n \sim 66 \) passing through a microwave cavity. Even though the microwave frequency (9.9 GHz) was only approximately 40% of the resonant frequency for a single-photon transition from level 66 to 67 and merely 1% of the photon frequency for excitation to the continuum, efficient ionization occurred when the strength of the field exceeded a threshold value of 20 V/cm. Moreover, the ionization rates were strongly dependent on the intensity of the oscillating electromagnetic field, but only weakly dependent on the frequency, thereby producing a quantum paradox.

Conventional quantum theory was unable to account for the experimental observations. Since the microwave frequency was smaller than the classical orbital frequency, Stark ionization at the peak values of the electrical field was initially considered as a possible explanation. However, the actual calculations yielded ionization rates sharply lower than those found in the experiment. Another likely
mechanism for the enhanced ionization was multiphoton absorption. One should realize that since almost one hundred photons are necessary to excite an electron into the continuum the corresponding perturbation theory would require one hundred orders of perturbation which renders this type of theoretical treatment intractable.

On the other hand, a numerical simulation by Leopold and Percival [24] showed that classical mechanics could reproduce the experimental data quite well. The physical mechanism responsible for the enhanced ionization was identified as the stochastic diffusion of electrons in phase space. In other words, the ionization takes place whenever the chaotic trajectories wander into the continuum. Kolmogorov-Arnold-Moser (KAM) theory guarantees that for small amplitude microwave fields most of the trajectories remain regular so that the strength of the perturbation must exceed a critical threshold before the classical orbits become sufficiently chaotic to cause significant ionization. The detailed investigation of the transition to global stochasticity was hindered by the fact that the electrons move in a six-dimensional phase space. To circumvent this problem Jensen [25-26] proposed to describe both classical and quantum dynamics with a much simpler one-dimensional Hamiltonian which in atomic units may be written as

\[ H = H_0 (x, p) + V(x, t) \]  

(2.1.1)

where

\[ H_0 = \frac{p^2}{2} + \begin{cases} \infty, & x \leq 0 \\ -\frac{1}{x}, & x > 0 \end{cases} \]  

(2.1.2)

and

\[ V = xFg(t) \cos (\Omega t). \]  

(2.1.3)

\( F \) is the peak amplitude of the driving force, \( \Omega \) is its frequency and \( g(t) \) is a slow slowly varying envelope function chosen to mimic the way in which the external
perturbation is turned on.

The Hamiltonian $H_0$ was originally used for the treatment of surface-state electrons which are weakly bound to the surface of liquid helium by their image charge. Grimes and his collaborators [27] studied these electrons under various conditions and showed that the effective binding potential depends exclusively on the relative distance $x$ between the electron and its image charge. To a good approximation it has the form $V_{\text{eff}} = -Ze/x$ where $Ze$ is the induced image charge. The Pauli exclusion principle makes the liquid helium surface act as an infinite repulsive wall. Classically, an electron oscillates between this infinite wall (helium surface) and the turning point of the one-dimensional attractive Coulomb potential.

Using Chirikov's resonance overlapping criterion Jensen [25-26] was able to derive the analytic estimate for the onset of the chaotic dynamics in the driven SSE model. He also worked out the excitation and ionization rates as functions of frequency and the intensity of the perturbation. These calculations were in good agreement with the experimental data for the ionization of the hydrogen atoms and consequently stimulated a great interest in this model. Moreover, the two and three dimensional numerical calculations yielded quite similar results which to some extent established the validity of the SSE model, at least in the classical domain. Quantum mechanical numerical calculations are intrinsically time consuming regardless of the method employed to solve the time-dependent Schrödinger equation. Only very recently Buchleitner and Delande [28] reported the first three-dimensional quantum calculations which confirmed that 1D quantum dynamics can mimic the 3D behavior reasonably well.

2.2 Classical properties

Classically the Hamiltonian (2.1.1) describes both bounded and unbounded dynamical behavior. In the former case the Hamiltonian may be rewritten in action-
angle variables \((I, \Theta)\) \(^{[29]}\) (See Appendix A1 for the complete derivation):

\[
H(I, \Theta) = -\frac{1}{2I^2} + 2I^2 F g(t) \sin^2(\eta) \cos(\Omega t) \tag{2.2.1}
\]

where the canonical variables \((x, p)\) can be expressed as

\[
x = 2I^2 \sin^2(\eta) \tag{2.2.2}
\]

\[
p = \frac{1}{I} \cot(\eta). \tag{2.2.3}
\]

The auxiliary variable \(\eta\) determines the angle variable by means of

\[
\Theta = 2\eta - \sin(2\eta). \tag{2.2.4}
\]

The unperturbed motion with constant action \(I_0\) has the Kepler frequency \(\omega = 1/I_0^3\) and the total energy \(E = -1/(2I_0^2)\) which is the familiar expression for the hydrogenic energy spectrum. The graph of the corresponding trajectory in action-angle space is a not particularly enlightening straight line, so that in Fig. 1 the orbits with action \(I_0 = 1, 5, 10\) are shown in ordinary phase space. Instead of drawing a continuous line a kind of stroboscopic technique was used to show that a Kepler electron spends most of the time in the vicinity of the turning point \(x_{I_0} = 2I_0^2, p_{I_0} = 0\). It can be seen from Fig. 1 that with the increasing action the classical trajectories are elongated in phase space along the position axis and simultaneously contracted along the momentum axis.

To facilitate further discussion in this paragraph we choose \(g(t)\) as a unit step function (alternatively, we could write this envelope function in the form \(g(\Omega t)\)). In this case Hamilton’s equations of motion generated by (2.2.1) have a useful scaling property: if \(I(t), \Theta(t)\) are the dynamical variables for the Hamiltonian with parameters \(F, \Omega\) and the initial conditions \(I_0, \Theta_0\) then \(\Theta'(t') = \Theta(t/I_0^3)\) and
\[ I(\tau') = I(t / I_0^2) / I_0 \] are the scaled variables for the Hamiltonian with the parameters

\[ F' = F l_0^4, \quad \Omega' = \Omega I_0^3 \tag{2.2.5} \]

and the initial conditions \( I, \Theta_0 \). Equivalently Hamiltonian (2.1.1) remains invariant under the transformation

\[ F' = F \gamma^4, \quad \Omega' = \Omega \gamma^3, \quad t' = t / \gamma^3, \quad x' = x / \gamma^2 \tag{2.2.6} \]

with \( \gamma \) being any real number.

Under appropriate conditions, the driven SSE system undergoes a transition to chaotic dynamics. This transition is associated with a profound change in the nature of most classical trajectories. Above a certain threshold value of the driving force the orbits become intricate and extremely sensitive to any perturbation. They erratically wander in phase space and usually ionize rapidly.

A qualitative estimate for the occurrence of chaos in a periodically forced nonlinear oscillator may be obtained from Chirikov's resonance overlap criterion [30]. This approach is heuristic but it is physically appealing because of the kind of arguments it evokes, even though in its original formulation it is mathematically rather abstruse.

The starting point of this analysis is the observation that the external force more effectively perturbs the undisturbed motion at the first-order resonances, i.e. at the values of the unperturbed action such that the external frequency \( \Omega \) resonates with the angular (Kepler) frequency \( \omega(I) \):

\[ \Omega = m \omega(I), \quad m = 1, 2... \tag{2.2.7} \]

However, \( \omega(I) \) is a nonlinear function of the action. Even though initially the perturbation may be very effective, as soon as it distorts the original orbit the reso-
nant condition (2.2.7) is no longer satisfied and nonlinear stabilization may occur. In that case the motion is confined to a neighborhood of the unperturbed trajectory called a resonance zone or resonance region. Note that for a linear oscillator the amplitude of the response is infinite at the resonant frequency. On the contrary, the amplitude of the nonlinear oscillator precisely at the resonant frequency is zero. The width of the resonance region may be estimated taking into account that within the resonance zone the response of the system is oscillatory, i.e., the nonlinear pendulum Hamiltonian fairly accurately describes the system's dynamics. As the strength of the driving force increases, the resonance zones become larger and eventually adjacent zones overlap each other. In that case the motion can be driven so far away from the original resonant value of the action that it falls under the influence of the nearby resonance. The same process may repeat so that the orbit may erratically wander anywhere in the accessible region of action-angle space.

The above analysis applied to the driven SSE model gives the following criterion for the overlap of the nonlinear resonances [31]

\[ F > \frac{1}{50\Omega^{1/3}}. \]  

(2.2.8)

It should be emphasized that this estimate is valid only for \( \Omega' > 1 \). If \( \Omega' < 1 \), i.e., in the region of the phase space where \( \Omega \) is smaller than the Kepler frequency, there are no the first-order resonances and consequently the motion is more stable. The transition to chaos may still occur due to the finite width of the resonance region at \( \Omega' = 1 \) but the higher order resonances

\[ n\Omega = m\omega \left( l \right), \quad n > 1, \quad n > m \]  

(2.2.9)

must be taken into account. High-order resonances also play a role in the chaotic transition for \( \Omega > 1 \) and their contribution was approximately taken into account in (2.2.8) by the choice of the numerical coefficient.
The classical equations of motions corresponding to the Hamiltonian (2.1.1) may be integrated only numerically. However, the calculations are complicated by the singularity of the potential at $x = 0$. To circumvent this difficulty the regularization method suggested by Leopold and Richards [32] may be applied. It is based upon the use of the extended-phase space in which time and energy are considered as two additional conjugate variables. In this way the theory of canonical transformations may be extended to include time [33] since it is one of the generalized coordinates. In the case of the driven SSE Hamiltonian the extended-phase space is four-dimensional $(x, p, t, p_2)$ with $p_2 = -H(x, p, t)$ being a generalized momentum conjugated to $t$. We introduce the new Hamiltonian given by:

$$\Gamma^* = p_2 + H(x, p, t)$$  \hspace{2cm} (2.2.10)

which is by definition identically equal to zero. If we parametrize the trajectories in the extended phase by $t^*$ one of the Hamilton's equations of motion reads

$$\frac{dt}{dt^*} = \frac{\partial}{\partial p_2} \Gamma^* = 1$$  \hspace{2cm} (2.2.11)

or

$$t = t^* + \text{const.}$$  \hspace{2cm} (2.2.12)

The remaining equations are the same as in standard Hamiltonian theory. In this formalism the time transformation is accomplished by multiplying $\Gamma^*$ by an arbitrary function. In order to remove the singularity at $x = 0$ the new Hamiltonian may be formed:

$$\Gamma = 4x\Gamma^* = 4xp_2 + 2xp^2 + 4Fg(t)x^2\cos(\Omega t) - 4.$$  \hspace{2cm} (2.2.13)

The canonical transformation

$$x = q_1^2, p_1 = 2q_1p$$  \hspace{2cm} (2.2.14)
and the change of notation $t \rightarrow q_2, \Gamma + 4 \rightarrow \Gamma$ enables one to write (2.2.13) as

$$\Gamma = \frac{1}{2} p_1^2 + 4 p_2 q_1^2 + 4 F g (q_2) q_1^4 \cos (\Omega q_2). \quad (2.2.15)$$

When $g(t)$ is chosen as a unit step function then the Hamiltonian $\Gamma$ yields the following equations of motion:

$$\dot{q}_1 = \frac{\partial \Gamma}{\partial p_1} = p_1 \quad (2.2.16)$$

$$\dot{p}_1 = -\frac{\partial \Gamma}{\partial q_1} = -8 q_1 p_2 - 16 F q_1^3 \cos (\Omega q_2) \quad (2.2.17)$$

$$\dot{q}_2 = \frac{\partial \Gamma}{\partial p_2} = 4 q_1^2 \quad (2.2.18)$$

$$\dot{p}_2 = -\frac{\partial \Gamma}{\partial q_2} = 4 F \Omega q_1^4 \sin (\Omega q_2). \quad (2.2.19)$$

To optimize the numerical calculations the set of equations (2.2.16-19) may be used in the vicinity of the singularity and the standard Hamiltonian equations of motions may be integrated elsewhere.

2.3 Quantum properties

Throughout this Section atomic units are consistently used. The Schrödinger equation corresponding to the unperturbed Hamiltonian (2.1.2) then reads

$$-\frac{1}{2} \frac{d^2}{dx^2} \Phi (x) - \frac{1}{x} \Phi (x) = \epsilon \Phi (x), x \geq 0 \quad (2.3.1)$$

where $\Phi (x) = \langle x | \Phi \rangle$ is the coordinate representation of the eigenfunction $|\Phi \rangle$. The boundary condition at $x = 0$ implies that $\Phi (x) = 0$ for $x < 0$. The solution to (2.3.1) may be conveniently found in the momentum representation [34]. Introducing the momentum space or $p$-space wave function
where \( \Phi_\varepsilon (x) = \langle x | \Phi_\varepsilon \rangle \) is the coordinate representation of the eigenfunction \( |\Phi_\varepsilon \rangle \) and the boundary condition at \( x = 0 \) implies that \( \Phi_\varepsilon (x) = 0 \) for \( x < 0 \). The solution to (2.3.1) may be conveniently found in the momentum representation [34]. Introducing the momentum space or \( p \)-space wave function

\[
\Phi_\varepsilon (p) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \Phi_\varepsilon (x) e^{-ipx} dx
\]

one may transform (2.3.1) into the first-order differential equation

\[
(\varepsilon - p^2/2) \frac{d\Phi_\varepsilon}{dp} = (p + i) \Phi_\varepsilon.
\]

It follows from (2.3.2) that the integral path of the inverse Fourier transform should be in the lower half of the \( p \)-plane.

For the bounded states (\( \varepsilon = -|\varepsilon| \)) the direct integration of (2.3.3) gives

\[
\Phi_\varepsilon (p) = \frac{B}{(|\varepsilon| + p^2/2)} e^{[i/2/|\varepsilon| \text{acot} (p/2|\varepsilon|)]}
\]

where the constant \( B \) may be determined from the normalization of the wave function. Since \( \Phi_\varepsilon (p) \) must be singled valued and \( \text{acot} \) has the period of \( \pi \) the following condition must be satisfied

\[
\sqrt{2/|\varepsilon|} \pi = 2n\pi, n = 1, 2, \ldots
\]

which implies that the negative energies are discrete \( \varepsilon_n = -1/(2n^2) \). The corresponding normalized eigenfunction is given by

\[
\Phi_n (p) = \frac{2n}{\sqrt{n}} \frac{1}{\sqrt{1 + n^2 p^2}} e^{[2in \text{acot} (np)]} = \frac{2n}{\sqrt{n}} \frac{(np + i)^{n-1}}{(np - i)^{n+1}}.
\]
The second form of the eigenfunction in (2.3.6) may be obtained with the help of the relation

\[ \text{acot}(z) = -\frac{1}{2i} \ln \left( \frac{1 + z i}{1 - z i} \right). \]  

(2.3.7)

The examples of the eigenfunctions \( \Phi_n(p) \) are provided in Fig. 2 and one may see that while their real parts are even functions of \( p \) their imaginary parts are odd functions.

In Appendix A2 the eigenvalue problem for the SSE Hamiltonian \( H_0 \) is solved using the standard power series method. It is found that the coordinate representation of the eigenfunction \( |\Phi_n\rangle \) is given by

\[ \Phi_n(x) = \frac{2}{n^{3/2}} xe^{-x/n} L_n^{(1)} \left( \frac{2x}{n} \right), \]  

(2.3.8)

\( L_n^{(1)} \) in (2.3.8) are associated Laguerre polynomial. In principle this formula may be derived by taking the inverse Fourier transform of (2.3.6). The eigenfunctions (2.3.8) are closely related to the hydrogenic radial functions \( R_{n,l}(r) \):

\[ \Phi_n(x) = R_{n,0}(x)/x \]  

(2.3.9)

where the Cartesian distance \( x \) replaces the radial distance \( r \) as the argument of \( R_{n,l} \). Fig. 3 shows the graphs of the eigenfunctions \( \Phi_n(x) \) for the principal quantum numbers used in Fig. 2.

The Schrödinger equation for the driven SSE model may be written as

\[ i \frac{\partial}{\partial t} |\Psi\rangle = -\frac{1}{2} \frac{\partial^2}{\partial x^2} |\Psi\rangle - \frac{1}{x} |\Psi\rangle + x F_g(t) \cos(\Omega t) |\Psi\rangle \]  

(2.3.10)

There is no analytical solution to (2.3.10) and numerical methods must be used to obtain the time-evolution of the wave function. In the most straightforward ap-
The approach to the wave function is expanded in the basis of eigenfunctions $|\Phi_n\rangle$ of the unperturbed Hamiltonian (2.1.2):

$$|\Psi(t)\rangle = \sum_n c_n(t) |\Phi_n\rangle e^{-i\varepsilon_n t}. \quad (2.3.11)$$

Then (2.3.10) leads to the set of coupled differential equations for the expansion coefficients $c_n(t)$:

$$i\dot{c}_n(t) = \sum_{n'} e^{i\omega_{nn'} t} f_g(t) \cos (\Omega t) x_{nn'} c_{n'}(t) \quad (2.3.12)$$

$$\omega_{nn'} = \varepsilon_n - \varepsilon_{n'}, \quad x_{nn'} = \langle \Phi_n | \hat{Q} | \Phi_{n'} \rangle. \quad (2.3.13)$$

The diagonal matrix element of the $\hat{Q}$ operator is found analytically to be

$$x_{nn} = \frac{3}{2} n^2. \quad (2.3.13)$$

To obtain the off-diagonal matrix elements $x_{nn'}$ we employed the convenient method originally proposed by Susskind and Jensen [34] which relies on the momentum space representation of the basis function (2.3.6) and the observation

$$\langle \varepsilon_n - \varepsilon_{n'} | \hat{Q} | \Phi_{n'} \rangle = i \langle \Phi_n | \hat{P} | \Phi_{n'} \rangle. \quad (2.3.14)$$

The above formula may be obtained by computing the matrix elements of $[\hat{Q}, \hat{H}_0] = i\hat{P}$ between the eigenfunctions of $\hat{H}_0$. Using (2.3.6) and (2.3.14):

$$x_{nn'} = -\frac{8}{\pi} \frac{(nn')^{5/2}}{(n^2 - n'^2)} \int_0^\infty p \sin [2n \text{acot} (np) - 2n' \text{acot} (n'p)] \frac{(1 + n^2p^2) (1 + n'^2p'^2)}{(1 + n^2p^2) (1 + n'^2p'^2)} dp. \quad (2.3.15)$$

However expansion (2.3.11) does not take into account the excitation into the continuum and numerical tractability requires the use of a truncated basis. For the strength of the driving force considered in this work continuum effects have been
found to be negligible [31,35]. The main consequence of the use of the finite basis is the possible modification of probability when the levels close to the edge of the basis set become significantly populated. This affect may considerably distort the results of the numerical simulations. To assess how the results are influenced by the truncated basis approximation it is necessary to perform the calculations with several different sizes of the basis.

Both quantum and classical temporal evolutions strongly depend on the form of the envelope function $g(t)$. When the driving force is applied instantaneously ($g(t)$ is the unit step function) the periodicity of the Hamiltonian (2.1.1) may be exploited within the framework of the Floquet formalism [29,36-42]. In this case the time evolution of the wave function is completely determined by a one-cycle unitary propagator $\hat{C}$

$$|\Psi((N+1)T)\rangle = \hat{C}|\Psi(NT)\rangle$$

(2.3.16)

where $T = 2\pi/\Omega$. The eigenvalue problem for $\hat{C}$ may be written as

$$\hat{C}|x_n\rangle = e^{-iE_n} |x_n\rangle$$

(2.3.17)

where the $E_n$, called quasi energies, are real and their corresponding eigenvectors are frequently called Floquet or quasienergy states (QES). To obtain the matrix representation of $\hat{C}$ in the basis of the $\hat{H}_0$ eigenfunctions we notice that

$$\langle \Phi_j \lvert \Psi(T) \rangle = \sum_k \langle \Phi_j \lvert \hat{C} \lvert \Phi_k \rangle \langle \Phi_k \lvert \Psi(0) \rangle$$

(2.3.18)

and if we choose the initial state such that

$$\langle \Phi_k \lvert \Psi(0) \rangle = \delta_{k,j}$$

(2.3.19)

then
\[ \langle \Phi_j | \Psi(T) \rangle = \langle \Phi_j | \hat{C} | \Phi_j \rangle. \] (2.3.20)

Thus the \( j \)’ column of the matrix representation of \( \hat{C} \) may be calculated using the initial conditions (2.3.19) and integrating the time-dependent Schrödinger equation over one period of the perturbation. We can then numerically solve the eigenvalue problem (2.3.17).

For times \( t = NT \) the wave function may be written as:

\[ |\Psi(NT)\rangle = \sum_n e^{-iE_n N} |\chi_n\rangle \langle \chi_n | \Psi(0) \rangle \] (2.3.21)

It is apparent from (2.3.21) that only the Floquet states overlapping the initial wavefunction contribute to its subsequent time evolution. Moreover, when the initial state is a pure state with \( c_{m_0}(0) = 1 \) then the amplitude \( c_m(NT) \) to excite any given state \( |\Phi_m\rangle \) after \( N \) cycles of the perturbation is given by

\[ c_m(NT) = \sum_n \langle \Phi_m | \chi_n \rangle e^{-iE_n N} \langle \chi_n | \Phi_{m_0} \rangle. \] (2.3.22)

In order to induce a \( |\Phi_{m_0}\rangle \rightarrow |\Phi_{m'}\rangle \) transition there has to be at least one Floquet state which connects \( |\Phi_{m_0}\rangle \) with \( |\Phi_{m'}\rangle \). Thus the degree of localization of the Floquet states affects the efficiency with which the systems absorbs the external energy.

The propagation of a wave packet is described herein by the quantum uncertainty \( U \) which is the product of the position uncertainty \( \Delta X \) and the momentum uncertainty \( \Delta P \):

\[ U = \Delta X \Delta P. \] (2.3.23)

The position uncertainty is given by the variance
\[ \Delta X(t) = \sqrt{\langle \Psi(t) | \dot{Q}^2 | \Psi(t) \rangle - (\langle \Psi(t) | \dot{Q} \Psi(t) \rangle)^2} \]  

(2.3.24)

and the momentum uncertainty is given by the variance

\[ \Delta P(t) = \sqrt{\langle \Psi(t) | \dot{P}^2 | \Psi(t) \rangle - (\langle \Psi(t) | \dot{P} \Psi(t) \rangle)^2}. \]  

(2.3.25)

Using the expansion (2.3.11) we may write the moments in (2.3.24) and (2.3.25) generically as

\[ \langle \Psi(t) | \dot{O} | \Psi(t) \rangle = \sum_{i,j} c_i^*(t) c_j(t) \langle \Phi_i | \dot{O} | \Phi_j \rangle e^{i\omega t}, \]  

(2.3.26)

where \( \dot{O} = \dot{Q}, \dot{Q}^2, \dot{P}, \dot{P}^2, \) etc. The above coefficients \( c_i(t) \) are either solutions to equations (2.3.12) or for times equal to multiples of period \( t = NT \) may be obtained by the application of the Floquet mapping. The non-diagonal matrix elements of the \( \dot{Q} \) operator are given by (2.3.15) and employing (2.3.14) the non-diagonal matrix elements for the \( \dot{P} \) operator may easily be calculated:

\[ p_{nn'} = \langle \Phi_n | \dot{P} | \Phi_{n'} \rangle = i q_{nn'} (\epsilon_n - \epsilon_{n'}), \]  

(2.3.27)

while

\[ p_{nn} = 0. \]  

(2.3.28)

The calculation of the matrix elements for \( \dot{Q}^2 \) and \( \dot{P}^2 \) may be efficiently performed in the momentum space representation, using (2.3.6) one obtains

\[ \begin{align*}
\dot{P}_{nn'}^2 &= \frac{4 \sqrt{nn'}^\infty_0 p^2 \cos \left[ \frac{2n \text{acot}(np) - 2n' \text{acot}(n'p)}{1 + n^2 p^2} \right]}{(1 + n^2 p^2) (1 + n'^2 p^2)} dp, \\
\dot{P}_{nn}^2 &= \frac{1}{n^2}. 
\end{align*} \]  

(2.3.29)
To evaluate the matrix elements of $\hat{Q}^2$ one additionally employs its momentum space representation $-\frac{\partial^2}{\partial p^2}$ to arrive at

$$x^2_{nn'} = \frac{8n^2\sqrt{nn'}}{\pi} \int_0^\infty \frac{(3n^2p^2 - 2n^2 - 1)\cos(f) - 6n^2psin(f)}{(1 + n^2p^2)^3(1 + n^2p^2)} dp$$

(2.3.31)

$$f = 2n'\text{acot}(n'p) - 2n\text{acot}(np),$$

$$x^2_{nn} = \frac{n^2(1 + 5n^2)}{2}. \quad (2.3.32)$$

Using (2.3.13), (2.3.28), (2.3.30), (2.3.32) it is possible to derive the following formula for the position uncertainty $\Delta X_n$, the momentum uncertainty $\Delta P_n$ and the total uncertainty $U_n$ of the eigenstate $|\Phi_n\rangle$ of the unperturbed Hamiltonian $\hat{H}_0$: 

$$\Delta X_n = n\sqrt{\frac{1}{2} + \frac{1}{4}n^2} \quad (2.3.33)$$

$$\Delta P_n = \frac{1}{n} \quad (2.3.34)$$

$$U_n = \sqrt{\frac{1}{2} + \frac{1}{4}n^2}. \quad (2.3.35)$$

From equation (2.3.35) we can see that for large $n$ the quantum uncertainty grows approximately linearly with $n$. The integrals in (2.3.6), (2.3.29) and (2.3.31) have been calculated numerically and in some cases tested against the analytical results obtained with the help of the symbolic algebra packages (e.g. Mathematica). In the case of the dipole matrix elements $x_{nn'}$ the following approximate formula, derived by Blümel and Smilansky [43], was found useful during
the development of the relevant software:

\[ x_{nn}^{(a)} = -C \left( \frac{\varepsilon_n \varepsilon_{n'}}{|\varepsilon_n - \varepsilon_{n'}|} \right)^{3/4} \left( 1 + D \frac{\varepsilon_n + \varepsilon_{n'}}{|\varepsilon_n - \varepsilon_{n'}|^{2/3}} \right) \]  

(2.3.36)

where \( C \approx 1.162, D \approx 0.2177 \). The relative error of the matrix elements calculated in this way is uniformly less than \( 1.6 \times 10^{-2} \) for all \( n \) and \( n' \). Moreover, it is a rapidly decreasing function of \( |n - n'| \). Blümel and Smilansky also considered the modified version of (2.3.36)

\[ x_{nn'}^{(m)} = (1 + \tau_{|n - n'|}) x_{nn'}^{(a)} \]  

(2.3.37)

where \( \tau_{|n - n'|} \) are the "experimental" correction parameters (listed in their paper) used to enhance the accuracy of the matrix elements for which \( |n - n'| < 10 \). The relative error in this case is less than \( 4.2 \times 10^{-3} \) for all \( n \) and \( n' \).

The properties of the SSE Hamiltonian are conveniently described in terms of the scaled parameters (2.2.5) and in the quantum case the initial action \( I_0 \) is replaced by the principal quantum number \( n_0 \) of the initial state. One should realize, however, that the quantum system does not obey the classical scaling relations.

Evaluating the commutator of the quantal operators \( \hat{Q}' \) and \( \hat{P}' \) associated with the classically scaled position and momentum, cf. (2.2.6), one obtains

\[ \{ \hat{Q}', \hat{P}' \} = \frac{i\hbar}{n_0} = i\tilde{h}_{\text{eff}} \]  

(2.3.38)

and \( \tilde{h}_{\text{eff}} = \tilde{\hbar}/n_0 \) may be interpreted as an effective Planck's constant. Thus, with fixed \( n_0^3\Omega \) and \( n_0^4F \), it is possible to control the value of \( \tilde{h}_{\text{eff}} \) simply by varying the initial principal quantum number. It is interesting that the existing technology allows us in principle to change \( \tilde{h}_{\text{eff}} \), in the experiments with the Rydberg hydrogen
atoms, by at least one order of magnitude. The technical details of this problem are briefly discussed by Koch [44].

With increasing scaled frequency $\Omega'$ the differences between classical and quantum dynamics become apparent [31]. When $\Omega' \gg 1$ the chaotic, diffusive behavior present in the classical system for a sufficiently strong perturbation (fairly well estimated by (2.2.8)) appears to be completely inhibited in the quantum domain. The "diffusive behavior" in the quantum case may only be observed after the application of a perturbation which is much stronger than that required in the classical system. This striking property of the driven SSE model focused sharp attention on high scaled frequency experiments with the Rydberg hydrogen atoms. The subsequent measurements [45,46] confirmed the numerical and theoretical predictions. However, the detailed theoretical explanation of these experiments is the subject of continuing controversy in the literature.

From (2.2.6) it is apparent that one can increase the value of the scaled frequency simply by choosing an initial state with a higher principal quantum number and maintaining the frequency of the driving force. Since the typical principal quantum numbers are usually high, this contradicts the intuition that the results of quantum mechanics and classical mechanics should converge in the limit of high quantum numbers or equivalently for small values of Planck's constant.

The quantum mechanical inhibition of classical diffusive energy growth (quantum suppression of chaos) was first observed in the numerical experiments on the periodically kicked quantum rotator [47]. This phenomenon is also known as "dynamical localization" since it is possible to establish a rather formal analogy with Anderson localization of the electronic wavefunction in disordered solids. This equivalence has been established both for the kicked rotator and with some approximations also for the driven SSE model. However, Anderson localization is known to be peculiar to one-dimensional tight-binding Hamiltonian and in higher
dimensional cases extended states can be found [48]. The latest three-dimensional numerical quantum calculations performed by Buchleitner and Delande [28] provided the first evidence of persistence of the dynamical localization in higher-dimensional systems.
CHAPTER THREE

DISTRIBUTION FUNCTIONS IN QUANTUM MECHANICS

3.1 Introduction

Properties of systems governed by classical mechanics are conveniently studied in a phase space representation. However, the uncertainty principle precludes the direct transfer of this concept and that of distribution functions to quantum mechanics. Said differently, since a particle cannot simultaneously have a well-defined position and momentum it is not possible to define a phase space probability density that a particle has a specific position \( q \) and momentum \( p \). Nonetheless so-called quasiprobability distribution functions have been found to be useful as calculation tools and to provide deep insight into the connection between classical and quantum mechanics.

Quantum mechanics in its usual form is concerned with the properties of vectors and operators in a Hilbert space: each state of a system corresponds to a vector, each observable quantity to an operator [49]. Quantum mechanical distribution functions provide a framework for an exact reformulation of quantum mechanics in which ordinary functions in a phase space are associated with both states and observable quantities.

The most complete and systematic phase space representation of quantum mechanics was achieved with the use of the Wigner function [50] originally introduced in 1932 for a treatment of quantum corrections to thermodynamics. Although the Wigner function has very interesting properties it is not positive definite, so that formally it cannot be considered to be a probability density function. For this reason non-negative distribution functions related to the Wigner distribution were pursued. As early as 1940 Husimi [51] introduced one such non-nega-
tive distribution, now commonly referred to as the Husimi distribution. It may be defined as a convolution of the Wigner distribution with a Gaussian smoothing function. The Husimi function is the simplest example of a more general scheme of generating non-negative distribution functions by smoothing (coarse-graining or smearing) the original Wigner distribution with another function. This method was proposed by Cohen [52] and further examined by Summerfield and Zweifel [53]. Different choices of smearing functions define different special classes of non-negative distribution functions, each of them may be used for a unique phase space reformulation of quantum mechanics.

The development of the phase space formalism based on the Husimi concept turned out to be surprisingly slow. For example, the time evolution law and the Bloch equation were derived by O'Connell et al more than forty years after Husimi's original work [54,55].

Many authors have considered other distribution functions the most commonly being that of Glauber [56,57] and Sudarshan [58] which found extensive applications in quantum optics. In the further discussion of the quantum phase space formalism herein the emphasis is put on the Wigner and Husimi distribution functions.

This Chapter is organized as follows: in Section 2 the concept of the Weyl transform, which constitutes the mathematical foundation of the Wigner formalism, is introduced. In Section 3 the fundamental properties of the Wigner function are reviewed. In Section 4 the coarse-graining process of the Wigner function which leads to the Husimi representation is elucidated. The important differences between these two formulations are also discussed. Section 5 concerns the concept of the characteristic function used to define a general class of quasiprobability distributions comprising the Wigner, Husimi and Glauber functions. Section 6 provides examples of the Wigner and Husimi distributions for the eigenstates of
the SSE Hamiltonian.

3.2 Weyl transformation

In the traditional formulation of quantum mechanics a state of the system is represented by a vector in a Hilbert space while a physical quantity corresponds to an operator in this space. The alternative description of quantum mechanics, preserving the whole physical content of the usual approach, is based upon the mapping of both state vectors and operators into ordinary functions in phase space. In the next two Sections an example of such a representation which has become known as Wigner-Weyl Phase Space Representation (WWPSR) [50,59-64] is reviewed.

The discussion in this Section is based upon the approach presented by Leaf [63,64] and de Groot et al [49] and for brevity is confined to a particle in one dimension. Generalization to multiparticle, multidimensional cases is straightforward but requires the introduction of indices labeling particles and summation signs which makes equations much longer. Some numerical coefficients related to space dimensionality are obviously different.

A few formulae of ordinary quantum mechanics are listed below to facilitate the following derivations. It is assumed in this Section that the limits of integration are infinite except where explicitly stated.

The momentum and coordinate operators \( \hat{P} \) and \( \hat{Q} \) obey the commutation relations:

\[
[\hat{p}, \hat{P}] = 0, \quad [\hat{Q}, \hat{Q}] = 0, \quad [\hat{Q}, \hat{P}] = i\hbar
\]  
(3.2.1)

Their eigenvectors \( |p\rangle \) and \( |q\rangle \) are defined by the eigenvalue equations

\[
\hat{P} |p\rangle = p |p\rangle, \quad \hat{Q} |q\rangle = q |q\rangle
\]  
(3.2.2)
and form complete orthogonal basis in Hilbert space

\[ \int dp \langle p | p \rangle = I, \int dq \langle q | q \rangle = I \]  

(3.2.3)

\[ \langle p | p' \rangle = \delta (p - p'), \langle q | q' \rangle = \delta (q - q'). \]  

(3.2.4)

The eigenfunctions of the momentum operator in the coordinate representation are given by

\[ \langle q | p \rangle = \frac{1}{\sqrt{2\pi \hbar}} e^{ipq}. \]  

(3.2.5)

The trace of an arbitrary quantum mechanical operator \( \hat{A} \) may be expressed in terms of the complete sets \( | p \rangle \) and \( | q \rangle \) as

\[ Tr[\hat{A}] = \int dp \langle p | \hat{A} | p \rangle = \int dq \langle q | \hat{A} | q \rangle. \]  

(3.2.6)

For two operators \( \hat{A}, \hat{B} \) which commute with their commutator, i.e.

\[ [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0 \]  

the Hausdorff-Baker relation holds

\[ e^{\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{\hat{A}} e^{1/2 [\hat{A}, \hat{B}]} . \]  

(3.2.7)

The Dirac delta function has the following integral representation

\[ \delta (x) = \frac{1}{2\pi} \int e^{ikx} dk. \]  

(3.2.8)

By using the closure relations (3.2.3) one may obtain the following identity for an arbitrary operator \( \hat{A} \)

\[ \hat{A} = \int dp' dp'' dq' dq'' |q''\rangle \langle q''| \langle p''| \hat{A} | p' \rangle \langle p'| q' \rangle \langle q' |. \]  

(3.2.9)

After the change of variables \( p' = p - u/2, p'' = p + u/2, q' = q - v/2, q'' = q + v/2 \) with the corresponding Jacobian equal to unity (3.2.9) may be
written as
\[ \hat{A} = \frac{1}{\hbar} \int dp dq a_w(p, q) \hat{A}(p, q) \quad (3.2.10) \]

where
\[ a_w(p, q) = \int d\nu e^{\frac{i}{\hbar} \nu (p + \frac{1}{2} u | \hat{A} p - \frac{1}{2} u)} \quad (3.2.11) \]

and the Hermitian operator \( \hat{\Delta}(p, q) \) independent of \( \hat{A} \) is given by
\[ \hat{\Delta}(p, q) = \int d\nu e^{\frac{i}{\hbar} \nu (q + \frac{1}{2} v | \hat{A} q - \frac{1}{2} v)} . \quad (3.2.12) \]

The function \( a_w(p, q) \) is called the Weyl transform of the operator \( \hat{A} \). In this way each operator may be associated with, in general, a complex valued phase-space function. However, if \( \hat{A} \) is Hermitian \( a_w(p, q) \) is real. This can easily be seen if one notices that the rhs of (3.2.11) is a Fourier transform of
\[ a(u) = \langle p + \frac{1}{2} u | \hat{A} | p - \frac{1}{2} u \rangle \]
and
\[ a(-u) = \langle p - \frac{1}{2} u | \hat{A} | p + \frac{1}{2} u \rangle = \langle p + \frac{1}{2} u | \hat{A} | p - \frac{1}{2} u \rangle^* = a^*(u) \quad (3.2.13) \]

which follows from the hermiticity of \( \hat{A} \). Thus it stems from (3.2.13) that \( a_w(p, q) \) is real.

Throughout this Chapter the correspondence between an operator and its Weyl transform is denoted by the symbol \( (\ldots)_W \).

Interchanging the roles of \( q \) and \( p \) in (3.2.9) one obtains a new identity
\[ \hat{A} = \int dp' dp'' dq' dq'' | p'' \rangle \langle p'' | q'' \rangle \langle q'' | \hat{A} | q' \rangle \langle q' | p' \rangle | p' \rangle \quad (3.2.14) \]
which with the help of the same arguments yields the counterpart of (3.2.11)

\[ a_w(p, q) = \int dve^\hbar \left< q - \frac{1}{2} v \right| \hat{\Lambda} \left| q + \frac{1}{2} v \right> \]  

(3.2.15)

and (3.2.12)

\[ \hat{\Lambda}(p, q) = \int dve^\hbar \left| p - \frac{1}{2} u \right> \left< p + \frac{1}{2} u \right| \]  

(3.2.16)

It is possible to derive a symmetrical form of (3.2.12) with respect to $q$ and $p$.

First one should notice that

\[ |q + \frac{1}{2} v\rangle = e^{\frac{i}{\hbar} v p} |q - \frac{1}{2} v\rangle \]  

(3.2.17)

which may be proved by multiplication with $|p\rangle$ and the use of (3.2.2) and (3.2.5). If (3.2.17) is substituted into (3.2.12) one encounters the projection operator

\[ \left| q - v/2 \right> \langle q - v/2 \right| \]  

which may be rewritten with the help of identity

\[ |q\rangle \langle q| = \frac{1}{\hbar} \int e^{\hbar} du. \]  

(3.2.18)

The validity of the above equation may be verified by letting it act on $|q\rangle$ and employing (3.2.2), (3.2.4) and (3.2.8). In this way (3.2.12) becomes

\[ \hat{\Lambda}(p, q) = \frac{i}{\hbar} \int dudve^\hbar \frac{(p - \hat{\hat{p}}) v - i (q - \hat{\hat{q}}) u - \frac{i}{2} uv}{e^{\hbar} e^{2\hbar}}. \]  

(3.2.19)

With the help of the Hausdorff-Baker relation (3.2.7) one arrives at the final form

\[ \hat{\Lambda}(p, q) = \frac{1}{\hbar} \int dudve^\hbar \frac{|(q - \hat{\hat{q}}) u + (p - \hat{\hat{p}}) v|}{e^{\hbar} e^{2\hbar}}. \]  

(3.2.20)
If one uses (3.2.20) as the representation of the \( \hat{A}(p,q) \) operator then formula (3.2.10) becomes

\[
\hat{A} = \frac{1}{\hbar^2} \int dp dq dudv a_w(p,q) e^{\frac{i}{\hbar} (q - \hat{Q}) u + (p - \hat{P}) v}. \tag{3.2.21}
\]

One immediately recognizes the Fourier transform \( \tilde{a}_w(u,v) \) of \( a_w(p,q) \):

\[
\tilde{a}_w(u,v) = \frac{1}{\hbar^2} \int dp dq a_w(p,q) e^{\frac{i}{\hbar} (qu + pv)}. \tag{3.2.22}
\]

The inverse Fourier transform is given by

\[
a_w(p,q) = \int du dv \tilde{a}_w(u,v) e^{-\frac{i}{\hbar} (qu + pv)}. \tag{3.2.23}
\]

Thus (3.2.21) may be written as

\[
\hat{A} = \int du dv \tilde{a}_w(u,v) e^{-\frac{i}{\hbar} (\hat{Q} u + \hat{P} v)}. \tag{3.2.24}
\]

The last two equations (3.2.23) and (3.2.24) show the correspondence between an operator and its Weyl transform in a particularly elegant way. It is also apparent that if the quantum operator is a function only of \( \hat{P} \) or \( \hat{Q} \) then its Weyl transform is the same function of \( p \) or \( q \) respectively.

The Weyl transform may also be written in another useful form. With the help of a simple identity:

\[
\langle p' | \hat{A} | p'' \rangle = Tr(\hat{A} \ | p'' \rangle \langle p' |) \tag{3.2.25}
\]

and (3.2.16), equation (3.2.11) may be expressed as

\[
a_w(p,q) = Tr [ \hat{A} \hat{\Delta}(p,q) ]. \tag{3.2.26}
\]
It is apparent that the operator $\hat{A}(p, q)$ plays a significant role in the Weyl correspondence. By choosing for $\hat{A}$ in (3.2.10) the operator $\hat{A}(p', q')$ one finds that the Weyl transform of $\hat{A}(p', q')$ is essentially a product of delta functions:

$$ (\hat{A}(p', q'))_W = \hbar \delta(p - p') \delta(q - q'). \quad (3.2.27) $$

The trace of the operator $\hat{A}(p, q)$ and of products of $\hat{A}(p, q)$ operators are frequently used in the further discussion. In particular, one finds from (3.2.6), (3.2.12) and (3.2.4) that

$$ Tr[\hat{A}(p, q)] = 1. \quad (3.2.28) $$

Furthermore from (3.2.26) with $\hat{A} = \hat{A}(p', q')$ and (3.2.27) one has

$$ Tr[\hat{A}(p, q) \hat{A}(p', q')] = \hbar \delta(p - p') \delta(q - q'). \quad (3.2.29) $$

The trace of an arbitrary operator may be expressed in terms of its Weyl transform. Making use of (3.2.10) and (3.2.28) one has

$$ Tr[\hat{A}] = \frac{1}{\hbar} \int dp dq a_W(p, q). \quad (3.2.30) $$

In a similar way taking (3.2.29) instead of (3.2.28) one obtains

$$ Tr[\hat{A}\hat{B}] = \frac{1}{\hbar} \int dp dq a_W(p, q) b_W(p, q). \quad (3.2.31) $$

In quantum mechanics commutators and anticommutators play a significant role. In order to find their Weyl transforms the transform of a product of two operators needs to be considered. It is demonstrated in Appendix A3 that

$$ (\hat{A}\hat{B})_W = e^{\left[\frac{\hbar}{2i} \left( \frac{\partial(a)}{\partial p} \frac{\partial(b)}{\partial q} - \frac{\partial(a)}{\partial q} \frac{\partial(b)}{\partial p} \right)\right]} a_W(p, q) b_W(p, q). \quad (3.2.32) $$
superscripts $a$ and $b$ indicate the phase function on which the corresponding differential operator acts. One can see from the above equation that in general the Weyl transform of the product $\hat{A}\hat{B}$ is not equal to the product of their Weyl transforms.

The Weyl transform of the commutator and anticommutator may be derived from (3.2.32):

$$([\hat{A}, \hat{B}])_W = 2i \sin \left[ \frac{\hbar}{2} \left( \frac{\partial^{(a)}(a)}{\partial p} - \frac{\partial^{(a)}(b)}{\partial p} \right) \right] a_W(p, q) b_W(p, q),$$

(3.2.33)

$$([\hat{A}, \hat{B}])_W = 2 \cos \left[ \frac{\hbar}{2} \left( \frac{\partial^{(a)}(a)}{\partial p} - \frac{\partial^{(a)}(b)}{\partial p} \right) \right] a_W(p, q) b_W(p, q).$$

(3.2.34)

Equation (3.2.33) was originally derived by Moyal and it is frequently called the Moyal bracket. One should notice that the Weyl transform of $[\hat{A}, \hat{B}] / i\hbar$ begins with the Poisson bracket of the transforms $a_W(p, q), b_W(p, q)$ while the Weyl transform of $\{\hat{A}, \hat{B}\} / 2$ starts off with the product $a_W(p, q) b_W(p, q)$.

An arbitrary operator $\hat{A}$ may in principle be determined from its Weyl transform using (3.2.10) with any of the formulae (3.2.12), (3.2.16), (3.2.20) or from (3.2.23) with (3.2.24). There is, however, another method which is often much more convenient. From (3.2.10) with (3.2.20) and the Hausdorff-Baker relation (3.2.7) it follows that

$$\hat{A} = \frac{1}{\hbar^2} \int dq dp du dv a_W(p, q) e^{i\frac{\hbar}{2} (q - \hat{Q}) u} e^{i\frac{\hbar}{2} (p - \hat{P}) v} e^{\frac{i\hbar}{2} uv} e^{2\hbar}.$$

(3.2.35)
The product $uv$ may be replaced by $-\hbar^2 \frac{\partial^{(l)}}{\partial q} \frac{\partial^{(l)}}{\partial p}$ acting on the first two exponentials, or after a partial integration by the same operator (there is no change of sign due to double integration) acting on $a_w(p, q)$. Then integration over $u, v$ yields

$$\hat{A} = \int dq dp \delta(q - \hat{Q}) \delta(p - \hat{P}) a_o(p, q)$$

(3.2.36)

where

$$a_o(p, q) = e^{2i\hat{q}\hat{p}} a_w(p, q).$$

(3.2.37)

Hence, in order to obtain $\hat{A}$ from its Weyl transform $a_w(p, q)$ it suffices to calculate $a_o(p, q)$ from (3.2.37) and replace $q, p$ by $\hat{Q}, \hat{P}$ respectively, always writing the coordinate operators to the left of the momentum operators. In Appendix A4 an example of this procedure is provided for a frequently encountered type of the Weyl transform:

$$a_w(p, q) = f(q)p^n.$$ 

(3.2.38)

It is proved that

$$f(q)p^n = \left( \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} \hat{P}^k f(\hat{Q}) \hat{P}^{n-k} \right)_w.$$ 

(3.2.39)

Using (3.2.39) one may construct

$$pq = \left( \frac{1}{2} \left( \hat{P} \hat{Q} + \hat{Q} \hat{P} \right) \right)_w$$

(3.2.40)

$$p^2q = \left( \frac{1}{4} \left( \hat{Q}^2 \hat{P}^2 + 2\hat{P} \hat{Q} \hat{P} + \hat{P}^2 \hat{Q} \right) \right)_w$$

(3.2.41)

$$p^2q^2 = \left( \frac{1}{4} \left( \hat{Q}^2 \hat{P}^2 + 2\hat{P} \hat{Q} \hat{P} \hat{Q} + \hat{P}^2 \hat{Q}^2 \right) \right)_w.$$ 

(3.2.42)
3.3 Wigner distribution function

The state of a quantum mechanical system may be described by means of a density operator or density matrix:

\[ \hat{\rho} (t) = |\Psi (t)\rangle \langle \Psi (t)|. \quad (3.3.1) \]

The expectation value of an operator may be written in terms of the density operator as

\[ \langle \hat{A} \rangle_q = Tr [\hat{\rho} (t)]. \quad (3.3.2) \]

However, using (2.2.31) one may also write

\[ \langle \hat{A} \rangle_q = \int dq dp \rho_w (p, q) \rho_w (p, q; t) \quad (3.3.3) \]

where \( h \rho_w (p, q; t) \) is the Weyl transform of the density operator

\[ \rho_w (p, q; t) = \hbar \rho_w (p, q; t). \quad (3.3.4) \]

The function \( \rho_w (p, q; t) \) is called a Wigner distribution function or Wigner function for short and it follows from (3.2.15) and (3.3.1) that

\[ \rho_w (p, q; t) = \frac{1}{\hbar} \int dq \frac{e^{ipq}}{\hbar} \Psi^* (q + \frac{1}{2} v; t) \Psi (q - \frac{1}{2} v; t), \quad (3.3.5) \]

in terms of the wave function in the coordinate representation. Alternatively using (3.2.11) instead of (3.2.15) \( \rho_w (p, q; t) \) may be expressed as

\[ \rho_w (p, q; t) = \frac{1}{\hbar} \int dq \frac{e^{iqu}}{\hbar} \Psi^* (p - \frac{1}{2} u; t) \Psi (p + \frac{1}{2} u; t) \quad (3.3.6) \]

in terms of the wave function in the momentum representation.

Formula (3.3.3) shows that the Weyl formalism enables one to cast quantum mechanical averages in the form used in classical mechanics. Thus one may ask
whether the Wigner function satisfies all requirements imposed on an ordinary phase-space distribution function. The trace of the density operator is equal to unity so that (3.2.30) shows immediately that \( \rho_W(p, q; t) \) is properly normalized.

\[
\int dq dp \rho_W(p, q; t) = 1.
\] (3.3.7)

It is also bounded, the application of the Schwartz inequality

\[
\left| \int f^* g dx \right|^2 \leq (\int |f|^2 dx \int |g|^2 dx)
\] (3.3.8)

to (3.3.5) gives

\[
|\rho_W(p, q)|^2 = \frac{1}{\hbar^2} \int dq e^{i\frac{p}{\hbar} q} \left| \int dq^* \psi(q) \left( q - \frac{1}{2} \right) \right|^2 \psi(q + \frac{1}{2})^2 \] (3.3.9)

so that performing the trivial change of variables and making use of the normalization of the wave function one finds that (3.3.9) is just the square of

\[
|\rho_W(p, q)| \leq \frac{2}{\hbar}.
\] (3.3.10)

The Wigner function is normalized, cf. (3.3.7), so that \( \rho_W(p, q) \) is different from zero in the region of phase space with volume at least \( \frac{\hbar}{2} \). It is apparent that it cannot be sharply localized both in \( q \) and \( p \). This is just a manifestation of the uncertainty principle which precludes the quantum distribution from being a Dirac delta function simultaneously in both \( p \) and \( q \).

Integration of the Wigner function with respect to one variable yields a quantum probability density. Using (3.3.5) and the integral representation of delta function (3.2.8) one finds

\[
\int dp \rho_W(p, q; t) = |\Psi(q, t)|^2.
\] (3.3.11)
Likewise taking (3.3.6) instead of (3.3.5) gives

\[ \int dq \rho_W(p, q) = |\Psi(p, t)|^2. \tag{3.3.12} \]

However, \( \rho_W(p, q; t) \) itself cannot be considered to be a probability density since it may be negative. This can be shown as follows. Let \( \psi_W \) and \( \varphi_W \) be two Wigner functions corresponding to wavefunctions \( \Psi \) and \( \Phi \). With the help of (3.3.5) one may write the following expression

\[ I = \int dq dp \psi_W(p, q) \psi_W(p, q) = \frac{1}{\hbar^2} \int dq dp dx dy \exp \left( \frac{i}{\hbar} (y + x)p \right) \]

\[ \Phi^* \left( q + \frac{x}{2} \right) \Psi \left( q + \frac{y}{2} \right) \Phi \left( q - \frac{x}{2} \right) \Psi^* \left( q - \frac{y}{2} \right). \tag{3.3.13} \]

Integration over \( p \) yields a delta function, subsequent change of variables \( \xi = q + \frac{x}{2}, \eta = q - \frac{x}{2} \) enables one to express (3.3.13) as

\[ I = \frac{1}{\hbar} \int d\xi d\eta \Phi^* (\xi) \Psi (\xi) \Phi (\eta) \Psi^* (\eta) = \frac{1}{\hbar} |\langle \Phi | \Psi \rangle|^2. \tag{3.3.14} \]

Finally, one gets

\[ \int dq dp \varphi_W(p, q) \psi_W(p, q) = \frac{1}{\hbar} |\langle \Phi | \Psi \rangle|^2. \tag{3.3.15} \]

If we choose \( \Psi \) and \( \Phi \) to be orthogonal then \( \psi_W \) and \( \varphi_W \) cannot be both positive definite.

The time evolution of the Wigner function is a direct consequence of the equation involving the Hamiltonian operator \( \hat{H} \)

\[ \frac{\partial \varphi}{\partial t} = \frac{1}{i \hbar} [\hat{H}, \varphi] \tag{3.3.16} \]
which governs the time evolution of the density operator. Calculating the Weyl transform of both sides of this equation and employing (3.2.33) one obtains

\[
\frac{\partial p_W}{\partial t} = \frac{2}{\hbar} \sin \left( \frac{\hbar}{2} \left( \frac{\partial (h)}{\partial q} \frac{\partial (p)}{\partial p} - \frac{\partial (h)}{\partial p} \frac{\partial (p)}{\partial q} \right) \right) h_W(p, q) \rho_W(p, q)
\]

(3.3.17)

where \( h_W(p, q) \) is the Weyl transform of the Hamiltonian \( \hat{H} \). If \( \hat{H} \) may be written as

\[
\hat{H} = \hat{T} + \hat{V}(\hat{Q})
\]

(3.3.18)

where \( \hat{T} \) and \( \hat{V} \) stand for the kinetic energy operator and potential energy operator respectively, then (3.3.17) may be written as

\[
\frac{\partial p_W}{\partial t} = \{ h_W, \rho_W \} + \sum_{k=3, odd}^{\infty} \frac{1}{k!} \left( \frac{\hbar}{2i} \right)^k \left[ \frac{\partial^k}{\partial q^k} V(q) \right] \frac{\partial^k p_W}{\partial p^k}.
\]

(3.3.19)

Hence, the equation of motion can be expressed as a power series of the Planck constant \( \hbar \) which is made up of the classical Poisson bracket and "quantum contributions". This feature of the dynamic evolution becomes particularly interesting whenever semiclassical approximations need to be performed. It seems that in the limit of small \( \hbar \) the series in (3.3.19) may be truncated to yield a Liouville formula for the time development of the distribution function. However, using (3.3.5) the \( k \) th order partial derivative \( \frac{\partial^k p_W}{\partial p^k} \) is estimated to be of order \( 1/\hbar^k \)

so that any expansion term with \( k \geq 3 \) becomes of the order \( 1/\hbar^k \). Consequently, for \( \hbar \to 0 \) the convergence of (3.3.19) to the classical equation of motion is problematic, with the trivial exception of linear systems where the derivative of the potential vanishes for \( k \geq 3 \).
So far the properties of the Wigner function has been considered within the framework of the Weyl transform. A question arises as to what are the physical requirements which uniquely determine the Wigner function, as defined by (3.3.5). This problem has been addressed by Hillery et al [65] who give the following list of properties:

(i) \( \rho_W(p, q) \) should be a Hermitian form of the state vector |\( \Psi \rangle \)

\[
\rho_W(p, q) = \langle \Psi | \hat{M}(p, q) | \Psi \rangle
\]  

(3.3.20)

where \( \hat{M}(p, q) \) is a self-adjoint operator depending on \( p \) and \( q \). Therefore, \( \rho_W(p, q) \) is real;

(ii)

\[
\int dp \rho_W(p, q; t) = |\Psi(q, t)|^2 = \langle q | \hat{p} | q \rangle, \tag{3.3.21}
\]

\[
\int dq \rho_W(p, q; t) = |\Psi(p, t)|^2 = \langle p | \hat{p} | p \rangle, \tag{3.3.22}
\]

\[
\int dq dp \rho_W(p, q; t) = 1 = \text{Tr} (\hat{p}); \tag{3.3.23}
\]

(iii) \( \rho_W(p, q) \) should be Galilei invariant, i.e. if \( \Psi(q) \rightarrow \Psi(q + a) \) then \( \rho_W(p, q) \rightarrow \rho_W(p, q + a) \) and if \( \Psi(q) \rightarrow \exp(\frac{i p' q}{\hbar}) \Psi(q) \) then \( \rho_W(p, q) \rightarrow \rho_W(p - p', q) \);

(iv) \( \rho_W(p, q) \) should be invariant with respect to space and time reflections, i.e. if \( \Psi(q) \rightarrow \Psi(-q) \) then \( \rho_W(p, q) \rightarrow \rho_W(-p, -q) \) and if \( \Psi(q) \rightarrow \Psi^*(q) \) then \( \rho_W(p, q) \rightarrow \rho_W(-p, q) \);

(v) In the force-free case the equation of motion is classical
\[ \frac{\partial \rho_W}{\partial t} = -\frac{p}{m} \frac{\partial \rho_W}{\partial q}. \tag{3.3.24} \]

Properties (i)-(v) determine the distribution function completely, alternatively (i)-(iv) along with previously discussed property (3.3.15) may also be used to define the Wigner function.

### 3.4 Husimi distribution function

It has already been pointed out that the Wigner function cannot be interpreted as a probability distribution. Even though it is real it is not positive definite and due to its oscillatory nature the existence of a proper classical limit is problematic. It is possible, however, to obtain a distribution function lacking all of the previously mentioned deficiencies by a proper coarse-graining or smoothing of the Wigner function. This idea was originally put forward by Husimi [51] who considered a simple Gaussian smoothing

\[ \rho_H(p, q) = \frac{2}{\hbar} \int dp' dq' e^{-\frac{\xi}{\hbar} (q' - q)^2 - \frac{1}{\xi} (p' - p)^2} \rho_W(p', q') \tag{3.4.1} \]

where \( \xi \) is so far an unspecified real parameter.

Furthermore, if one notices that the Wigner function of a coherent state

\[ \Phi_\alpha(x) = \langle x|\alpha \rangle = \langle x|pq \rangle = \left( \frac{e}{\pi\hbar} \right)^{1/4} e^{-\frac{\xi}{\hbar} (q - x)^2 + i\frac{p}{\hbar} (x - q)} \tag{3.4.2} \]

is just a Gaussian

\[ (\Phi_\alpha)_W = \frac{2}{\hbar} e^{-\frac{\xi}{\hbar} (q' - q)^2 - \frac{1}{\xi} (p' - p)^2} \tag{3.4.3} \]

then the alternative definition of \( \rho_H \) follows from (3.3.15)
\[ \rho_H(p, q) = \frac{1}{\hbar} |\langle pq|\Psi\rangle|^2. \]  (3.4.4)

It is apparent that a function defined in this way is non-negative.

Coherent states \(|pq\rangle\) also denoted by \(|\alpha\rangle\) correspond to minimum uncertainty wave packets. They are usually defined as eigenstates of the annihilation operator

\[ \hat{a} = \sqrt{\frac{\hbar}{2}} (\hat{Q} + i \frac{\hat{P}}{2}) \]  (3.4.5)

\[ \hat{a} |\alpha\rangle = \alpha |\alpha\rangle \]  (3.4.6)

where

\[ \alpha = \sqrt{\frac{\hbar}{2}} (q + i \frac{\hat{P}}{2}) . \]  (3.4.7)

For the purpose of further discussion let us also recall the definition of the creation operator \(\hat{a}^\dagger\)

\[ \hat{a}^\dagger = \sqrt{\frac{\hbar}{2}} (\hat{Q} - i \frac{\hat{P}}{2}) \]  (3.4.8)

whose eigenvalue is just \(\alpha^*\)

\[ \langle \alpha | \hat{a}^\dagger = \alpha^* \langle \alpha | . \]  (3.4.9)

Coherent states are not orthogonal to each other (they are eigenvectors of a non-hermitian operator) but they do form a complete set of states. Otherwise, they would not be very useful. In fact they form an overcomplete set, \(i.e\.) it is possible to choose a subset which is already complete. The completeness relation for the coherent state is given by

\[ \mathcal{I} = \int \frac{d^2\alpha}{\pi} |\langle \alpha |\rangle|^2 = \int \frac{dp dq}{\hbar} |pq\rangle \langle pq|. \]  (3.4.10)
If one puts (3.4.4) in a slightly different form

\[ \rho_H(p, q) = \frac{1}{\hbar} \langle \Psi | \Psi \rangle \langle \rho q | \rho q \rangle = \frac{1}{\hbar} \langle \rho q | \rho q \rangle \]  

(3.4.11)

and use property (3.4.10) it becomes apparent that the Husimi function is normalized to unity (note that \( \text{Tr} (\rho) = 1 \)). The last formula provides also another definition of the Husimi function as essentially the diagonal representation of the density matrix in the coherent state basis.

Thus, the process of coarse-graining of the Wigner function has generated the non-negative, normalized function \( \rho_H(p, q) \). One may ask how the other properties of the Wigner function discussed in the last Section are affected by this transformation. To address this problem a modified version of (3.4.11) is found more convenient. It may be derived in the following way [66]. After inserting the completeness relation (3.3.3) into (3.4.11) two times and using the coordinate representation of the coherent states (3.4.2) one obtains

\[ \rho_H(p, q) = \frac{1}{\hbar} \int dx dx' \langle \rho q | x' \rangle \langle x' | \Psi \rangle \langle \Psi | x \rangle \langle x | \rho q \rangle = \]

\[ \frac{1}{\hbar} \int dx dx' K(p, q;x', x) \Psi^w (x) \Psi (x') . \]  

(3.4.12)

The kernel of the transformation is given by

\[ K(p, q; x', x) = \left( \frac{\xi}{\pi\hbar} \right)^{1/2} \frac{\xi}{2} \frac{e^{-\frac{\xi}{2} \left[ (q-x)^2 + (q-x')^2 \right]}}{\hbar} + \frac{i \hbar}{\xi} (x-x') \]  

(3.4.13)

The structure of equation (3.4.12) shows that contrary to the properties of the Wigner function (3.3.11-12) integration of the Husimi distribution with respect to one variable does not yield the corresponding probability density, namely

\[ \int dp \rho_H(p, q) \neq |\Psi^w (q)|^2 , \]  

(3.4.14)
\[
\int dq \rho_H(p, q) \neq |\Psi(p)|^2.
\] (3.4.15)

The Galilei invariance of the Wigner function is not influenced by coarse-graining, cf. property (iii) in Section 2.3. To verify the first requirement of (iii) one replaces \( \Psi(x) \) by \( \Psi(x + a) \) in the rhs of (3.4.12)

\[
\int dx dx' K(p, q; x', x) \Psi^*(x + a) \Psi(x + a) = 
\]

\[
\int du dv K(p, q; v - a, u - a) \Psi^*(u) \Psi(v). \] (3.4.16)

However, the kernel (3.4.13) has the property

\[
K(p, q; v - a, u - a) = K(p, q + a; v, u) \] (3.4.17)

so that

\[
\int du dv K(p, q; v - a, u - a) \Psi^*(u) \Psi(v) = 
\]

\[
\int du dv K(p, q + a; v, u) \Psi^*(u) \Psi(v) = \rho_H(p, q + a). \] (3.4.18)

Substitution of \( \Psi(x) \) by \( \Psi(x) \exp\left(\frac{i p' x}{\hbar}\right) \) in the rhs of (3.4.12) leads to

\[
\int dx dx' K(p, q; x', x) e^{\frac{i p' (x - x')}{\hbar}} \Psi^*(x) \Psi(x') = 
\]

\[
\int dx dx' K(p - p', q; x', x) \Psi^*(x) \Psi(x') = \rho_H(p - p', q), \] (3.4.19)

where the second line is a consequence of the identity

\[
K(p, q; x', x) e^{\frac{i p' (x - x')}{\hbar}} = K(p - p', q; x', x). \] (3.4.20)

It follows from (3.4.18) and (3.4.19) that the Husimi function is in fact Galilei invariant.
Using the following properties of the kernel $K(p, q; x', x)$:

\begin{align*}
K(p, q, -x', -x) &= K(-p, -q, x', x) \quad (3.4.21) \\
K(p, q, x', x) &= K(-p, q, -x', x') \quad (3.4.22)
\end{align*}

one may easily demonstrate that the Husimi function is invariant with respect to space reflection and time reversal, cf. property (iv) in Section 3.3.

In order to find the Husimi representation $a_H(p, q)$ of an arbitrary operator $\hat{A}$ one postulates that

$$
\langle \hat{A} \rangle = Tr [\hat{A} \hat{\rho}] = \int dp dq a_H(p, q) \rho_H(p, q). \quad (3.4.23)
$$

In Appendix A5 it is demonstrated that the integral relation between the Husimi and Wigner distributions (3.4.1) is equivalent to

$$
\rho_H(p, q) = e^{\frac{i}{\hbar} \left( \frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{\partial^2}{\partial p^2} \right)} \rho_W(p, q). \quad (3.4.24)
$$

Plugging this formula into (3.4.23) and integrating by parts yields

$$
\langle \hat{A} \rangle = \int dp dq \rho_W(p, q) e^{\frac{i}{\hbar} \left( \frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{\partial^2}{\partial p^2} \right)} a_H(p, q) \quad (3.4.25)
$$

so that $a_H(p, q)$ may be derived from the Weyl transform of the operator $\hat{A}$

$$
a_H(p, q) = e^{\frac{i}{\hbar} \left( \frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{\partial^2}{\partial p^2} \right)} a_W(p, q). \quad (3.4.26)
$$

It is worth pointing out that the relation between the Husimi and Wigner distributions (3.4.24) is different from that of the Husimi and Wigner representations of operators (3.4.26).

The application of (3.4.26) gives
\[
(\hat{Q})_H = q \tag{3.4.27}
\]
\[
(\hat{P})_H = p \tag{3.4.28}
\]

and one can see that these representations coincide with the corresponding Weyl transforms. However,

\[
(\hat{Q}^2)_H = q^2 - \frac{\hbar}{2\xi} \tag{3.4.29}
\]
\[
(\hat{P}^2)_H = p^2 - \frac{\hbar\xi}{2} \tag{3.4.30}
\]

so that it is obvious that in general the Husimi representation \(a_H(p, q)\) explicitly involves the coarse-graining parameter \(\xi\).

Now we proceed to determine the time development of the Husimi function which follows from the time evolution of the density operator. Calculating diagonal matrix elements of both sides of (3.3.16) in the coherent state basis one gets

\[
\frac{\partial \rho_H}{\partial t} = \frac{\partial}{\partial t} \langle pq | \hat{\rho} | pq \rangle = \frac{1}{\hbar} \langle pq | [\hat{H}, \hat{\rho}] | pq \rangle \tag{3.4.31}
\]

It is convenient to introduce the following notation for the diagonal matrix elements \((...)_G = \langle pq | ... | pq \rangle\). The subscript \(G\) stands for Glauber and the meaning of this somewhat cumbersome notation shall become apparent in the next Section where quantum distribution functions are discussed within the framework of the boson operators formalism. The only exception to this notation is made for the Husimi function \(\rho_H = (\hat{\rho})_G\). Postponing the detailed discussion to Section 3.5 we note that

\[
a_G(p, q) = (\hat{A})_G = e^{\frac{\hbar}{4} \left( \frac{1}{\xi} \frac{\partial^2}{\partial q^2} + \frac{\xi}{\partial p^2} \right)} a_W(p, q). \tag{3.4.32}
\]
The comparison of (3.4.26) and (3.4.32) shows that \( a_G(p, q) \) may be obtained from regular Husimi representations simply by replacing \( \xi \) by \(-\xi\).

It is also shown in the next Section that the diagonal representation of the product of two operators may be written as

\[
(\hat{A}\hat{B})_G = e^{\frac{\hbar}{2} \left( \frac{1}{\xi} \frac{\partial}{\partial q} - i \frac{\partial}{\partial p} \right)} \left( \frac{1}{\xi} \frac{\partial}{\partial q} + i \frac{\partial}{\partial p} \right) a_G b_G \quad (3.4.33)
\]

or equivalently

\[
(\hat{A}\hat{B})_G = e^{\frac{\hbar}{2} \left( \frac{1}{\xi} \frac{\partial}{\partial q} + i \frac{\partial}{\partial p} \right)} e^{-\frac{\hbar}{2} \left( \frac{1}{\xi} \frac{\partial}{\partial q} + i \frac{\partial}{\partial p} \right)} a_G b_G. \quad (3.4.34)
\]

It follows either from (3.4.33) or (3.4.34) that the diagonal representation of the commutation relation \([\hat{A}, \hat{B}] / (i\hbar)\) becomes

\[
\left( \frac{1}{i\hbar} [\hat{A}, \hat{B}] \right)_G = 2 \frac{\hbar}{h} \text{Im} (\hat{A}\hat{B})_G. \quad (3.4.35)
\]

Application of this formula to (3.4.31) yields the time evolution of \( \rho_H(p, q) \)

\[
\frac{\partial \rho_H}{\partial t} = 2 \frac{\hbar}{h} \text{Im} (\hat{H}\hat{\rho})_G = \{ h_G, \rho_H \} + \frac{\hbar}{2} \left( \frac{1}{\xi} \frac{\partial^2}{\partial q^2} h_G - \xi \frac{\partial^2 \rho_H}{\partial q \partial p} + \right.
\]

\[
\sum_{l=3}^{\infty} \frac{1}{l!} \left( \frac{\partial h_G}{\partial q} \right)^l \text{Im} \left[ \frac{\hbar}{2} \left( \frac{1}{\xi} \frac{\partial}{\partial q} + i \frac{\partial}{\partial p} \right)^l \right] \rho_H. \quad (3.4.36)
\]

The second line in (3.4.36) is valid as long as the Hamiltonian of a system may be put in a form \( \hat{H} = \hat{T} + \hat{V}(\hat{Q}) \), where \( \hat{T} \) is the kinetic energy operator and \( \hat{V} \) is the potential energy operator. Then after the expansion of the second expo-
ential in (3.4.34) into a Taylor series one realizes that the presence of the partial
derivative \( \frac{\partial h_G}{\partial p^j} \) makes the terms of the order higher than two vanish.

The second term in (3.4.36) is a result of the coarse-graining and does not
have a quantum origin. It is apparent that even in the force-free case the time de-
velopment of the Husimi function does not coincide with the classical Liouville
equation. As a consequence the Husimi representation should not be compared
with classical mechanics but rather with its coarsed-grained equivalent. The pro-
cess of coarse-graining of classical mechanics is analogous to the method of gener-
ating the Husimi function, i.e. the coarsed-grained classical distribution function
reads

\[
\rho_{CG}(p, q) = \frac{2}{\hbar} \int dp' dq' e^{\frac{\xi}{\hbar} (q' - q)^2 - \frac{1}{\xi \hbar} (p' - p)^2} \rho_C(p', q').
\]  

(3.4.37)

The extensive numerical calculations [67] have shown that the Wigner func-
tion differs significantly from the classical distribution function \( \rho_C \) at any stage of
the evolution, even when the corresponding classical dynamics is regular. On the
other hand, the Husimi distribution initially agrees with \( \rho_{CG} \) quite well. This cor-
respondence, however, breaks down after some time when the quantum interfer-
ence effects become important. Fig. 4 elucidates the relations between the Wigner
and Husimi distributions and their classical counterparts \( \rho_C \) and \( \rho_{CG} \).

In this Section we discussed only the basic properties of the Husimi formal-
ism. A systematic formulation of quantum mechanics in terms of the Husimi func-
tion has been given relatively recently by Mizrahi [60,68-69] and independently
in a different way by Takahashi [67] and Lalovic et al [70].
3.5 General distribution function

Quantum distribution functions have been the subject of particularly extensive research in quantum optics. The primary purpose of this Section is to establish the connection between the Wigner and Husimi functions, discussed in the last two Sections, and quantum distributions expressed in terms of creation and annihilation operators. The application of boson operator formalism (inherent to quantum optics) seems to be artificial in the context of classical-quantum correspondence. However, using this approach one may gain considerable insight into the properties of the Wigner and Husimi functions. The boson operator formalism is also a powerful calculation tool which enables us to study some properties of distribution functions in a particularly elegant way.

Let us assume that an operator $\hat{A}(\hat{P}, \hat{Q})$ may be represented as a power series in $\hat{P}$ and $\hat{Q}$. Then using (3.4.5) and (3.4.8) one may always write this expansion in terms of $\hat{a}$ and $\hat{a}^\dagger$. In the most general form it reads [71]

$$\hat{A}(\hat{a}, \hat{a}^\dagger) = \sum_l \sum_m \sum_n L(l, m, ..., n) \hat{a}^l \hat{a}^m ... \hat{a}^n$$  

(3.5.1)

where $l, m, ...$ are positive integers or zero. It is possible, however, to apply the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$ repeatedly to rearrange the creation and annihilation operators among themselves. This procedure generates differently looking but otherwise equivalent forms of $\hat{A}(\hat{a}, \hat{a}^\dagger)$.

Suppose that one uses the commutation relation in such a way that all operators $\hat{a}$ in every term of sum (3.5.1) are to the right of all operators $\hat{a}^\dagger$. The function is then said to be in normal order.
A (a, \overline{a}) = A^{(n)} (a, \overline{a}) = \sum_{r,s} a^{(n)}_{r,s} \hat{a}^r \hat{a}^s \quad \text{(3.5.2)}

A superscript \( n \) stands for normal order and the expansion coefficients are independent of \( a \) and \( \overline{a} \). If the ordering of the creation and annihilation operators is just the opposite of (3.5.2) the function is said to be in antinormal order

\[ \hat{A} (a, \overline{a}^\dagger) = \hat{A}^{(a)} (a, \overline{a}^\dagger) = \sum_{r,s} a^{(a)}_{r,s} \hat{a}^r \overline{a}^s \quad \text{(3.5.3)} \]

which is indicated by superscript \( a \).

A product of \( m \) annihilation operators and \( n \) creation operators can be ordered in \( (n + m)! / n! m! \) ways. The symmetrically ordered product of this operators, denoted by \( \{ \hat{a}^\dagger^m \hat{a}^n \}_{\text{sym}} \), is just the average of all these differently ordered products. For example

\[ \{ \hat{a}^\dagger \hat{a} \}_{\text{sym}} = \frac{1}{2} (\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger) \quad \text{(3.5.4)} \]

or

\[ \{ \hat{a}^\dagger \hat{a}^2 \}_{\text{sym}} = \frac{1}{3} (\hat{a}^\dagger \hat{a}^2 + \hat{a} \hat{a}^\dagger \hat{a} + \hat{a}^2 \hat{a}^\dagger). \quad \text{(3.5.5)} \]

Thus the symmetric expansion of the operator \( \hat{A} \) reads

\[ \hat{A} (a, \overline{a}^\dagger) = \hat{A}^{(s)} (a, \overline{a}^\dagger) = \sum_{r,s} a^{(s)}_{r,s} \{ \hat{a}^\dagger^r \hat{a}^s \}_{\text{sym}} \quad \text{(3.5.6)} \]

Since the normal and antinormal forms of the operator expansion are unique it is possible to establish a one-to-one correspondence between \( \hat{A}^{(n)} (a, \overline{a}^\dagger) \) or \( \hat{A}^{(a)} (a, \overline{a}^\dagger) \) and the ordinary complex variable functions \( a^{(n)} (\alpha, \overline{\alpha}^*) \) or
\( a^{(a)}(\alpha, \alpha^*) \) simply by replacing \( \hat{a} \) by \( \alpha \) and \( \hat{a}^\dagger \) by \( \alpha^* \). These functions are frequently called normal and antinormal associated functions.

It follows from (3.5.2), (3.4.6) and (3.4.9) that the associated normal function is given by the diagonal matrix element in the coherent state representation

\[
a^{(n)}(\alpha, \alpha^*) = \langle \alpha | \hat{A} (\hat{a}, \hat{a}^\dagger) | \alpha \rangle.
\]

(3.5.7)

On the other hand, any suitably well behaved operator \( \hat{A} (\hat{a}, \hat{a}^\dagger) \) has the integral representation

\[
\hat{A} (\hat{a}, \hat{a}^\dagger) = \int \frac{d^2\alpha}{\pi} | \alpha \rangle \langle \alpha | \ a^{(a)}(\alpha, \alpha^*) \ .
\]

(3.5.8)

To prove this theorem it suffices to use (3.5.3) and the completeness relation for the coherent states (3.4.10) in the lhs.

Inserting (3.5.8) into (3.5.7) the following relation between the normal and antinormal associated functions may be found

\[
a^{(n)}(\alpha, \alpha^*) = \int \frac{d^2\alpha'}{\pi} | \alpha \rangle | \alpha' \rangle^2 a^{(a)}(\alpha', \alpha^*) \ .
\]

(3.5.9)

Further we notice that the trace of \( \hat{A} (\hat{a}, \hat{a}^\dagger) \) is given by

\[
Tr [ \hat{A} (\hat{a}, \hat{a}^\dagger) ] = \int \frac{d^2\alpha}{\pi} a^{(n)}(\alpha, \alpha^*)
\]

(3.5.10)

or

\[
Tr [ \hat{A} (\hat{a}, \hat{a}^\dagger) ] = \int \frac{d^2\alpha}{\pi} a^{(a)}(\alpha, \alpha^*)
\]

(3.5.11)

That is, the trace may be found by integrating either the normal or antinormal associated function in the complex \( \alpha \)-plane. The traces exist if the corresponding in-
integrals exist. Equation (3.5.10) may be proved by inserting the completeness relation in the lhs. To verify (3.5.11) one simply takes the trace of both sides of (3.5.8). In both cases one should note that $Tr[|u⟩⟨v|] = ⟨v|u⟩$.

For an arbitrary operator $\hat{A}(\hat{a}, \hat{a}^\dagger)$ and the density matrix $\hat{ρ}(\hat{a}, \hat{a}^\dagger)$ the following relations hold

$$Tr[\hat{A}\hat{ρ}] = \int \frac{d^2α}{π} a^{(n)}(α, α^*) \rho^{(a)}(α, α^*) \ , \ \ (3.5.12)$$

$$Tr[\hat{A}\hat{ρ}] = \int \frac{d^2α}{π} a^{(n)}(α, α^*) \rho^{(n)}(α, α^*) \ . \ \ (3.5.13)$$

To prove (3.5.12) one expands $\hat{ρ} = \hat{ρ}^{(a)}$ and $\hat{A} = \hat{A}^{(n)}$ into power series and uses the cyclic property of the trace, i.e. $Tr[\hat{A}\hat{B}\hat{C}] = Tr[\hat{C}\hat{B}\hat{A}] = Tr[\hat{B}\hat{C}\hat{A}]$

$$Tr[\hat{A}^{(n)}\hat{ρ}^{(a)}] = Tr\left[\sum_{k,l} a_{k,l}^{(n)} \hat{a}^k \hat{a}^l \rho^{(a)}(α, α^*) \hat{a}^r \hat{a}^s\right] =$$

$$\sum_{k,l} \sum_{r,s} a_{k,l}^{(n)} \rho^{(a)}(α, α^*) Tr[\hat{a}^{k+s} \hat{a}^{l+r}] \ . \ \ (3.5.14)$$

Since $\hat{a}^{k+s} \hat{a}^{l+r}$ is in normal order one may apply (3.5.10) to obtain

$$Tr[\hat{A}^{(n)}\hat{ρ}^{(a)}] = \int \frac{d^2α}{π} \sum_{k,l} a_{k,l}^{(n)} α^k α^l \sum_{r,s} \rho^{(a)}(α, α^*) \alpha^r \alpha^s =$$

$$\int \frac{d^2α}{π} a^{(n)}(α, α^*) \rho^{(a)}(α, α^*) \ . \ \ (3.5.15)$$

A similar proof holds for (3.5.13).
Hence, using the power series expansion of quantum mechanical operators in terms of creation and annihilation operators one may find associated functions and write quantum averages in the form resembling those found in the Wigner and Husimi formalisms. Moreover, taking into account that the Husimi distribution is defined essentially as the diagonal representation of the density operator in the coherent state basis one may conjecture using (3.5.9) and (3.5.13) that the Husimi representation of operators correspond to antinormal associated functions. To formally show this equivalence we need to introduce the concept of the characteristic function.

One is often interested in the moments of some operator \( \hat{A} \). Its \( l \) th moment is given by [71]

\[
\langle \hat{A}^l \rangle = \langle \Psi | \hat{A}^l | \Psi \rangle = \text{Tr} \left[ \hat{A}^l \hat{\rho} \right]
\]  

(3.5.16)

It is sometimes easier to evaluate the average

\[
C_A (\eta, t) = \langle e^{i \eta \hat{A}} \rangle
\]

(3.5.17)

than to calculate the moment (3.5.16) directly. Furthermore, all the moments of \( \hat{A} \) can be found from \( C_A (\eta) \) since it is evident that

\[
\langle \hat{A}^l \rangle = \frac{\partial^l}{\partial (i \eta)^l} C_A (\eta) \big|_{\eta = 0}.
\]

(3.5.18)

That is, the \( l \) th moment is obtained by differentiating \( C_A \) \( l \) times and then letting \( \eta = 0 \). \( C_A \) is called a moment generating function or the characteristic function of \( \hat{A} \). The characteristic function may be calculated either in the Schrödinger or Heisenberg representations, the choice is a matter of convenience.

If one considers the operator
already discussed in the context of the Weyl transformation, cf. (3.2.24), then with the help of (3.2.31) one may write

\[
C^{(W)}(u, v) = Tr[\hat{p}\hat{\mathcal{C}}] = \int dq dp \rho_W(p, q) e^{\frac{i}{\hbar} (qu + pv)} .
\]

Thus, the Wigner function is just the Fourier transform of the characteristic function \( C^{(W)}(u, v) \)

\[
\rho_W(p, q) = \frac{1}{\hbar^2} \int du dv C^{(W)}(u, v) e^{-\frac{i}{\hbar} (qu + pv)} .
\]

However, using the framework of annihilation and creation operators (3.4.5), (3.4.8) and defining

\[
\eta = \frac{1}{\hbar} \left( \frac{\sqrt{\hbar}}{2\xi} u - i \sqrt{\frac{\hbar}{2}} v \right)
\]

one may write

\[
\frac{1}{\hbar} (\hat{Q}u + \hat{P}v) = \eta \hat{a} + \eta^* \hat{a}^\dagger ,
\]

likewise, employing (3.4.7)

\[
\frac{1}{\hbar} (qu + pv) = \eta \alpha + \eta^* \alpha^* .
\]

It follows from (3.5.20) and (3.5.23) that

\[
C^{(W)}(u, v) = Tr \left[ \hat{p} e^{\frac{i}{\hbar} (\eta \hat{a} + \eta^* \hat{a}^\dagger)} \right] = C^{(W)}(\eta, \eta^*) .
\]

Substituting this result into (3.5.21) and using (3.5.24) one obtains
\[
\rho_W(p, q) = \frac{\hbar}{(2\pi \hbar)^2} \int d\eta d\eta^* e^{-i(\eta\alpha + \eta^* \alpha^*)} C^{(W)}(\eta, \eta^*) = \frac{1}{\hbar} \rho_W(\alpha, \alpha^*) .
\]

(3.5.26)

This equation is a convenient starting point for defining a generalized distribution function \( \rho \). It suffices to generalize the characteristic function and then define \( \rho \) as the inverse Fourier transform of the generalized characteristic function [72].

First one should observe that the application of the Hausdorff-Baker relation gives

\[
e^{i(\eta \hat{a} + \eta^* \hat{a}^t)} = e^{i\eta \hat{a}} e^{i\eta^* \hat{a}^t} e^{-\frac{1}{2}|\eta|^2} = e^{i\eta^* \hat{a}^t} e^{i\eta \hat{a}} e^{\frac{1}{2}|\eta|^2}
\]

(3.5.27)

If one defines the new characteristic functions \( C^{(a)} \) and \( C^{(n)} \):

\[
C^{(a)} = Tr \left[ \hat{\rho} e^{i\eta \hat{a}} e^{i\eta^* \hat{a}^t} \right] \quad (3.5.28)
\]

\[
C^{(n)} = Tr \left[ \hat{\rho} e^{i\eta^* \hat{a}^t} e^{i\eta \hat{a}} \right] \quad (3.5.29)
\]

then (3.5.27) enables us to relate them to \( C^{(W)} \)

\[
C^{(W)} = C^{(a)} e^{\frac{1}{2}|\eta|^2} = C^{(n)} e^{-\frac{1}{2}|\eta|^2} .
\]

(3.5.30)

\( C^{(a)} \), \( C^{(n)} \) are called antinormal and normal characteristic function respectively because of the ordering of the moments generated by them. The Wigner function \( C^{(W)} \) is often called symmetric.

A generalized characteristic function is defined as follows
\[ C^{(s)}(\eta, \eta^*) = Tr \left[ \hat{\rho} e^{s|\eta|^2 + i(\eta \hat{a} + \eta^* \hat{a}^\dagger)} \right] \] (3.5.31)

where \( s \) is a parameter. It is clear that the choice \( s = 0, -1, 1 \) corresponds to the Wigner \( C^{(W)} \), antinormal \( C^{(a)} \) and normal \( C^{(n)} \) characteristic function respectively.

In order to determine the relation between \( \rho \) and \( \rho_W \) it is necessary to express the former in terms of \( p, q \). First, since (3.5.22) implies that

\[ |\eta|^2 = \frac{1}{2\hbar} (\frac{1}{\xi} u^2 + \xi v^2) \] (3.5.32)

then

\[ C^{(s)}(u, v) = e^{\frac{s}{4\hbar} (\frac{1}{\xi} u^2 + \xi v^2)} C^{(W)}(u, v). \] (3.5.33)

The expression for \( \rho \) may be derived simply by replacing \( C^{(W)}(u, v) \) by \( C^{(s)}(u, v) \) in (3.5.26). If one further takes into account that \( u^2, v^2 \) inside the integrand may be replaced by \(-\hbar^2 \frac{\partial^2}{\partial q^2}\) and \(-\hbar^2 \frac{\partial^2}{\partial p^2}\) outside the integral sign one gets the final form

\[ \rho^{(s)}(p, q) = e^{\frac{-\hbar s}{4} (\frac{1}{\xi} \frac{\partial}{\partial q} + \xi \frac{\partial}{\partial p})} \rho_W(p, q). \] (3.5.34)

For \( s = -1 \) the above equation reads

\[ \rho^{(-1)} = \rho^{(n)}(p, q) = e^{\frac{-\hbar}{4} (\frac{1}{\xi} \frac{\partial}{\partial q} + \xi \frac{\partial}{\partial p})} \rho_W(p, q) \] (3.5.35)
which is identical to relation (3.4.24) obtained earlier for the Husimi function. The superscript $n$ in (3.5.35) suggests that $\rho^{(n)}$ corresponds to the antinormal characteristic function $C(a)$. This may be easily understood if one notices that the exponential operators in (3.5.28) are in antinormal order. Then it follows from (3.5.13) that $\rho^{(n)}$ is the inverse Fourier transform of $C(a)$.

Thus the Husimi function is equivalent to the normal associated function for the density operator while the Husimi representations of operators correspond to the antinormal associated functions.

The choice of $s = 1$ in (3.5.35) gives the well known distribution of Glauber and Sudarshan $\rho_G$ [56-58] which is the antinormal associated function for the density operator. In this formalism the representations of operators are the normal associated functions. The basic properties of the distributions discussed so far are collected in Table 1. It worth pointing out that only the Husimi function is positive definite.

<table>
<thead>
<tr>
<th>Distribution Function</th>
<th>Ordering of Distribution</th>
<th>Ordering of Phase Space Functions</th>
<th>Positive definite</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_w$</td>
<td>symmetric</td>
<td>symmetric</td>
<td>No</td>
</tr>
<tr>
<td>$\rho_H$</td>
<td>normal</td>
<td>antinormal</td>
<td>Yes</td>
</tr>
<tr>
<td>$\rho_G$</td>
<td>antinormal</td>
<td>normal</td>
<td>No</td>
</tr>
</tbody>
</table>

Now, let us find the Husimi representation of the product of two operators [66]. The usual derivation presented by Takahashi [67] relies on an identity originally obtained by O’Connell et al [72] and is rather awkward.
If the operators $\hat{A}, \hat{B}$ are functions of $\hat{P}, \hat{Q}$ it is possible to expand them in terms of normally ordered creation and annihilation operators:

$$\hat{A} = \sum_{r, s} a_{r, s}^{(n)} \hat{a}^\dagger \hat{a}^s, \quad \hat{B} = \sum_{r, s} b_{r, s}^{(n)} \hat{a}^\dagger \hat{a}^s. \quad (3.5.36)$$

Then using the notation already introduced in the previous Section the diagonal matrix element of $\hat{A}\hat{B}$ in the coherent state basis reads

$$(\hat{A}\hat{B})_G = \langle pq | \hat{A}\hat{B} | pq \rangle = \langle \alpha | \hat{A}\hat{B} | \alpha \rangle = \int \frac{d^2 \alpha'}{\pi} \langle \alpha | \hat{A} | \alpha' \rangle \langle \alpha' | \hat{B} | \alpha \rangle =$$

$$\int \frac{d^2 \alpha'}{\pi} |\langle \alpha' | \alpha \rangle|^2 a^{(n)}(\alpha', \alpha^*) b^{(n)}(\alpha, \alpha^*)$$

$$(3.5.37)$$

where

$$a^{(n)}(\alpha', \alpha^*) = \sum_{r, s} a_{r, s}^{(n)} \alpha'^r \alpha^s, \quad b^{(n)}(\alpha, \alpha^*) = \sum_{r, s} b_{r, s}^{(n)} \alpha^* r \alpha^s. \quad (3.5.38)$$

Now using the identity (Appendix A6)

$$|\langle \alpha' | \alpha \rangle|^2 = e^{-\frac{\partial^2}{\partial \alpha \partial \alpha^*}} \delta^{(2)}(\alpha - \alpha')$$

$$(3.5.39)$$

and recalling that

$$\delta^{(2)}(\alpha - \alpha') \equiv \delta(\alpha^* - \alpha'^*) \delta(\alpha - \alpha') = \delta(\alpha_r - \alpha'_r) \delta(\alpha_{im} - \alpha'_{im}) \quad (3.5.40)$$

(subscripts $r \ (im)$ stands for the real (imaginary) part of a complex number) one may write
\[
(\hat{A} \hat{B})_G = \int \frac{d^2 \alpha'}{\pi} \delta^{(2)}(\alpha - \alpha') \, e^{\frac{\delta^2}{\alpha \alpha^*}} \, [a^{(n)}(\alpha', \alpha^*) \, b^{(n)}(\alpha, \alpha^*)]
\]

or equivalently

\[
(\hat{A} \hat{B})_G = \int \frac{d^2 \alpha'}{\pi} \delta^{(2)}(\alpha - \alpha') \, e^{\frac{\delta^{(a)}}{\alpha \alpha^*}} e^{\frac{\delta^{(b)}}{\alpha^* \alpha}} \, a^{(n)}(\alpha', \alpha^*) \, b^{(n)}(\alpha, \alpha^*) .
\]

(3.5.42)

Carrying out the integration leads to

\[
(\hat{A} \hat{B})_G = e^{\frac{\delta^{(a)}}{\alpha \alpha^*}} e^{\frac{\delta^{(b)}}{\alpha^* \alpha}} \, a^{(n)}(\alpha, \alpha^*) \, b^{(n)}(\alpha, \alpha^*) \quad (3.5.43)
\]

and this equation may be cast into form given by (3.4.33) if one notes that

\[
\frac{\partial}{\partial \alpha} = \frac{\hbar}{i} \left( \frac{\partial}{\partial q} - i \xi \frac{\partial}{\partial p} \right). \quad (3.5.44)
\]

3.6 Wigner and Husimi distributions in the SSE Model

In this Section we attempt to elucidate the properties of the Wigner and Husimi distribution functions by calculating them for the non-trivial case of the eigenfunctions of the SSE Hamiltonian \( \hat{H}_0 \). In this case the distribution functions in general may be calculated only numerically so that some aspects of the computational methods are briefly discussed.

Using the definition of the Wigner function (3.3.5) and taking into account that \( \Phi_n(x) \) is real and identically equal to zero for \( x \leq 0 \) one obtains
\[\phi^n_W(p, q) = \frac{1}{\pi} \int_0^{2q} \Phi_n(q + \frac{1}{2} x) \Phi_n(q - \frac{1}{2} x) \cos(xp) \, dx \quad (3.6.1)\]

where Planck's constant was set to unity.

Hence \(\phi^n_W(p, q)\) is symmetrical with respect to the momentum axis in the quantum phase space. The integration in (3.6.1) must in general be carried out numerically and involves evaluation of the associated Laguerre polynomials cf. (2.3.8). For high quantum numbers \(n\) the only reliable method of computing the Laguerre polynomials is based upon the recurrence relation [73]

\[L^{(1)}_{n+1}(x) = (2 - \frac{x}{n+1})L^{(1)}_n(x) - L^{(1)}_{n-1}(x). \quad (3.6.2)\]

To avoid the accumulation of round-off errors the calculations should be performed in double precision arithmetic.

In Fig. 5 the Wigner function for \(|\Phi_5\rangle\) is presented. Even for such a low principal quantum number the oscillatory behavior of this distribution is apparent. This behavior is a source of serious numerical problems. In order to faithfully display the structure of the Wigner function one is forced to use a denser grid in the phase space with increasing principle quantum number. This is computationally inefficient although the resulting images are often quite spectacular.

The Husimi distribution corresponding to the eigenfunctions \(|\Phi_n\rangle\) can be evaluated with the help of definition (3.4.4) and formula (3.4.2):

\[\phi^n_H(p, q) = \frac{1}{2\pi} \left| \langle \Phi_n | \Phi_\alpha \rangle \right|^2 = \frac{1}{2\pi} \left| \int_0^\infty e^{-\frac{\xi}{2} (q-x)^2 + ip(x-q)} \Phi_n(x) \, dx \right|^2 \quad (3.6.3)\]
and again the Planck's constant was put equal to unity.

In principle it is possible to express Laguerre polynomials in (2.3.8) as a power series in \( x \) and then integrate each term in (3.6.3) separately which yields the representation of of \( q''_H \) by means of the parabolic cylinder functions [74]. However, the numerical integration in (3.6.3) is fairly straightforward. One should notice that due to the presence of a rapidly decaying exponential the integration may be effectively confined to a relatively small interval \([\text{Max}(0, q-x_u), q+x_u]\). The value of \( x_u \) is determined from the condition that the exponential in (3.6.3) takes on predetermined, very small values at the endpoints. For the calculations discussed here \( x_u \) was set to \( \sqrt{12/\xi} \) although satisfactory accuracy may be accomplished with a much smaller value.

As it has already been pointed out the definition of the Husimi distribution involves the coarse-graining parameter \( \xi \). The choice of \( \xi \) is not unique and setting its value to the natural frequency of the unperturbed system was originally proposed by Husimi. However, his arguments cannot be directly employed in the present context. The choice of the coarse graining parameter for the SSE Hamiltonian has been previously discussed [74] and is based on the following observation [75]. If \( \rho_H(q,p) \) is the Husimi representation of a wavefunction \( |\Psi\rangle \) then from (3.4.29) and (3.4.30)

\[
\langle q^2 \rangle_H = \int q^2 \rho_H(q,p) \, dq dp = \langle \hat{Q}^2 \rangle + \frac{1}{2\xi} \tag{3.6.4}
\]

and

\[
\langle p^2 \rangle_H = \int p^2 \rho_H(q,p) \, dq dp = \langle \hat{P}^2 \rangle + \frac{1}{2\xi}, \tag{3.6.5}
\]

where \( \langle \hat{Q}^2 \rangle = \langle \Psi | \hat{Q}^2 | \Psi \rangle \), \( \langle \hat{P}^2 \rangle = \langle \Psi | \hat{P}^2 | \Psi \rangle \). On the other hand,
\[ \langle q \rangle_H = \int \int q \rho_H(q, p) dq dp = \langle \hat{Q} \rangle \tag{3.6.6} \]
\[ \langle p \rangle_H = \int \int p \rho_H(q, p) dq dp = \langle \hat{P} \rangle \tag{3.6.7} \]

\[ \langle \hat{Q} \rangle = \langle \Psi | \hat{Q} | \Psi \rangle \quad \text{and} \quad \langle \hat{P} \rangle = \langle \Psi | \hat{P} | \Psi \rangle. \]

It is apparent from (3.6.4)-(3.6.5) that coarse-graining artificially increases quantum fluctuations. Note that the average of the Husimi representation \( a_H(q, p) \) with respect to the Husimi distribution \( \langle \cdots \rangle_H \) is identical with the average of the Wigner representation \( a_W(q, p) \) with respect to the Wigner distribution \( \langle \cdots \rangle_W \). \( \langle a_H \rangle_H = \langle a_W \rangle_W = \langle \hat{A} \rangle \), i.e. the quantum average of an observable is independent of the representation of the distribution function. However, the average of \( q^2 \), or any other phase-space function may change when evaluated in the Wigner and the Husimi representations separately, as indicated by (3.6.4)-(3.6.5). In order to obtain a reliable phase-space representation of \( \Psi \) we require that

\[ \langle \hat{Q}^2 \rangle = \frac{1}{2} \xi, \quad \langle \hat{P}^2 \rangle = \frac{1}{2} \xi \tag{3.6.8} \]

or

\[ \frac{1}{2} \langle \hat{Q}^2 \rangle \ll \xi \ll 2 \langle \hat{P}^2 \rangle. \tag{3.6.9} \]

It was shown previously that for large principle quantum numbers the expectation value \( \langle \Phi_n | \hat{Q}^2 | \Phi_n \rangle \) for the unperturbed eigenfunctions \( |\Phi_n \rangle \) is proportional to \( n^4 \) (cf. formula (2.3.32)) and the expectation value \( \langle \Phi_n | \hat{P}^2 | \Phi_n \rangle \) is proportional to \( 1/n^2 \) (cf. formula (2.3.30)). Thus the criterion (3.6.9) reads

\[ \frac{1}{2} n^4 \ll \xi \ll \frac{2}{n^2}. \tag{3.6.10} \]
If we choose the coarse graining parameter in (3.6.10) equal to the natural frequency of the state |Φ₅>: ξ = 1/n³ then this relation is satisfied. One should realize however that these arguments are valid only for a pure state.

Fig. 6 provides the example of the Husimi distribution of |Φ₅⟩ calculated with the coarse-graining parameter ξ₅ = 1/5³. It is clear from this figure that the process of smoothing has effectively suppressed the oscillatory behavior of the Wigner function. In Figure 7 both distributions are presented from a viewpoint chosen to emphasize that the Husimi function, unlike the Wigner function, is positive definite.

It is worth stressing that the maximum of the Husimi function is peaked at the turning point of the corresponding classical trajectory (cf. Fig. 1(b) and Fig. 6). With the increasing principle quantum number n the Husimi distribution of |Φₙ⟩ is stretched along the position axis and contracted along the momentum axis in the phase space reflecting the properties of classical trajectories. This provides also the simple geometrical interpretation of relations (2.3.33) and (2.3.34) for the position and momentum uncertainty of the eigenstates |Φₙ⟩.

Further insight into the choice of the coarse-graining parameter may be obtained by considering the asymptotic form of the Husimi distribution for ξ → ∞ and ξ → 0 [66].

Using (3.4.12) and (3.4.13) after integrating p_H over momentum and taking the limit ξ → ∞ one obtains

\[ \lim_{\xi \to \infty} \int p_H(p, q) \, dp = \lim_{\xi \to \infty} 2\pi \hbar \left( \frac{\xi}{\pi \hbar} \right)^{1/2} \int e^{-\frac{\xi}{\hbar}} |\Psi(x)|^2 \, dx = 2\pi \hbar |\Psi(q)|^2. \]
In the other limit it is convenient to express $\rho_H$ as

$$\rho_H(p, q) = \int dp_x dp_x' K(p, q; p_x, p_x') \Psi^*(p_x) \Psi(p_x)$$  \hspace{2cm} (3.6.12)

with the new kernel $K$ given by

$$\tilde{K}(p, q; p_x, p_x') = \frac{1}{(\pi \hbar \xi)^{1/4}} e^{-\frac{1}{2\xi} \left[ (p-p_x)^2 + (p-p_x')^2 \right] - \frac{iq}{\hbar} (p_x - p_x')}$$ \hspace{2cm} (3.6.13)

Formula (3.6.12) may be derived using the completeness relation for the momentum operator rather than for the coordinate operator in (3.4.12) and the momentum representation of the coherent state:

$$\langle p_x | q \rangle = \frac{1}{(\pi \hbar \xi)^{1/4}} e^{-\frac{(p-p_x)^2}{2\hbar \xi} - \frac{iq}{\hbar} (p_x - p_x)}.$$ \hspace{2cm} (3.6.14)

Employing (3.6.12) and (3.6.13) one may show that

$$\lim_{\xi \to 0} \int \rho_H(p, q) dq = 2\pi \hbar |\Psi(p)|^2.$$ \hspace{2cm} (3.6.15)

It can be seen from (3.6.15) and (3.6.11) that by choosing very small or very large value of the coarse-graining parameter one may obtain the distribution which resembles the probability density either in momentum or coordinate representation. In Fig. 8(a) the Husimi function $|\Phi_H\rangle$ corresponding to $\xi_s = \xi_s/100$ is presented. Fig. 8(b) shows the Husimi distribution for the same eigenfunction but with the much larger coarse-graining parameter $\xi_t = 100\xi_s$. The contour plots of the distributions from Fig. 8 are contrasted in Fig. 9 with the probability densities in momentum and coordinate representations, respectively. One can see from
this figure that the asymptotic behavior of the Husimi distribution given by (3.6.15) and (3.6.11) is already very well pronounced.
CHAPTER FOUR

NUMERICAL RESULTS FOR THE DRIVEN SSE MODEL

4.1 Quantum dynamics

In this Section we discuss the influence of the initial localization of a Gaussian wave packet (coherent state) in the quantum phase space of the driven SSE model on its subsequent time evolution [76,77]. In the primary classical and quantum simulations discussed here the perturbation was turned on suddenly ($g(t)$ is a unit step function), $\Omega = 1/(66)^3$ a.u. and $F = 0.03/(66)^4$ a.u. The calculations with the different values of the model's parameters and/or the type of the initial wave-function in most cases were performed to verify the conclusions drawn from the main numerical data.

In Fig. 10(a) the Poincaré surface of section of the classical phase space for $F = 0.01/(66)^4$ a.u. is shown. This picture was constructed using the trajectories originating from the turning points of the classical unperturbed orbits with an action $I$: $x_I = 2I^2, p_I = 0$ and $I$ is an integer selected from the interval $[60, 80]$. For every trajectory a point was plotted in the phase space every period $T$ of the perturbation for a total of 200 periods. These particular initial conditions have been chosen to elucidate the structure of the nonlinear resonance corresponding to the scaled frequency $\Omega' = 1$. One can see from Fig. 10(a) and the blowup of the central section in Fig. 10(b), that all the trajectories are apparently stable KAM tori.

Increasing the field strength to $F = 0.03/(66)^4$ a.u. induces an instability in the orbits resulting in the outermost KAM tori dissolving into a chaotic sea, and the more central tori retaining their stability, cf. Fig. 11(a). The stable region of Fig. 11(a) is enhanced in Fig. 11(b), where one can see that a number of the inner tori
have bifurcated into sequences of stable island chains. In further discussion we
call this central region the stability (regular) island or stability region. Note that
the phase space in Fig. 11(a) can clearly be divided into the regular and stochastic
(chaotic) parts. Most Hamiltonian systems investigated in the literature (with the
standard map being the paradigm) have this type of phase space which is dubbed
mixed phase space [78]. On the other hand, chaotic systems without the regular is-
lands do exist in physical applications. Following Bleheret et al [79] we use the
term "systems with fully developed chaos" as a generic name for chaotic systems
without regular islands.

In the quantum mechanical calculations presented herein three minimum un-

certainty wave packets, initially localized in the phase space at $q_1 = 8000$ a.u.,
$p_1 = 0; q_2 = 10000, a.u., p_2 = 0$ and $q_3 = 12000 a.u., p_3 = 0$, were used. They
are referred to as $P_1$, $P_2$ and $P_3$, respectively. The quantum dynamics of the wave
packet $P_4$, originally located at $q_4 = 7000 a.u., p_4 = 0$, is discussed separately in
Section 4.3. The Husimi functions for these packets differ only by their location
in phase space so that in Fig. 12 only the one corresponding to the packet $P_1$ is
displayed. The comparison of Fig. 12 with the structure of the classical phase
space in Fig. 11(b) (the vertical gridlines in this picture refer to the initial position
localization of the packets) shows that the packet $P_1$ is well embedded in the sta-
bility island while the packet $P_2$ just barely overlaps with the island. On the other
hand, the packet $P_3$ is totally outside the stability region, in the chaotic portion of
the phase space. The projection of the packets $P_1$, $P_2$ and $P_3$ on the basis state
$|\Phi_n\rangle$ of the SSE Hamiltonian is given in Fig. 13. In Figs. 14-16 the time evolution
of these wave packets in the Husimi representation is presented. The range of posi-
tion $q$ ($0, 20000 a.u.$) and momentum $p$ ($-0.03 a.u., 0.03 a.u.$) used in the present-
ed pictures comprises only a small portion of the phase space. We have already
mentioned that the Husimi distribution of the eigenstate \(|\Phi_n\rangle\) peaks in the phase space at \(2n^2\). Thus the maximum value of position 20000 a.u. corresponds to the maximum of the Husimi distribution for \(n = 100\). One can see from Fig. 13 that the basis expansion of the packets \(P_1, P_2\) and \(P_3\) are peaked at \(n_1 = 64, n_2 = 72\) and \(n_3 = 79\), respectively. In the course of time the distribution function of the strongly perturbed packets may spread outside the indicated region of phase space which can be clearly seen as bumps at the edges of the pictures. The scales for the value of the Husimi distribution were chosen for maximum resolutions and usually differ from one picture to the other. In the accompanying contour plots six contour lines, uniformly spaced between zero and the maximum value of the Husimi function, were used. It should be noticed that the Husimi distributions were calculated at times which correspond to the maximum strength of the driving force so that the pictures are usually not symmetric with respect to the \(p\) axis. This is distinct from the results presented by Stevens and Sundaram [74], who investigated the time evolution of the distribution function for the driven SSE Hamiltonian initially prepared in an eigenstate \(|\Phi_n\rangle\). The symmetry of all their depicted Husimi functions with respect to momentum suggests that the expectation value
\[
\langle \Psi(t) | \hat{P} | \Psi(t) \rangle
\]
would be identically equal to zero. Inspection of equations (2.3.26) and (2.3.27), however, as well as our numerical calculations contradict this conjecture.

Figs. 14-16 reveal a significant influence of the structure of the classical phase space on the quantum dynamics. The packet \(P_1\) depicted in Fig. 14 originally located within the stability island, remains very well localized even after 100 cycles of the driving force, cf. Figs. 14(a)-14(d). The packets \(P_2, P_3\), on the other hand, undergo complicated evolution as shown in Figs. 15 and 16. It is clear that they spread out to cover the region of the phase space occupied by the classical trajectories. This spreading is particularly rapid and persistent for the packet \(P_3\). Howev-
er, the time scale of the motion is short so that the presented snapshots cannot fully describe the nature of the quantum dynamics. This is demonstrated more clearly by the time evolution of the autocorrelation function or survival probability

\[ S(t) = \left| \langle \Psi(t) | \Psi(0) \rangle \right|^2 \]

(4.1.1)
given in Fig. 17. Only values for times equal to multiples of the period \( T \) are plotted.

The packet \( P_1 \) in Fig. 17(a) exhibits a very interesting kind of fast collapse and revival whose amplitudes are slowly varying function of time. The envelope of the revivals begins to decrease immediately after the perturbation is switched on. The minimal value of 0.53 occurs at \( t = 60T \). From that moment revivals become stronger and stronger and at \( t = 141T \) the survival probability achieves the value 0.92. On the other hand, the minimum of the envelope of the collapses drops to 0.02 at \( t = 3T \) and steadily grows to the maximum of 0.22 observed at \( t = 70T \). Then it decays gradually so that at \( t = 1327 \) it is equal again to 0.02.

The autocorrelation function is frequently used to extract information about the coherence of the quantum dynamics. The very low envelope of collapses at the early stage of the time evolution of the packet \( P_1 \) are somewhat surprising since there is very little spreading apparent in Fig. 14. The resolution of this problem is provided in Fig. 18(a) where the Husimi function for the packet \( P_1 \) at \( t = 3T \) is shown.

The extremely low value of the autocorrelation function is primarily a result of the coherent displacement of the packet from its initial position. Another example of this type of behavior is given in Fig. 18(b) which shows the distribution function for the packet \( P_2 \) at \( t = 2T \) when the survival probability is equal to 0.01. In this case besides the coherent displacement a noticeable amount of spreading may also be observed. While the time development of the survival probability of the packet
$P_1$ is quite regular the other packets $P_2$ and $P_3$ quickly lose the correlation with the initial state and their subsequent evolution seems to be erratic [cf. Fig. 17(b), 17(c)]. Despite this irregular behavior the autocorrelation function may be as high as $0.44$ at $t = 116T$ for the packet $P_2$ and $0.42$ at $t = 81T$ for the packet $P_3$ which demonstrates the presence of strong quantum mechanical correlations. Analyzing Fig. 17(b) we discover in the initial evolution and later at $t = 100T$ the ghost of the quasiperiodic behavior of the packet $P_2$. There is no similar behavior in Fig. 17(c) which corresponds to the packet $P_3$. This observation provides additional evidence that the quantum dynamics is affected by the structure of the classical trajectories in phase space.

A quantitative measure of the spreading observed in the above pictures is given by the quantum uncertainty [cf. (2.3.23-26)]. In Fig. 19(a) the change in $U(t)$ over time is graphed for $P_1$, $P_2$ and $P_3$. It is clear from this figure that there is essentially no change from the initial uncertainty in $P_1$, that the uncertainty in $P_2$ is substantially larger and that in $P_3$ is the greatest of the three. If we examine the position uncertainty and momentum uncertainty separately in Figs. 19(b) and 19(c) we can see that the large oscillations in $U(t)$ are primarily due to abrupt changes in the momentum uncertainty over time.

The character of the temporal evolution of momentum uncertainty may be elucidated if one realizes that the minimum uncertainty wave packet is the linear combination of many unperturbed basis states each having a different natural frequency. The superposition of motions with the different frequencies yields the observed erratic behavior. This interpretation was confirmed in our numerical calculations performed on the driven SSE Hamiltonian initially prepared in the pure state $|\Phi_n\rangle$. If the external perturbations is strong enough to significantly populate several basis states the momentum uncertainty exhibits irregular evolution.
Otherwise it is a slowly varying function of time. In Fig. 20 the quantum uncertainty, position uncertainty and momentum uncertainty are plotted for the "high frequency" numerical experiment with $|\Phi_{s0}\rangle$ perturbed by the driving force with the scaled frequency $\Omega' = 2.8$ and the scaled amplitude $F' = 0.03$. One can see from this figure that the external perturbation causes only minor distortions of the wavefunction as shown by the slow variation of $U(t)$, $AX(t)$, $AP(t)$ around the initial values. The additional evidence is provided in Fig. 21 where the Husimi distributions of the wavefunctions at $t = 0$ and $t = 30T$ are compared. It is clear that the wavefunction and consequently its Husimi distributions essentially remains "frozen" which exemplifies typical quantum mechanical dynamics in the high frequency regime at moderate field strengths.

There is some short time variation in the position uncertainty in Fig 19(b), but its time evolution is dominated by an apparent diffusion process. If we disregard the transient, the position uncertainty of $P_2$ and $P_3$ grows ballistically with time $\Delta X \propto t$. Note that this is not the diffusive mechanism discussed by Casati et al [31] and later by Jensen et al [35]. They discussed the diffusion of action in action-angle space using a Fokker-Planck equation with an action dependent diffusion coefficient. Here the "diffusion" is in configuration space.

To test whether this ballistic behavior is not a result of a particular choice of the coherent states as the initial wavefunction the additional quantum mechanical calculations were performed for the system prepared in the eigenstates $|\Phi_n\rangle$ with $n = 64, 72, 79$. These values of the principle quantum number correspond to the maximum of the occupation probability for the expansion of the wave packets $P_1$, $P_2$ and $P_3$ in the unperturbed basis (cf. Fig. 13). The quantum uncertainty, position uncertainty and momentum uncertainty for these supplementary runs are given in Fig. 22. The time development of the relevant survival probabilities are shown in Fig. 23. It is apparent from Fig. 22(b) that in the numerical experiments
with $|\Phi_{72}\rangle$ and $|\Phi_{79}\rangle$ the growth of the position uncertainty is also ballistic. The straight lines in this figure were drawn to guide the eye. On the other hand, in the experiment with $|\Phi_{64}\rangle$ the spreading is very limited and the question arises whether the quantum dynamics in this case resembles that of the wave packet $P_1$. However, the erratic behavior of the survival probability in Fig. 23(b) and the large oscillations of the momentum uncertainty in Fig. 22(c) shows that the dynamics is much more involved. In this case the Husimi distribution erratically “wanders” around quite large but nevertheless bounded parts of the quantum phase space cf. Fig. 24. This in sharp contrast with quite regular behavior of the wave packet $P_1$ which, as we recall from Fig. 14, is effectively trapped inside the stability island. Note that the Husimi distribution of the eigenfunction $|\Phi_{64}\rangle$, given in Fig. 24(a), unlike that of the wave packet $P_1$ is fairly broad and it is not confined to the stability region. This observation, to some extent, may be used to qualitatively elucidate the quantum dynamics found in the experiment with $|\Phi_{64}\rangle$. We will return to this problem in Section 4.3.

Finally we may attempt to draw the conclusion that the quantum dynamics may be stabilized in the vicinity of the regular regions in the classical phase space. This behavior was also found in the driven double-well oscillator [17] and in the case of the driven SSE Hamiltonian prepared in the pure state $|\Phi_n\rangle$ discussed earlier by Jensen et al [35]. However, both Lin and Ballentine [17,18] and Takahashi and Saito [80,81] found that if the wave packet is located in a classically chaotic region it spreads to cover the entire chaotic sea. The comparison of the Husimi functions shown in Fig. 16 with the structure of the classical phase space Fig. 11 suggests that this scenario is also applicable to the perturbed SSE Hamiltonian. We should realize however that the time evolution of the Husimi function is the intricate interplay of “classical” and “quantum” terms in equation (3.4.36). This interplay was discussed by Bonci et al [82,83] with regard to the evolution of
the Wigner distribution in their discussion of a two-level atomic system interacting with a coherent radiation field. As a result of this interplay the portion of the phase space accessible to the quantum wave packet is in the present study reduced compared to the classical trajectories. Moreover, despite the spreading the wave packet retains its quantum properties as is clearly reflected in the time development of the survival probability. The presence of quantum interference is also manifested in the structure of the Husimi distribution which does not uniformly cover the phase space but is usually made up of several “islands”.

To emphasize the quantum nature of the wave packet dynamics we performed a “time reversal” experiment reversing the direction of the time evolution at the point when the spreading of the packets was almost complete. As far as the numerical calculations are concerned the “time reversal” may be accomplished either by changing the direction of time during the numerical integration of the set of equations (2.3.12) or while using the Floquet method by replacing the evolution operator \( \hat{C} \) by the adjoint operator \( \hat{C}^\dagger \). In Fig. 25(a) we see that at \( t = 507 \), the point at which the evolution was reversed, the position uncertainty of the packet \( P_3 \) retraces its path as shown by the symmetry of the curve. This reversibility is a clear manifestation of quantum coherence throughout the “diffusion” of this packet. In the same way the corresponding correlation function (survival probability) depicted in Fig. 25(b) denotes the time reversibility of the evolution process. Thus we see that the term “diffusion” in this context is misleading and ought to be abandoned.

4.2 Floquet analysis

The importance of Floquet theory goes beyond the numerical efficiency which becomes significant only when the number of periods of integration is much larger than the number of basis states. There is general consensus [6, 84] about the functional form of the distribution of nearest neighbor quasienergy level spacing.
When the corresponding classical system undergoes a transition from integrable motion to chaotic motion it is reflected in the change of level statistics from Poisson-like to Wigner-like (avoided level crossing distribution). Moreover, it was shown by Graffi et al. [85] that the threshold for avoided level crossing coincides with that predicted by Chirikov's resonance criterion [30] for the onset of stochastic behavior in classical Hamiltonian systems. The overlap of resonances is also associated with the change of the structure of some quasienergy states. For example, in the double-resonance model studied by Lin and Reichl [84] the Floquet states are well localized below the overlap threshold of the perturbation. When the overlap takes place the quasienergy states in the region of the phase where two resonances interact become extended. Their extension grow with the increasing strength of the perturbation.

The Floquet approach was used to estimate the threshold for the onset of ionization in driven SSE Hamiltonian [43, 86-88]. For small perturbations the Floquet eigenvectors overlapping the initial wave packet are well localized about the unperturbed hydrogen eigenfunctions. When the strength of the perturbation exceeds a critical value quasienergy vectors spread out which via equation (2.3.22) leads to a rapid delocalization of the initial wave packet. Jensen et al. [20] have shown that the kind of Husimi representation of quasienergy states excited at the end of the slow switch-on of the perturbation are highly localized near unstable periodic orbits in the chaotic classical phase space. It was suggested that this provides an explanation for the existence of the anomalously stable states found in the experiments with microwave-perturbed highly excited hydrogen atoms. This is reminiscent of the scarred wave functions found by Heller [11] in the stadium billiard or the wavefunctions of Rydberg atoms in a strong magnetic field [89].

We have already pointed out (2.3.21) that only Floquet states initially overlapping the wavefunction contribute to its time development. We define the Floquet spectrum as
\[ I(E) = \sum_i |\langle \Psi(0)| \chi_i \rangle|^2 \delta(E - E_i) \]  

(4.2.1)

\( I(E) \) is given in Fig. 26 for the three cases studied. The spectrum of \( P_1 \) as shown in Fig. 26(a) is dominated by two QES \( E_1 = 2.477 \) with \( I_{P_1}(E_1) = 0.546 \) and \( E_2 = 1.452 \) with \( I_{P_2}(E_2) = 0.281 \). The Husimi representation of these states are shown in Fig. 27. We can see from this picture that both states are very well localized. The total uncertainty is equal \( \Delta U_{E_1} = 4.1 \) a.u. for the state \( E_1 \) and \( \Delta U_{E_2} = 3.6 \) a.u. for the state \( E_2 \). These values of the quantum uncertainty are very low in comparison with the uncertainty of the eigenfunctions \( |\Phi_n\rangle \) peaked in the same region of the phase space. Calculating (2.3.35) for \( n = 64 \) we obtain the uncertainty of 32 a.u. Moreover, the comparison with the portrait of the classical phase space Fig. 11(b) shows that these Floquet states are embedded in the stability island. While the dynamics of \( P_1 \) is determined by a very small number of QES, the time evolution of \( P_2 \) and \( P_3 \) involves a great number of them. Figure 28 shows the Husimi distribution of the QES \( E_3 = 0.476 \) [cf. Fig. 26(b)] with the largest overlap with the packet \( P_2, I_{P_2}(E_3) = 0.189 \). The total uncertainty of this state is \( \Delta U_{E_3} = 4.7 \) a.u. It happens that the Floquet state from Fig. 27(b) also significantly overlaps with the packet \( P_2, I_{P_2}(E_2) = 0.185 \). The Husimi representations of two Floquet states from the spectrum of \( P_3, E_4 = 2.522 \) with

\[ I_{P_3}(E_4) = 0.255 \] and \( E_5 = 0.415 \) with \( I_{P_3}(E_5) = 0.155 \) are presented in Fig. 29.

The spatial extension of the distribution functions from Fig. 29 is much greater than those from Figs. 27 and 28. This is clearly reflected by the total uncertainty which for the state \( E_4 \) is equal \( \Delta U_{E_4} = 79.3 \) a.u. and for \( E_5 \) is equal \( \Delta U_{E_5} = 77.8 \) a.u. The significant difference between the QES from the spectrum of the packet \( P_3 \) and those from the spectrum of \( P_2 \) becomes apparent when we compare the
values of the total uncertainty for five dominant Floquet states from Fig. 26(b) and 26(c). For the packet $P_2$ the uncertainty varies from $4.1 \, a.u.$ to $11.6 \, a.u.$ while for the packet $P_3$ varies from $27.1 \, a.u.$ to $84.2 \, a.u.$ We would like to stress another feature of the Husimi functions in Fig. 29 namely the long tails mimicking the structure of the classical trajectories. This observation may be used as a heuristic explanation of the migration of the packet $P_3$ into the region of the phase-space corresponding to low quantum numbers.

We conclude this section with a brief discussion of the general properties of the quasienergy states of the driven SSE Hamiltonian. Bardsley et al. [86] classified the Floquet states into three groups on the basis of their expansion over the eigenfunctions $|\Phi_n\rangle$:

(I) states which primarily overlap with a single low $n$ state and thus do not differ significantly from $|\Phi_n\rangle$,

(II) transitional states,

(III) states which mainly overlap with high $n$ states and whose expansion coefficients decay as a power of $n$ for large $n$.

The examples of the basis expansion of several Floquet states are given in Fig. 30. Note that the presence of well localized quasienergy vectors and close to the end of the basis is the numerical artifact. This may be verified by the diagonalization of the evolution operator $\hat{\mathcal{C}}$ in the larger basis. However, the basis expansion of all Floquet states discussed in this Section is peaked far away from the end of the basis and should not be affected by the basis truncation. Nevertheless, the calculations with a smaller basis, made up of 150 states, were carried out and yielded the same results.
Type I and II states are always present in the spectrum of the Floquet operator \( \hat{\mathcal{C}} \). The range of the transitional states depends upon the strength of the perturbation. The spectrum of the packets \( P_1 \) and \( P_2 \) is composed of the very well localized transitional states with low values of the quantum uncertainty. We have found the distribution functions of the most localized states to be centered over the classical stability island [cf. Fig. 12] which shows the way in which the structure of the Floquet states reflects the properties of the classical phase space.

4.3 KAM quantum dynamical barriers

On the basis of the KAM theorem it is now clear that a classical motion may be confined to a region of the phase space delineated by the invariant KAM tori [90]. Due to the uniqueness of the solution of the Hamilton equations tori cannot be crossed by a classical trajectory. Thus, KAM tori constitute the impenetrable barriers for the flow in the phase space and consequently may significantly influence the transport properties of the Hamiltonian systems. This is particularly strongly pronounced in two dimensional phase space which may be partitioned by tori into disjoint regions. We restrict further discussion to systems with two degrees of freedom. However, the KAM theorem guarantees the existence of tori only for sufficiently small perturbations. With the increasing perturbation they eventually are destroyed and transformed into Cantori (broken tori). Cantori are quasi periodic orbits with irrational winding numbers similar to those of the original tori. Unlike tori they do not fill a line in the Poincaré surface of section but only a fractal object - Cantor set and as a result are permeable to classical trajectories. Once the last confining KAM torus that partitions phase space is broken the stochastic orbits may wander around all accessible regions of the phase space. These orbits may be strongly influenced by the small stable regions or islands, identical in nature to that shown in Fig. 11(b), which are characteristic feature of the phase space of Hamiltonian systems with two degrees of freedom. These islands, also known as KAM islands, originate as a result of a break up of unper-
turbed periodic orbits with rational winding number $r/s$ where both $r$ and $s$ are integers. The Poincaré-Birkhoff theorem [90] (frequently referred to as the fixed point theorem) states that only an even number of periodic points $2ks, k = 1, 2, \ldots$ of the rational orbits will survive under sufficiently small perturbation. Half of them are elliptic (stable) and half hyperbolic (unstable). The elliptic points are surrounded by a family of invariant curves. This family itself is the subject of the KAM theorem so that its rational members will break up according to the Poincaré-Birkhoff theorem. This means that inside the island there are both stochastic layers, associated with hyperbolic points, and new island chains. The repetitive application of the above analysis to all new elliptic points yields the spectacular self-similar structure.

A particle which erratically moves in the phase space may spend a considerable amount of time in the vicinity of a KAM island [91-93]. After this “quiescent” period it resumes its chaotic motion and eventually may again stick to another island. This “hopping” process results in the slow (algebraic) decay of correlation functions. Moreover, a group of particles launched from the part of the phase space containing KAM islands escape from the predefined region according to the algebraic law $N(t) = 1/t^z$ where $N(t)$ is the number of the remaining particles after a time $t$ and $z$ is the decay exponent. $N(t)$ is proportional to the classical “survival” probability. Lai et al [94] showed that this algebraic decay law holds also for a driven SSE model. Moreover, they found that the decay exponent may decrease as the strength of the perturbation is increased. This is somewhat surprising since one expects the larger driving force to facilitate migration of the electrons out of a given region. Lai et al were able to relate this unusual behavior to the metamorphosis of the phase space structure. Under sufficiently small perturbations the phase space is made up of KAM islands immersed in two distinct chaotic regions separated by the confining KAM tori. When these tori are destroyed and transformed into Cantori new layers of the KAM islands become accessible to
the erratically roaming electrons. After this metamorphosis the time evolution of
the classical "survival" probability may be still described by the power law but
with different decay exponents for small and large times. In the latter case the de-
cay exponent is smaller than that before the metamorphosis. Lai et al demonstrat-
ed that the trajectories of the electrons which escape after longer time are trapped
by the joint action of the Cantori and the newly accessible islands.

Now one may pose an intriguing question. Since the Correspondence Principle
requires quantum mechanics to recover classical properties in the limit $\tilde{\hbar} \to 0$, is it
possible to find a quantum analogue to KAM tori or Cantori? Do they also play
the role of dynamical barriers in quantum mechanics?

This problem was first addressed in the case of the quantum kicked rotator
where a single confining KAM torus may be isolated. Geisel et al [95,96] demon-
strated that both tori and Cantori can inhibit the spreading of the wavefunction.

The penetration depth of a KAM torus was found to scale as $\tilde{\hbar}^{-0.66}$ and the penetra-
tion probability as $\tilde{\hbar}^{-2.5}$. Amazingly enough, classically penetrable Cantori can
completely arrest the spreading of the wave packet. Thus Cantori appear to act as
quantum dynamical barriers even more drastically than in classical domain. The
plausible explanation relies on the fact that the fractal structure of the Cantor set
in the quantum phase space is resolved only to the length scale of the order $\tilde{\hbar}$. Gei-
sel et al conclude that the classical KAM tori and Cantori are the origins of a
KAM localization mechanism which is entirely different from the quantum inter-
ference dynamic (Anderson) localization already discussed in Section 2.3. As far
as the driven SSE model is concerned the good agreement of the ionization rates
obtained from the classical and quantum calculations in the low-frequency regime
suggests that also in this model the classical dynamical barriers may persist in the
quantum domain. The purpose of this Section is to investigate how the prominent
KAM island displayed in Fig. 11(b) affects the propagation of the Husimi distribution in the quantum phase space.

The first observation comes from the dynamics of the wave packet $P_1$. As it has already been pointed out in Section 4.1 this packet remains confined within the stability island. The regular quantum dynamics, in this case, is a result of the existence of the Floquet states whose Husimi representations are extremely well localized in the stability region. We also speculated that the profoundly different dynamics in the experiment with $|\Phi_{64}\rangle$ may be attributed to the large spatial extension of the Husimi distribution of $|\Phi_{64}\rangle$. In the context of the Floquet analysis presented in the last Section this conjecture seems to be justified now. The initial wavefunction in this experiment is simply coupled to many quasienergy states which results in the erratic but otherwise confined time development of the Husimi distribution and the dynamical variables.

The question arises whether the dynamics of the wave packet $P_1$ provides convincingly enough evidence for the role of the KAM tori as quantum dynamical barriers. We were not quite certain so that we carried out another numerical experiment this time with the wave packet $P_4$ initially localized at $q_4 = 7000$ a.u. The inspection of the classical phase space in Fig. 11(b) shows that the Husimi distribution of this wave packet is essentially outside the stability island. What is even more important the width of the island at this part of the phase space is comparable to that of the packet. Hence, if KAM tori persist in the quantum phase space the dynamics of the wave packet $P_4$ should be strongly affected.

Fig. 31 shows the Floquet spectrum for the packet $P_4$. One can see that there are several quasienergy states with the comparable overlap so that the "random" character of the time evolution of the survival probability in Fig. 32 or the momentum uncertainty in Fig. 33(c) is not surprising. On the other hand, the graph of the
quantum uncertainty Fig. 33(a) or the position uncertainty Fig. 33(b) shows that the spreading of the wave packet is limited. Now let us focus our attention on the propagation of the Husimi distribution displayed in Fig. 34. It is quite astonishing how clearly the presence of the KAM island is manifested in the quantum phase space. In all presented plots the wavepacket does not invade the classically inaccessible region but rather wraps around it. Note that the excitation of the wave packet is possible through relatively narrow channels determined by the borders of the stability island and the curve which delineates the energetically allowed portion of the phase space. This results in the squeezing of the wave packet under the action of the driving force. The influence of the KAM tori on the structure of the Floquet states is also very straightforward. In Fig. 35 the Husimi representation of five dominant quasienergy states in the spectrum of $P_4$ are presented. They clearly may be classified into two groups. Husimi distributions of the Floquet states from Figs. 35(b) and 35(d) do not differ much from those corresponding to the eigenfunctions $|\Phi_n\rangle$ and they are peaked outside the stability region. The distributions of the quasienergy states from Figs. 35(a), 35(c) and 35(e) are quite similar to each other with very characteristic three peaks. These distributions wrap around the stability island and their minima are centered over the island. This provides a quite suggestive interpretation of the packet’s dynamics shown in Fig. 34.

4.4 Conclusions and proposed future research work

In this thesis we have investigated the influence of the structure of the classical phase space on the quantum dynamics of certain minimum uncertainty wave packets. We have found that the packets initially overlapping the regular regions of phase space remain localized, while the packets centered on the classical chaotic sea spread rapidly. The quantum dynamics was analyzed using the Floquet formalism and it was determined that the Floquet spectrum of the stable packets are dominated by a few quasienergy states whose Husimi distributions are very well localized in the classical stability islands. Moreover, it has been found that the
most localized Floquet states are peaked in the vicinity of the stable island. The spectrum of the most unstable wave packet is made up of the greatest number of the QES whose corresponding distribution functions are usually very elongated thereby mimicking the shape of classical trajectories. To elucidate the complicated nature of the quantum evolution the quantum uncertainty was introduced as a dynamical variable. In the presence of the spreading of the wave packet the time development of its quantum uncertainty is determined by the monotonic growth of position uncertainty and the erratic oscillations of the momentum uncertainty. Surprisingly enough, the position uncertainty increases ballistically with time \( \Delta X \propto t \) until the packet fills the available portion of the phase space. We stress that apart from significant spreading the quantum interference effects are clearly pronounced both in the time evolution of the survival probability and in the structure of the Husimi distributions. Finally, it has been demonstrated that the prominent KAM island persists in the quantum phase space as a dynamical barrier which hinders the wave packet from exploring the classically inaccessible region. We argue that the KAM localization along with the scarring previously discussed by Jensen et al [20] might be responsible for the existence of the anomalously stable states observed in the experiments with the microwave driven Rydberg hydrogen atoms.

In this work we analyzed the differences between quantum dynamics in the regular and chaotic regions of the classical phase space of the driven SSE model. However, more profound understanding of the correspondence between the classical and quantum mechanics of this system may be provided by extraction of purely classical contribution from evolution of both the Husimi distribution function and averages of quantal observables. In particular, the comparison of the Husimi function with the coarse-grained classical distribution \( \rho_{CG} \) would allow us to thoroughly investigate quantum penetration of KAM dynamical barriers. The influence of classical dynamics upon the evolution of expectation value of operators may be particularly conveniently studied within the framework of the Wigner
representation. For an arbitrary operator $\hat{A}(\hat{P}, \hat{Q})$ the semiclassical approximation of $\langle \psi(t) | \hat{A}(\hat{P}, \hat{Q}) | \psi(t) \rangle$ may be obtained just by solving the Hamilton equations of motion and averaging the Weyl transform $A_w(p, q, t)$ over the initial distribution function $\rho_w(p, q, 0)$ [19,82,83] (Note that in the Husimi representation the analogous method cannot be implemented because of the presence of the coarse-graining term in the equation governing time evolution of the Husimi distribution cf. (3.4.36)). With the help of this approach we would like to find out whether the ballistic growth of the position uncertainty in the driven SSE model may be associated with the properties of the classical dynamics. We have already stated in Chapter 1 that, both from historical and conceptual point of view, semiclassical methods have been significantly useful for calculating stationary eigenfunctions and eigenvalues and for elucidating quantum mechanical properties. Thus it is quite natural to expect that a semiclassical theory may yield valuable insights into the concepts of quasienergies and Floquet states. However, a systematic approach to a semiclassical Floquet theory has been developed only very recently. Breuer and Holthaus [97] used the Maslov construction of the canonical operator in the extended phase space to derive quantization rules for quasienergies and Floquet states of a generic periodically time-dependent system. These rules are analogous to the well known Einstein-Brillouin-Keller (EBK) quantization conditions for autonomous systems [1]. Breuer and Holthaus tested their theory for a class of strongly driven anharmonic oscillators whose classical phase space may be clearly divided into an almost regular and a stochastic region. Semiclassical quantization rules were found to provide excellent approximation to the exact quasienergies and Floquet states. The independent confirmation of these results came from the calculations performed by Bensch et al for periodically driven Duffing (quartic) oscillator [98]. The formalism developed by Breuer and Holthaus may be applied to elucidate the nature the quasienergy states localized within the stability island of the driven SSE model. It is apparent that this technique cannot be used in the
chaotic portion of the phase space where tori are rare or absent at all. In this case
semiclassical periodic orbit theories as developed, for example by Gutzwiller [1],
might shed light on the intricate relations between nonlinear classical dynamics
and linear quantum dynamics.
APPENDIX A1

DRIVEN SURFACE STATE ELECTRON HAMILTONIAN IN ACTION
ANGLE VARIABLES
The Hamilton-Jacobi equation for the bounded motion in the SSE model is given by

$$\frac{1}{2} \left( \frac{\partial W}{\partial x} \right)^2 - \frac{1}{x} = -|\epsilon| \quad (A1.1)$$

where $W$ is Hamilton's principle function. Defining $\beta = |\epsilon|x$, one has

$$\frac{\partial W}{\partial x} = \begin{cases} \sqrt{2|\epsilon|} \left( \frac{1}{\sqrt{\beta}} - 1 \right), & p > 0 \\ -\sqrt{2|\epsilon|} \left( \frac{1}{\sqrt{\beta}} - 1 \right), & p < 0. \end{cases} \quad (A1.2)$$

This differential equation can be easily solved to yield

$$W = \begin{cases} \sqrt{\frac{2}{|\epsilon|}} \left( \sqrt{\beta} - \beta^2 + \text{asin} \sqrt{\beta} \right) + C_1, & p > 0 \\ C_2 - \sqrt{\frac{2}{|\epsilon|}} \left( \sqrt{\beta} - \beta^2 + \text{asin} \sqrt{\beta} \right), & p < 0. \end{cases} \quad (A1.3)$$

At the outer turning point $x_t$ of the motion $p = 0$. Therefore $-|\epsilon| = -1/x_t$ and $\beta_t = 1$. It is convenient to normalize $W$ in such a way that $W(0) = 0$ which implies $C_1 = 0$. At the outer turning point the function $W$ must be continuous and we get $C_2 = \pi \sqrt{2/|\epsilon|}$. The action variable $I$ is introduced in the usual way

$$I = \frac{1}{2\pi} \int p \, dx \quad (A1.4)$$

and the integral in the above equation may be calculated explicitly. With $p = \frac{\partial W}{\partial x}$

$$I = 2 \frac{1}{2\pi} \int_0^{x_t} \frac{\partial W}{\partial x} \, dx = \frac{1}{\pi} [W(1) - W(0)] = \frac{1}{\sqrt{2|\epsilon|}}. \quad (A1.5)$$

This yields the familiar hydrogenic expression of the energy in terms of the action:
\( \varepsilon = -1/(2l^2) \). Equation (A1.5) shows that the action \( I \) is a constant of motion. Thus, the canonical transformation to the variables where \( I \) is the new generalized momentum integrates the dynamics of \( H_0 \) and obviously \( H_0 = -1/(2l^2) \). This may be accomplished with the help of the generating function \( F_2(x, I) \), a function of the old coordinate and the new momentum. \( F_2(x, I) \) is just Hamilton's principal function \( W \) expressed in terms of \( x \) and \( I \). Using \( \beta = x/2l^2 \) one obtains

\[
F_2(x, I) = 2n \begin{cases} \sqrt{\beta - \beta^2} + \text{asin} \sqrt{\beta}, & p > 0 \\ \pi - \sqrt{\beta - \beta^2} - \text{asin} \sqrt{\beta}, & p < 0. \end{cases} \tag{A1.6}
\]

The conjugate variable of the action, the angle variable \( \Theta \) is given by

\[
\Theta = \frac{\partial}{\partial I} F_2(x, I) = 2 \begin{cases} \text{asin} \sqrt{\beta - \beta^2}, & p > 0 \\ \pi - \text{asin} \sqrt{\beta + \beta^2}, & p < 0. \end{cases} \tag{A1.7}
\]

Since \( \beta \) is positive and varies from 0 to 1 and back to 0 in one cycle of the motion, one may parametrize \( \beta = \sin^2(\eta), \ 0 \leq \eta \leq \pi \). Hence, \( x \) may be expressed as

\[
x = 2n^2 \sin^2(\eta) \tag{A1.8}
\]

and (A1.7) yields \( \Theta = 2\eta - \sin(2\eta), \ 0 \leq \eta \leq \pi \). \( \Theta \) is unique function of \( \eta \) for \( 0 \leq \Theta \leq 2\pi \). The momentum \( p \) is given by

\[
p = \frac{\partial}{\partial x} F_2(x, I) = \frac{1}{l} \cot(\eta). \tag{A1.9}
\]

Finally, using (A1.8) and (A1.9) the driven Hamiltonian (2.1.1) may be written as

\[
H(I, \Theta) = -\frac{1}{2l^2} + 2l^2 Fg(t) \sin^2(\eta) \cos(\Omega t). \tag{A1.10}
\]
APPENDIX A2

SOLUTION OF EIGENVALUE PROBLEM FOR THE SSE HAMILTONIAN $\hat{H}_0$
The Shrödinger equation corresponding to the unperturbed Hamiltonian $\hat{H}_0$ reads

$$\frac{d^2 \Phi}{dx^2} + 2 \left( \frac{1}{x} + \epsilon \right) \Phi = 0 \quad (A2.1)$$

since $\exp(-x\sqrt{-2\epsilon})$ is the asymptotic solution of (A2.1) for $x \to \infty$ one may write

$$\Phi(x) = e^{-x\sqrt{-2\epsilon}} R(x). \quad (A2.2)$$

Upon substitution of (A2.2) into (A2.1) the following differential equation is obtained

$$xR''(x) - 2x\sqrt{-2\epsilon} R'(x) + \frac{2}{x} R(x) = 0. \quad (A2.3)$$

If $R(x)$ is expressed as a power series [73,99]

$$R(x) = x^s \sum_{k=0}^{\infty} a_k x^k \quad (A2.4)$$

with $a_0 \neq 0$ then (A2.3) leads to

$$\frac{s(s-1)}{x} a_0 = 0 \quad (A2.5)$$

and

$$[s(s-1) + 2s] a_1 = (2\sqrt{-2\epsilon} - 2) a_0. \quad (A2.6)$$

The last two equations may be simultaneously satisfied only if $s = 1$. Then, the recurrence relation for the coefficients $a_k$ reads

$$a_{k+1} = \frac{2\sqrt{-2\epsilon}(k+1) - 2}{(k+1)(k+2)} a_k \quad (A2.7)$$

The power series in (A2.4) terminates only if
\[ \varepsilon = \frac{1}{2 (k + 1)^2}, \quad k = 0, 1, \ldots \quad (A2.8) \]

or using standard notation

\[ \varepsilon_n = \frac{1}{2n^2}, \quad n = 1, 2, \ldots \quad (A2.9) \]

If one writes \( \Phi (x) \) as \( x e^{-x^2/2} L(x) \) and plugs this form into the original Schrödinger equation (A2.1) one obtains

\[ xL''(x) + (2 - \frac{2}{n} x) L'(x) + \frac{2}{n} (n - 1) L(x) = 0. \quad (A2.10) \]

The comparison of this equation with the well known relation for the associated Laguerre polynomials [73, formula 13.45]

\[ xL''_n^{(k)}(x) + (k + 1 - x) L'^{(k)}_n(x) + nL^{(k)}_n(x) = 0 \quad (A2.11) \]

enables us to express the eigenfunction \( \Phi_n \) as

\[ \Phi_n(x) = \frac{x}{n} e^{-x/2} L^{(1)}_{n-1} \left( \frac{2x}{n} \right). \quad (A2.12) \]

The normalized eigenfunction

\[ \Phi_n(x) = \frac{2}{\sqrt{n/2}} x e^{-x/2} L^{(1)}_{n-1} \left( \frac{2x}{n} \right) \quad (A2.13) \]

may be found with the help of the normalization integral for the associated Laguerre polynomials [73, formula 13.52]

\[ \int_0^\infty e^{-x} x^{k+1} L^{(k)}_n L^{(k)}_m \, dx = \frac{(n+k)!}{n!} \frac{1}{(2n+k+1)}. \quad (A2.14) \]
APPENDIX A3

DERIVATION OF THE WEYL TRANSFORM OF THE PRODUCT OF TWO OPERATORS
In order to find the Weyl transform of the product of two operators equation (3.2.32) it is necessary to determine the trace of the product of three \( \hat{A} \) operators. Employing (3.2.12), the property of the delta function

\[
\int \delta(a-x) \delta(x-b) \, dx = \delta(a-b)
\]

and (3.2.6) one gets

\[
Tr [\hat{A}(p, q) \hat{A}(p', q') \hat{A}(p'', q'')] = \int dq_1 dq_2 dq_3 e^{\frac{i}{\hbar} [pq_1 + p'q_2 + p''q_3]}
\]

\[
\delta(q'' - q + \frac{q_1 + q_3}{2}) \delta(q - q' + \frac{q_1 + q_2}{2}) (q'' - q' + \frac{q_2 + q_3}{2})
\]  

(A3.1)

Performing the change of variables \( x = (q_1 + q_3)/2, y = (q_1 + q_2)/2, \)

\( z = (q_2 + q_3)/2 \) with the corresponding Jacobian equal to \( 2^2 \) one arrives at

\[
Tr [\hat{A}(p, q) \hat{A}(p', q') \hat{A}(p'', q'')] = 2^2 e^{\frac{2i}{\hbar} \left( p(q'' - q') + p'(q - q'') + p''(q' - q) \right)}
\]

(A3.2)

Equation (3.2.26) for the product \( \hat{A}\hat{B} \) with the help of (3.2.10) and (A3.3) may be written as

\[
\langle \hat{A} \hat{B} \rangle_w = \frac{2^2}{\hbar^2} \int dq' dp' dq'' dp'' a_w(p', q') b_w(p'', q'') e^{\frac{2i}{\hbar} \left( p(q'' - q') + p'(q - q'') + p''(q' - q) \right)}
\]

(A3.4)

The change of variables \( \tilde{p} = p'' - p, \tilde{q} = q'' - q \) and the Taylor expansion of \( b_w(p + \tilde{p}, q + \tilde{q}) \) around \( (p, q) \) yields
\[
\begin{align*}
(\hat{A}\hat{B})_W &= \frac{2^2}{\hbar^2} \int dq' dp' d\tilde{q} d\tilde{p} a_W(p', q') \\
&= \frac{2^2}{\hbar^2} \left[ \frac{2i}{\hbar} \left( (q' - q) \frac{\partial}{\partial p'} - (p' - p) \frac{\partial}{\partial q'} \right) \right] e^{\frac{\hbar}{2i} \frac{\partial}{\partial q} \frac{\partial}{\partial p}} b_W(p, q)
\end{align*}
\] (A3.5)

In the last exponential we may replace \( \tilde{p} \) by the differential operator \( \frac{\hbar}{2i} \frac{\partial}{\partial q} \) and likewise \( \tilde{q} \) by \( \frac{\hbar}{2i} \frac{\partial}{\partial p} \) both acting to the left as indicated by superscript (l). Then the integration over \( \tilde{p} \) and \( \tilde{q} \) gives delta function so that the integration with respect to \( q', p' \) may also be performed. Finally, (A3.5) takes the form

\[
(\hat{A}\hat{B})_W = a_W(p, q) e^{\frac{\hbar}{2i} \frac{\partial}{\partial q} \frac{\partial}{\partial p}} b_W(p, q)
\]  

(A3.6)

More common notation is obtained by replacing the indices (l) and (r) by (a) and (b) respectively

\[
(\hat{A}\hat{B})_W = e^{\frac{\hbar}{2i} \frac{\partial}{\partial q} \frac{\partial}{\partial p}} a_W(p, q) b_W(p, q)
\]  

(A3.7)
APPENDIX A4

DERIVATION OF FORMULA (3.2.39)
In this Appendix a quantum mechanical operator corresponding to the following Weyl transform

\[ a_w(p, q) = f(q) p^n \]  

(A4.1)

is found where \( f \) is an arbitrary function and \( n \) a natural number. Application of (3.2.37) gives

\[ a_o(p, q) = \sum_{k=0}^{n} \binom{n}{k} \left( \frac{\hbar}{2i} \right)^k \frac{d^k f(q)}{dq^k} p^{n-k} \]  

(A4.2)

and the corresponding operator is given by

\[ \hat{A} = \sum_{k=0}^{n} \binom{n}{k} \left( \frac{\hbar}{2i} \right)^k \frac{d^k \hat{f}(\hat{Q})}{d\hat{Q}^k} \hat{P}^{n-k}. \]  

(A4.3)

The above equation may be rewritten as

\[ \hat{A} = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} \hat{P}^k \hat{f}(\hat{Q}) \hat{P}^{n-k} \]  

(A4.4)

As may be seen in the following way. From the commutation relations (3.2.1) one finds

\[ \hat{P}^k \hat{f}(\hat{Q}) = \sum_{j=0}^{k} \binom{h}{j} \binom{k}{j} \frac{d^j \hat{f}(\hat{Q})}{d\hat{Q}^j} \hat{P}^{k-j} \]  

(A4.5)

Inserting this expression into (A4.3) and using the identities

\[ \binom{n}{k} \binom{k}{j} = \binom{n}{j} \binom{n-j}{k-j}, \frac{1}{2^m} \sum_{n=0}^{m} \binom{m}{n} = 1 \]  

(A4.6)

(A4.4) is recovered. Finally, one may write
\[ f(q) p^n = \left( \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} \tilde{p}^k f(\tilde{q}) \tilde{p}^{n-k} \right) \quad w. \] (A4.7)
APPENDIX A5

DERIVATION OF FORMULA (3.4.24)
In order to prove (3.4.24) one inserts the Taylor expansion of the Wigner function
\[
\rho_H(p', q') = \sum_{m,n=0}^{\infty} \frac{\partial^{m+n}}{\partial q^m \partial p^n} \rho_W(p, q) \frac{(q' - q)^m (p' - p)^n}{m!n!} \quad (A5.1)
\]
into the integral representation of the Husimi function (3.4.1) to obtain
\[
\rho_H(p, q) = \frac{1}{\hbar} \sum_{m,n=0}^{\infty} \frac{\partial^{m+n}}{\partial q^m \partial p^n} \rho_W(p, q) \frac{1}{m!n!} \int_{-\infty}^{\infty} (q' - q)^m e^{-\frac{\xi}{\hbar} (q' - q)^2} \int_{-\infty}^{\infty} (p' - p)^n e^{-\frac{(p' - p)^2}{\xi \hbar}} dp'. \quad (A5.2)
\]
It is apparent that only terms with even \(m\) and \(n\) contribute, using
\[
\int_{0}^{\infty} x^{2n} e^{-px^2} dx = \frac{(2n-1)!!}{2 (2p)^n} \sqrt{\frac{\pi}{p}}, \quad p > 0, \quad n = 0, 1, 2... \quad (A5.3)
\]
[100, equation (3.461.2)] and noting that
\[
\frac{(2n-1)!!}{(2n!)} = \frac{1}{2^n n!} \quad (A5.4)
\]
one arrives at
\[
\rho_H(p, q) = \sum_{m,n=0}^{\infty} \frac{\xi^{n-m} \hbar^{m+n}}{4^m 4^n m!n!} \frac{\partial^{2m+2n}}{\partial q^{2m} \partial p^{2n}} \rho_W(p, q) = e^{\frac{\hbar}{4} \left( \frac{1}{\xi} \frac{\partial^2}{\partial q^2} + \frac{1}{\xi} \frac{\partial^2}{\partial p^2} \right)} \rho_W(p, q) \quad (A5.5)
\]
APPENDIX A6

DERIVATION OF IDENTITY (3.5.39)
Before proving identity (3.5.39) one need to show that the relation between the normally and antinormally ordered product of the delta functions is given by

$$\delta (\alpha^* - \hat{\alpha}^\dagger) \delta (\alpha - \hat{\alpha}) = e^{-\frac{\partial^2}{\partial \alpha^* \partial \alpha}} \delta (\alpha - \hat{\alpha}) \delta (\alpha^* - \hat{\alpha}^\dagger) \quad \text{(A6.1)}$$

Starting from the normally ordered form

$$\delta (\alpha^* - \hat{\alpha}^\dagger) \delta (\alpha - \hat{\alpha}) = \frac{1}{\pi^2} \int d^2 \zeta e^{-i \zeta^* (\alpha^* - \hat{\alpha}^\dagger) e^{-i \zeta (\alpha - \hat{\alpha})}} \quad \text{(A6.2)}$$

and using the following relation (which is a direct consequence of the Hausdorff-Baker relation (3.2.7))

$$e^{-i \zeta^* \hat{\alpha}^\dagger} e^{-i \zeta \hat{\alpha}} = e^{-i \zeta^* \hat{\alpha}^\dagger} e^{-i \zeta \hat{\alpha}} \quad \text{(A6.3)}$$

one arrives at

$$\delta (\alpha^* - \hat{\alpha}^\dagger) \delta (\alpha - \hat{\alpha}) = \frac{1}{\pi^2} \int d^2 \zeta e^{-i \zeta^* \hat{\alpha}^\dagger} e^{-i \zeta \hat{\alpha}} \quad \text{(A6.4)}$$

This equation after substitution

$$e^{-i \zeta^* \hat{\alpha}^\dagger} e^{-i \zeta \hat{\alpha}} = e^{-\frac{\partial^2}{\partial \alpha^* \partial \alpha}} e^{-i \zeta^* \hat{\alpha}^\dagger} e^{-i \zeta \hat{\alpha}} \quad \text{(A6.5)}$$

gives (A6.1).

Now one may easily prove that the square overlap $|\langle \alpha | \alpha' \rangle|^2$ may be written as

$$|\langle \alpha | \alpha' \rangle|^2 = e^{-\frac{\partial^2}{\partial \alpha^* \partial \alpha}} \delta (\alpha - \alpha') \quad \text{(A6.6)}$$

After calculating

$$\langle \alpha' | \delta (\alpha - \hat{\alpha}) \delta (\alpha^* - \hat{\alpha}^\dagger) | \alpha' \rangle =$$
one inserts the completeness relation (3.4.10) into the lhs to get

\[ \int \frac{d^2 \alpha''}{\pi} |\langle \alpha'' | \alpha' \rangle|^2 \delta^{(2)}(\alpha - \alpha'') = e^{\frac{\partial^2}{\partial \alpha \partial \alpha^*}} \delta^{(2)}(\alpha - \alpha') \quad (A6.8) \]

which after integration of the lhs gives (A6.6).
FIGURES
Figure 1. Classical orbits of the SSE Hamiltonian with action: (a) $I_0 = 1$, (b) $I_0 = 5$ and (c) $I_0 = 10$. 
Figure 2. Eigenfunctions $\Phi_n(p)$ of the SSE Hamiltonian: (a) $n = 1$, (b) $n = 5$, (c) $n = 10$. Left column shows the real part of the eigenfunctions and right column shows the imaginary part.
Figure 3. Eigenfunctions $\Phi_n(x)$ of the SSE Hamiltonian: (a) $n = 1$, (b) $n = 5$, (c) $n = 10$. 
Figure 4. Relations between the Wigner and Husimi distribution functions $\rho_W$ and $\rho_H$ and their classical counterparts $\rho_C$ and $\rho_{CG}$. 
Figure 5. Wigner distribution of the eigenfunction $|\Phi_5\rangle$ of the SSE Hamiltonian $H_0$. 
Figure 6. Husimi distribution of the eigenfunction $|\Phi_3\rangle$ of the SSE Hamiltonian $H_0$. 
Figure 7. Comparison of the Wigner and Husimi distribution functions corresponding to the eigenfunction $|\Phi_3\rangle$ of the SSE Hamiltonian $H_0$. 
Figure 8. Husimi distributions of the eigenfunction $|\Phi_5\rangle$ with different values of the coarse-graining parameter (a) $\xi = 1/(100 \times 5^3)$, (b) $\xi = 100/5^3$. 
Figure 9. The upper left contour plot corresponds to the Husimi distribution from Fig. 8(a), the upper right to that from Fig. 8(b). The lower left graph shows the probability density for the eigenfunction $|\Phi_5\rangle$ in the momentum space representation, the lower right the corresponding density in the coordinate representation.
Figure 10. (a) Poincaré surface of section for $\Omega = 1/ (66)^3$ a.u. and $F = 0.01/ (66)^4$ a.u., (b) magnified central part of the Fig. 10(a).
Figure 11. (a) Poincaré surface of section for $\Omega = 1/(66)^3$ a.u. and $F = 0.03/(66)^4$ a.u. (b) The regular part of the classical phase space is enlarged to reveal the structure of nonlinear resonances. The vertical gridlines correspond to the position localization of four minimum uncertainty wave packets used in quantum calculations. The packet $P_1$ was initially localized at $q_1=8000$ a.u., the packet $P_2$ at $q_2=10000$ a.u., $P_3$ at $q_3=12000$ a.u. and $P_4$ at $q_4=7000$ a.u.
Figure 12. Husimi function of the packet $P_1$ at $t = 0$. 
Figure 13. The projection of three minimum uncertainty wave packets on the basis states of the SSE Hamiltonian $\hat{H}_0$. Dotted line corresponds to the packet $P_1$ dashed lined to the packet $P_2$ and solid line to $P_3$. 
Figure 14. Time evolution of the wave packet $P_1$ initially localized at the regular part of the classical phase space. The times plotted are (a) $5T$, (b) $20T$, (c) $50T$, (d) $100T$. 
Figure 14 continued
Figure 14 continued
Figure 14 continued
Figure 15. Time evolution of the wave packet $P_2$ initially overlapping the regular part of the classical phase space. The times plotted are (a) $5T$, (b) $20T$, (c) $50T$, (d) $100T$. 
Figure 15 continued
Figure 15 continued
Figure 15 continued
Figure 16. Time evolution of the wave packet $P_3$ initially localized in the chaotic region of the classical phase space. The times plotted are (a) $5T$, (b) $20T$, (c) $50T$, (d) $100T$. 
Figure 16 continued
Figure 16 continued
Figure 16 continued
Figure 17. Survival probability for (a) wave packet $P_1$, (b) wave packet $P_2$ and (c) wave packet $P_3$. 
Figure 18. Husimi function of (a) the wave packet $P_1$ at $t = 3T$, (b) the wave packet $P_2$ at $t = 2T$. 
Figure 18 continued
Figure 19. Time evolution of (a) quantum mechanical uncertainty, (b) position uncertainty, (c) momentum uncertainty. Dotted line corresponds to the packet $P_1$, dashed line to the packet $P_2$ and solid line to the packet $P_3$. 
Figure 20. Time evolution of (a) quantum mechanical uncertainty, (b) position uncertainty, (c) momentum uncertainty for the experiment with $|\Phi_{80}\rangle$. 
(a) $t=0$

Figure 21. (a) Husimi function of $|\Phi_{80}\rangle$, (b) Husimi function at $t = 30T$ in the numerical experiment with $|\Phi_{80}\rangle$. 
Figure 21 continued
Figure 22. Time evolution of (a) quantum uncertainty, (b) position uncertainty, (c) momentum uncertainty. Dotted line corresponds to the experiment with \( |\Phi_{64}\rangle \), dashed line to the experiment with \( |\Phi_{72}\rangle \) and solid line to that of \( |\Phi_{79}\rangle \).
Figure 23. Time evolution of the survival probability in the numerical experiments with (a) $|\Phi_{64}\rangle$, (b) $|\Phi_{72}\rangle$, (c) $|\Phi_{79}\rangle$. 
Figure 24. Time development of the Husimi function in the experiment with $|\Phi_{64}\rangle$. Times plotted are (a) $t = 0$, (b) $t = 5T$, (c) $t = 20T$, (d) $t = 50T$. 
Figure 24 continued
Figure 24 continued
Figure 24 continued
Figure 25. "Time reversal" experiment for the wave packet $P_3$ (a) time evolution of position uncertainty. At $t = 50T$ the time evolution was reversed. The symmetry of the curve shows the reversibility of the quantum dynamics. (b) Time evolution of survival probability.
Figure 26. Floquet spectra corresponding to the wave packets (a) $P_1$, (b) $P_2$, (c) $P_3$. 
Figure 27. Husimi representation of two quasienergy states significantly overlapping the packet $P_1$: (a) $E_1 = 2.477$, $I_{P_1}(E_1) = 0.546$, (b) $E_2 = 1.452$, $I_{P_1}(E_2) = 0.281$. 
Figure 27 continued
Figure 28. Husimi representation of the quasienergy state significantly overlapping the packet $P_2$: $E_3 = 0.476$, $I_{P_2}(E_3) = 0.189$. This packet overlaps also the QES from Fig. 27(b), in this case $I_{P_2}(E_2) = 0.185$. 
Figure 29. Husimi representation of two quasienergy states significantly overlapping the packet $P_3$: (a) $E_4 = 2.522$, $I_{P_3}(E_4) = 0.255$. (b) $E_5 = 0.415$, $I_{P_3}(E_5) = 0.155$. 
Figure 29 continued
Figure 30. Basis expansion of selected Floquet states.
Figure 31. Floquet spectrum of the wave packet $P_4$.

Figure 32. Time evolution of the survival probability for the wave packet $P_4$. 
Figure 33. Time evolution of (a) quantum uncertainty, (b) position uncertainty, (c) momentum uncertainty for the wave packet $P_4$. 
Figure 34. Time evolution of the Husimi distribution of wave packet $P_4$. Times plotted are (a) $5T$, (b) $10T$, (c) $20T$, (d) $50T$, (e) $100T$. 
Figure 34 continued
Figure 34 continued
Figure 34 continued
Figure 34 continued
Figure 35. Husimi representation of the quasienergy states significantly overlapping the packet $P_4$. 
Figure 35 continued
Figure 35 continued
Figure 35 continued
Figure 35 continued


