

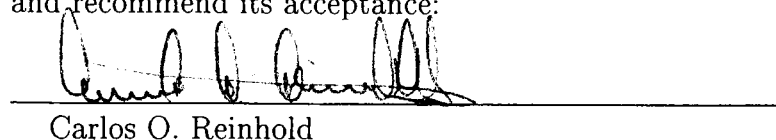
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I am submitting herewith a dissertation written by Shuhei Yoshida entitled "Quantum chaos in the periodically kicked Rydberg atom". I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Physics.



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**Quantum chaos in the periodically
kicked Rydberg atom**

A Dissertation

Presented for the

Doctor of Philosophy Degree

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Shuhei Yoshida

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Abstract

A theoretical study of classical-quantum correspondence in the periodically kicked Rydberg atom is presented. Experimental measurements of the Rydberg atom survival probability have found a broad maximum for pulse repetition frequencies near the classical orbital frequency. Comparisons with a detailed classical analysis show that this behavior provides an unambiguous signature of dynamical stabilization. The classical simulations further show that the kicked atom is, depending on the pulse repetition frequency, chaotic or characterized by a mixed phase space with various families of fully stable islands within which the atom is stable against ionization. When the classical Rydberg atom is stable, classical-quantum correspondence is observed, i.e., the quantum counterpart closely mimics the classical phase space structure on the Husimi distribution of the system, which is a quantum wave function projected onto phase space. On the other hand, the quantum system is found to be stable even when the classical system becomes chaotic and leads to a fast ionization rate. In such cases, the corresponding quantum wave functions show enhanced amplitudes along the paths of unstable periodic orbits, which are classical regular motions hidden within disordered chaotic orbits. These enhanced regular motions, stabilize the quantum system against the ionization of the classical atom. In the study of the kicked atom, it is necessary to perform numerical simulations of the quantum system. In practice, only a finite number of basis states can be used in order to explore the solution of the time-dependent Schrödinger equation in the whole Hilbert space. This finite basis set subtends a finite subspace within the Hilbert space. Artificial reflections at the effective "wall" which is the boundary of the finite subspace, and reentering of probability flux into the subspace represent a major limitation for the study of long time evolution of the ionization process in the kicked Rydberg atom. We propose a new method called the repetitive projection method (RPM) and discuss its applicability compared to other conventional methods.

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List of Acronyms

a.u.		atomic unit
CR		complex rotation
CTMC		classical trajectory Monte Carlo
DVR		discrete variable representation
HCP		half-cycle pulse
LDOS		local density of state
RPM		repetitive projection method
srff		slow rise fast fall-off
TDSE		time-dependent Schrödinger equation

Chapter 1

Introduction

Since the discovery of quantum mechanics, many scientists have been trying to understand this new world of physics. Basically, quantum mechanics describes phenomena on a small scale, such as an atomic scale, where the disturbance accompanied by the act of observation becomes non-negligible. Since science is concerned only with observables and we can observe an object only by letting it interact with some outside influence, this disturbance is unavoidable. We may define an object to be big or small depending on whether the disturbance is negligible or not. The concepts of big and small are, however, purely relative and refer to the gentleness of our means of observation as well as to the object being observed. In order to give an absolute meaning to the scale – the concepts of big and small – we have to assume that there is a limit to the finiteness of our powers of observation and the smallness of the accompanying disturbance. Since our physical intuition is grounded in classical mechanics where the observation doesn't affect any physical phenomena, quantum mechanics, in a sense, resides in the world beyond our intuition. According to the “correspondence principle,” quantum mechanics must go over into classical mechanics in the classical limit which is defined by letting the Planck constant approach zero, $\hbar \rightarrow 0$, and which is identical to letting the limit of the observation approach zero. With the aid of the “correspondence principle,” we

expect to understand the crossover region called the “semi-classical” regime and build a bridge between two different worlds of physics, classical and quantum mechanics.

One of the most interesting subjects of study in classical-quantum correspondence is a system whose classical dynamics becomes “chaotic” or “disordered.” It has been found that a very simple mathematical non-linear system can have very complicated trajectories classically. Not only is their behavior exceedingly sensitive to precise initial conditions, but they also never settle to any reasonable final state with a recognizable fixed pattern. This field, termed “chaos”, has been studied extensively and has been rapidly growing with the development of numerical simulations and the rapid growth of computing powers in last three decades. Quantum mechanics is linear in the wave function i.e. the time evolution of the wave function, $|\psi(t)\rangle = \sum a_n(t)|\phi_n\rangle$, is governed by the linear differential equation

$$i\hbar\dot{\mathbf{a}}(t) = \hat{H}\mathbf{a}(t) \quad (1.1)$$

The question arises: what implications does chaotic classical dynamics, which is a result of non-linear dynamics, have for the quantum description of the system, particularly in the semi-classical regime? This field of study is called “quantum chaos” and it has been studied for various systems. Some well-known works, which are closely related to this thesis, are introduced in the next few sections.

1.1 Quantum chaos

In this section, two of the most important discoveries in the field of “quantum chaos” are introduced. They will be revisited in Chapter 5. One is known as ‘scars’ of the wave function, which were found by Heller [1] for a classically chaotic, bounded, time-independent system. Consider the case of a free point particle bouncing in a closed hard-walled two-dimensional region, the so-called ‘billiard problem’. In the case of the

stadium billiard (fig. 1.1), it is known that the classical system becomes strongly chaotic [2] and the periodic orbits are densely distributed in phase space. However, they are unstable and their measure is zero. Nevertheless, quantum eigenfunctions of the system have been found to have an enhanced amplitude along the path of unstable periodic orbits, different eigenfunctions corresponding to different periodic orbits (fig. 1.1). These wave functions are called scarred wave functions, and an enhanced amplitude along an unstable orbit is called the ‘scar’ of the wave function.

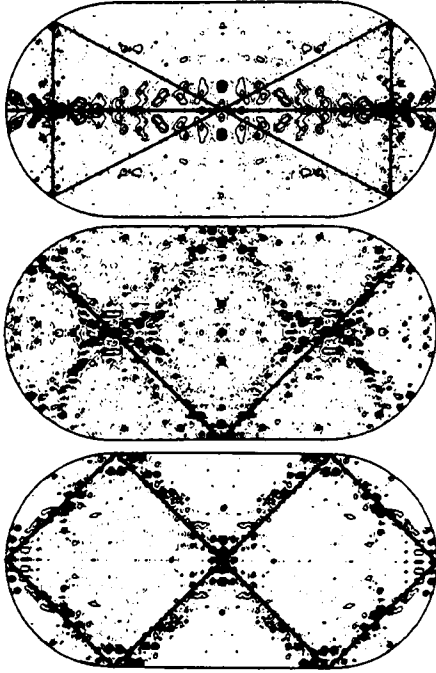


Figure 1.1: Unstable periodic orbits and semi-classical wave functions in the stadium billiard [1]

Another discovery in quantum chaos has been that of quantum localization of periodically perturbed systems. The kicked rotor is a well-known system in this category [3, 4]. The system is described by the Schrödinger equation [5],

$$i\tilde{\hbar}\frac{\partial}{\partial t}|\psi\rangle = H_{rot}|\psi\rangle \quad (1.2)$$

with

$$H_{rot} = \frac{\tilde{\hbar}^2}{2}p_\theta^2 + K_{rot}\cos\theta \sum_k \delta(t-k) \quad (1.3)$$

where $\tilde{\hbar}$ is a “dimensionless” Planck constant. Classically, the equations of motion associated with this Hamiltonian are reduced to the standard map [5, 6], which, for large enough K_{rot} , is known to become chaotic and yield diffusion in the angular momentum p_θ space with an increasing average energy as a function of time,

$$\tilde{\hbar}^2 \langle p_\theta^2/2 \rangle \sim \frac{K_{rot}^2}{4}t. \quad (1.4)$$

The corresponding quantum system was studied by Casati et al. [3]. A result of their numerical simulations is schematically illustrated in fig. 1.2. The quantum motion diffuses just as in the classical case but only during a finite interval of time, k^*T , after which quantum effects become important and the classical diffusion is suppressed. Further investigation [4] has shown that this phenomenon is mathematically the analogue of the suppressed electrical conductivity in systems with random scattering potentials [7]. A

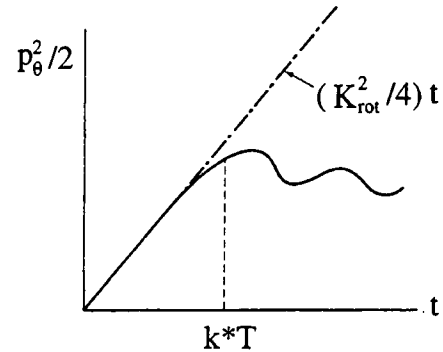


Figure 1.2: Schematic picture of Anderson localization for the kicked rotor problem [3, 5]

classical particle in such a potential makes a random walk, and eventually diffuses a distance whose square is proportional to the time. However, a quantum particle does not necessarily behave in this way and remains in the vicinity of its own initial position. This phenomenon is called Anderson localization and has been studied extensively. The experimental realization of the kicked rotor system has only recently been achieved by subjecting cooled atoms to modulated standing waves, and has confirmed the existence of quantum localization [8].

Another well-studied periodically perturbed system is that of a Rydberg atom subject to a microwave field [9, 10, 11]. In atomic systems, unconstrained chaotic motion leads to ionization of the atom, or alternatively, bounded periodic (or regular) motion leads to stabilization. Thus, chaotic motion can be observed as ionization of the atom. Analogously to the kicked rotor system, quantum localization was found first theoretically [9, 10] and subsequently verified experimentally [11]. It was proved to be identical to Anderson localization. In addition, the localization in this microwave system has been found to involve scarred wave functions. The relation between these two topics, quantum localization and scarred wave functions, is, however, not yet clear.

The main topic of this thesis is the kicked atom system [12, 13, 14, 15, 16, 17] which

is also a periodically perturbed system. Because of the simplicity of the theoretical treatment compared to the microwave system, the kicked atom is expected to provide a good testing ground for the study of quantum chaos and a deeper insight into physics. Before going into details, the basic ideas about the realization of the kicked atom are introduced.

1.2 Realization of the kicked atom

When we speak of a “kicked atom”, the first question that arises is “what is a ‘kick’ ? ” The word “kick” is usually used to describe the physical phenomenon of delivering an impulse to an object in such a short interaction time that the object doesn’t move. For example, when you kick a ball, the time period during which the foot touches the ball is so short that the ball doesn’t move much.

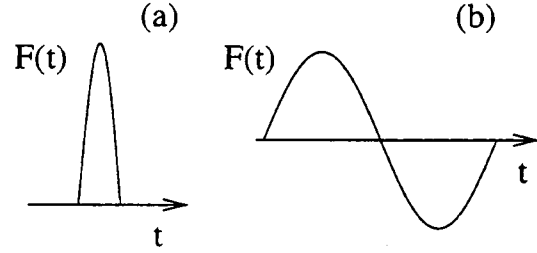


Figure 1.3: (a) Half-cycle pulse (b) sinusoidal pulse

However, the ball will subsequently start moving due to the momentum transferred by the “kick”. In the kicked atom, the “kick” can be realized using a so-called half-cycle pulse (HCP) [18, 19, 20, 21]. Note that the system is called the “kicked atom” but the object which is kicked is an electron in the atom and not the atom itself. A HCP is a pulsed unidirectional electric field which is characterized by the pulse duration T_p (fig. 1.3), and its peak field F_p . The name half-cycle pulse originates in the fact that it resembles half of a cycle of a sinusoidal pulse.

Consider a system where a single HCP interacts with a Rydberg atom with a principal quantum number n_i . The time scale that determines whether the pulse is short or long is given by the orbital period of the electron in the atom. If the pulse duration T_p is much shorter than the orbital period T_{n_i} of the excited electron, a single HCP $F(t)$

delivers an impulsive momentum transfer

$$\Delta \mathbf{p} = - \int dt \mathbf{F}(t) \quad (1.5)$$

to the excited electron¹. Since a HCP is a unidirectional pulse, the absolute value of $\Delta \mathbf{p}$ is finite. In contrast, $\Delta \mathbf{p}$ is zero on average for a sinusoidal pulse (fig. 1.3). In practice, producing a HCP with T_p of the order of the orbital period T_n is not an easy task. Such a system has been realized in two different ways: by making the pulse duration shorter, i.e., using subpicosecond pulses and relatively low Rydberg levels ($n_i \sim 30$) [18] or, alternatively, by making the orbital period longer, i.e., using nanosecond pulses and very-high- n states ($n_i \sim 400$) [19]. The latter pulses can be generated using conventional pulse generators. Therefore, it is possible to manipulate the shape, the duration, and the strength of a pulse, or even to superimpose several pulses and create various kinds of “designer” pulses. One important example is that of a periodic train of pulses which can be generated by superimposing several narrow HCPs equally-spaced in time. The basic scheme of this experiment is displayed in fig. 1.4. In the first stage, the Rydberg atom ($n_i = 388$) is created by photoexciting ground-state potassium or rubidium atoms using a frequency-stabilized laser beam. The atoms are then subject to a train of equispaced HCPs. The number of Rydberg atoms remaining in the experimental volume after application of the pulse train is determined by field ionization. Measurements with no pulse train applied are interspersed at routine intervals during data acquisition to monitor the number of Rydberg atoms initially created by the laser.

In this process, momentum is periodically transferred to the electron in the atom. Intuitively, the atom should gain a large amount of energy and should finally become ionized. The question is whether the atom is always ionized or can be stabilized in any way. The quantum description as well as the classical description of this fully chaotic system is investigated in this thesis.

¹See Appendix D for a numerical example.

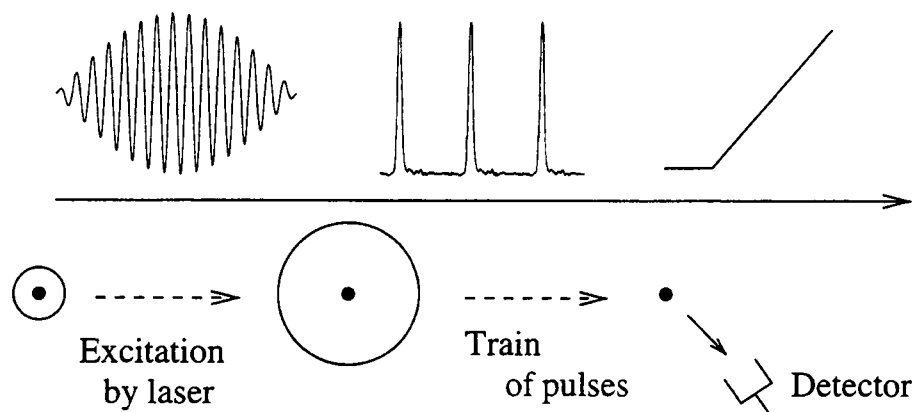


Figure 1.4: Schematic picture of the experiment of the kicked atom system. From the left to the right: laser excitation, a sequence of HCPs, and field ionization.

1.3 Overview

In the next chapter, the classical dynamics of the kicked atom is analyzed. Similarities between a real three-dimensional system and a simplified one-dimensional system are discussed. Using this simplified model, a clear picture of the stabilization and ionization of the classical atom is found.

In chapter 3, methods for the quantum numerical simulations are discussed. The time-dependent Schrödinger equation cannot be solved easily either analytically or numerically, which is the biggest obstacle especially for the long-time propagation of the quantum system. A new technique, the “Repetitive Projection Method” (RPM), is developed. This method is compared with other conventional methods and its applicability to the kicked atom is discussed.

In chapter 4, the quantum dynamics of the kicked atom is discussed. We analyze the stabilization of the quantum system for conditions that classical-quantum correspondence is expected. Since this system is periodic in time, the wave function is expanded in a periodic basis set composed of Floquet states, and the stability of each Floquet state is analyzed.

In chapter 5, the quantum localization of the kicked atom is discussed. It is shown

that quantum localization is manifested as scars of localized Floquet states. The localization characteristics are analyzed using the energy distribution of the populated excited states.

A major part of this thesis has already been published [16, 17, 22, 23]. The kicked atom model has also been used to describe the stochastic dynamics of atomic states of fast atoms traveling through matter [24, 25], which is beyond the scope of this thesis.

Atomic units (a.u.) are used throughout this thesis unless stated otherwise. In these units, $\hbar = 1$, $m = 1$ (electron rest mass), $e = -1$ (charge of the electron), $r_B = \hbar^2/me^2 = 1$ (Bohr radius), and $v_B = e^2/\hbar = 1$ (Bohr velocity). Therefore, a Rydberg atom in a given n level has a binding energy $E_n = -1/2n^2$, an average radius $r_n = \langle 1/r \rangle^{-1} = n^2$, an average momentum $p_n = \sqrt{\langle p^2 \rangle} = n^{-1}$, an average Coulomb field $F_n = \langle 1/r \rangle^2 = n^{-4}$, and an orbital period $T_n = 2\pi n^3$.

Chapter 2

Classical analysis of the kicked atom

In the kicked atom, both experimental and theoretical results show not only ionization but also stabilization of the atom under the influence of a train of pulses. In this chapter, the classical dynamics of the kicked atom is analyzed, and both ionization and stabilization of the atom are discussed.

2.1 Three-dimensional model

Consider the electron in a three-dimensional (3-D) hydrogen atom that is subject to a periodic train of impulses $\Delta\mathbf{p} = \Delta p \mathbf{e}_z$ where $\mathbf{e}_z$ is a unit vector directed towards the positive z -axis. The Hamiltonian for this problem in cylindrical coordinates is

$$H^{3D} = H_{at}^{3D} + V(t)$$

with

$$H_{at}^{3D} = \frac{p^2}{2} - \frac{1}{r} = \frac{p_z^2 + p_\rho^2}{2} + \frac{L_z^2}{2\rho^2} - \frac{1}{\sqrt{z^2 + \rho^2}}$$

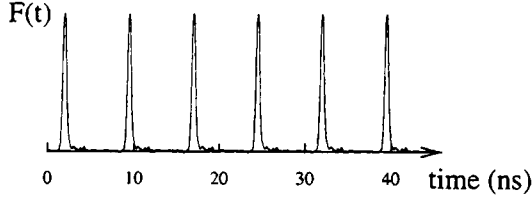


Figure 2.1: Experimental profile of a train of HCPs

$$V(t) = zF(t), \quad (2.1)$$

where we use a coordinate system centered at the atomic nucleus, $\mathbf{r} = (x, y, z)$ and $\mathbf{p} = (p_x, p_y, p_z)$ are the position and momentum of the electron, $\mathbf{L} = \mathbf{r} \times \mathbf{p} = (L_x, L_y, L_z)$ is the angular momentum, $\rho^2 = x^2 + y^2$, and $p_\rho = (xp_x + yp_y)/\rho$. Fig. 2.1 displays a typical experimental profile for a train of pulses which can be written as

$$F(t) \simeq \sum_{k=0}^{K-1} F_{HCP}(t - kT) \quad (2.2)$$

where F_{HCP} is the profile of a single HCP, K is the total number of pulses, and T is the period of the train (frequency $\nu = 1/T$). Since the perturbation $F(t)$ is along the $\hat{z}$ direction, L_z is a constant of motion.

The time evolution of the system can be calculated by numerically integrating the Hamilton's equations of motion,

$$\begin{aligned} \frac{d\mathbf{r}}{dt} &= \mathbf{p}, \\ \frac{d\mathbf{p}}{dt} &= -\frac{\mathbf{r}}{r^3} - e_z F(t), \end{aligned} \quad (2.3)$$

using the Runge-Kutta method and the experimental pulse profile (fig. 2.1) as an input data for the external field $F(t)$.

At $t = 0$ the initial quantum state of a Rydberg atom can be mimicked using an ensemble of points in phase space with well defined binding energy, average angular

momentum, etc. The survival probability of the atom can be estimated statistically by letting a large but finite ensemble of initial conditions evolve in time following Hamilton's equations (eq. (2.3)), and evaluating the probability for the ensemble to remain in bound states ($H_{at} < 0$),

$$P_s(t) = \frac{\text{Number of trajectories with a negative energy at time } t}{\text{Number of initial conditions}}. \quad (2.4)$$

This approach is called the classical trajectory Monte Carlo (CTMC) approach¹. Fig. 2.2 shows an example of the survival probability as a function of the frequency, ν , of the train of pulses. Both CTMC (solid line) and experimental results (squares) reveal a broad maximum in the survival probability for pulse repetition frequencies near the classical orbital frequency, $2\pi \times 388^3(\text{a.u.}) \simeq 110(\text{MHz})$. In this figure, frequencies are also given in scaled units. Scaled units are indicated by the subscript "0" throughout this thesis. In scaled units all variables are referred to the initial state of the atom. For example,

$$\begin{aligned} r_0 &= \frac{r}{r_{n_i}} = \frac{r}{n_i^2} \\ p_0 &= \frac{p}{p_{n_i}} = p n_i \\ t_0 &= \frac{t}{T_{n_i}} = \frac{t}{2\pi n_i^3} \\ \nu_0 &= \frac{\nu}{\nu_{n_i}} = 2\pi n_i^3 \nu. \end{aligned} \quad (2.5)$$

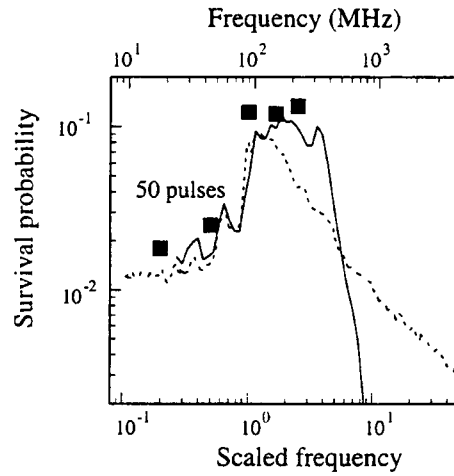


Figure 2.2: Survival probability of the kicked K(388p) atom as a function of the frequency of a train of 50 pulses with $F_p = 60 \text{ mV/cm}$. Squares are experimental results, and the solid line and the dashed line are classical results with the experimental pulse profile and δ -function impulses with $\Delta p_0 = 0.36$, respectively [16].

¹See Appendix A for details

Initial ensembles with different energies become identical by this scaling and, therefore, the dynamics also become identical². This classical scaling invariance is very useful to compare the dynamical properties associated with different initial energy levels and to test classical-quantum correspondence.

The Hamilton's equations for finite-width pulses can be solved numerically. Therefore, it is not computationally feasible to investigate the long-term stability in the limit of the number of pulses $K \rightarrow \infty$ (typically $K \gtrsim 10^6$), and to perform a detailed analysis of classical phase space. Thus, to further examine the origin of the maximum observed in the survival probability, calculations for the "kicked" hydrogen atom have also been performed assuming that each HCP can be replaced by a δ -function impulse,

$$V(t) = -z\Delta p \sum_{k=0}^{K-1} \delta(t - kT). \quad (2.6)$$

where Δp is the integral of a single HCP in the train (eq. (1.5)). In this limit, the time evolution is decomposed into periods of free evolution ($kT + \epsilon < t < (k+1)T - \epsilon$) and kicks ($kT - \epsilon < t < kT + \epsilon$) where $\epsilon \rightarrow 0$. During a free evolution, the electron follows a Kepler motion and is constrained to a plane; this motion is analytically solvable (Appendix C). In turn, a kick is just a momentum transfer simply described by

$$p_z|_{t=kT+\epsilon} = p_z|_{t=kT-\epsilon} + \Delta p \quad (2.7)$$

with the other variables unchanged. Therefore, the computation of the time evolution is reduced to an analytical map and is relatively stable for a long time. The survival probability of this kicked atom is also given in fig. 2.2. This simplified model reproduces the observed overall structures in the survival probability although the stability is somewhat reduced. This is the result of the finite width of each experimental HCP cutting off the higher frequencies in the perturbation which enhance the stability of the

²See Appendix B .

orbit³. The similarities between the different calculations and the experiment suggest that the stabilization can be analyzed in detail in terms of the “kicked” atom.

Fig. 2.3 shows clear evidence of the dynamical stabilization of the kicked atom, where the survival probability as a function of K is plotted for a fixed frequency of the train of kicks. The frequencies are chosen from the pronounced peaks in fig. 2.2, $\nu_0 \sim 1.3, 0.6, 2.1$, and from the valleys, $\nu_0 \sim 0.7, 1.9, 6.2$. From the fact that the survival probability is still finite after a million kicks, these pronounced peaks in fig. 2.2 can be identified as stabilization, as opposed to slow ionization, of the atom under the influence of the train of pulses.

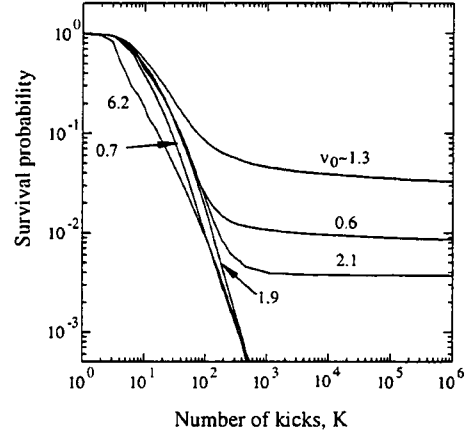


Figure 2.3: Classical survival probability for the kicked hydrogen atom with $L_0 \simeq 0$ and $\Delta p_0 = 0.3$ at various frequencies ν_0 as a function of the number of kicks [16].

2.2 One-dimensional model

In this section, we analyze theoretically the dynamics of the simplest system, the one dimensional (1-D) kicked atom, and we discuss the conditions for which the evolution of the electron is regular or chaotic. Subsequently, we show the similarity between the 3-D and the 1-D systems and the validity of the 1-D model to analyze the stabilization of the 3-D system.

Consider the electron in a 1-D hydrogen “atom” that is subject to a periodic train of impulses Δp with a frequency ν (period $T = 1/\nu$). The dynamics of the atom is governed by the Hamiltonian

$$H(q, p, t) = H_{at}(q, p) + V(q, p, t) \quad (2.8)$$

³See Appendix D

with

$$\begin{aligned} H_{at}(q, p) &= \frac{p^2}{2} + \frac{\Lambda^2}{2q^2} - \frac{1}{q}, \\ V(q, p, t) &= -q\Delta p \sum_{k=0}^{K-1} \delta(t - kT) \end{aligned} \quad (2.9)$$

where q and p denote the position and momentum of the electron. The 1-D atom is described by an unperturbed Hamiltonian H_{at} and includes an effective centrifugal barrier with a quasi angular momentum Λ . We take the limit $\Lambda \rightarrow 0$ and, therefore, the only role of this potential is to provide an infinite barrier at $q = 0$ such that the motion is confined to the $q > 0$ region of phase space. Clearly, the Hamiltonian in this limit becomes equivalent to the 3-D Hamiltonian for $\rho = 0$, $p_\rho = 0$, and $L_z = 0$. Like the 3-D model, the 1-D model can be solved accurately by splitting the time evolution per period into two parts: a free Coulomb evolution described by a map M_{Coul} (Appendix C), and a kick described by a map M_{kick} , i.e.,

$$\begin{aligned} (q_{k+1}, p_{k+1}) &= M(q_k, p_k) \\ &= M_{Coul} \circ M_{Kick}(q_k, p_k), \end{aligned} \quad (2.10)$$

where (q_k, p_k) denotes the phase space coordinates just before the k -th kick.

One interesting feature which is unique for the 1-D system is that the dynamics of the system is completely different depending on the sign of the momentum transfer [13]. For $\Delta p < 0$, pronounced peaks can be seen in the survival probability as a function of ν_0 (fig. 2.4), thereby providing a good candidate for an analogue system of the 3-D kicked atom system. The peaks are observed at frequencies similar to those at which stabilization is predicted for the 3-D kicked atom, and they become more pronounced than those for the 3-D calculation. The survival probability as a function of K (fig. 2.4) shows stabilization of the atom at the frequencies corresponding to the pronounced peaks ($\nu_0 = 0.616, 1.07$, and 2.12) and ionization at the frequencies corresponding to the valleys ($\nu_0 = 0.7, 1.98$, and 5.55).

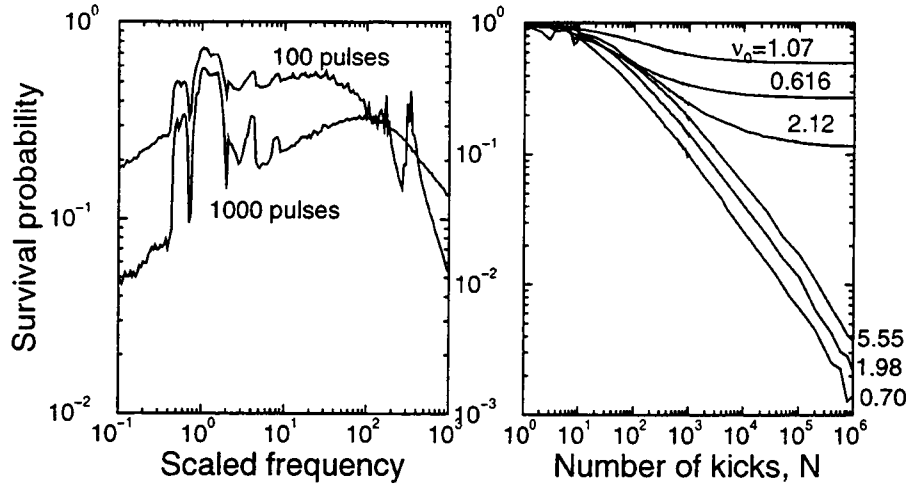


Figure 2.4: Classical survival probability of a 1-D kicked atom as a function of scaled frequency (left) following application of 100 and 1000 kicks with $\Delta p_0 = -0.3$ and as a function of the number of kicks (right) at various frequencies ν_0 of the train with a same momentum transfer [16].

In fig. 2.5, on the other hand, no pronounced peak is found at any frequency for a positive momentum transfer ($\Delta p > 0$) and power law decay of the survival probability is observed [13]. Both figures in fig. 2.5 prove that the system is fully chaotic in this case.

2.3 Analysis of the stabilization of the atom

2.3.1 Poincaré map

In high dimensional systems, it is very difficult to visualize classical trajectories in phase space. The Poincaré map (or the Poincaré surface of section) is a tool to visualize classical trajectories by projecting them onto a lower dimensional phase space and to reveal the dynamical properties of each trajectory.

For example, consider the case in which trajectories are confined to a three-dimensional manifold spanned by three independent variables (x_1, x_2, x_3) . Normally, a system with

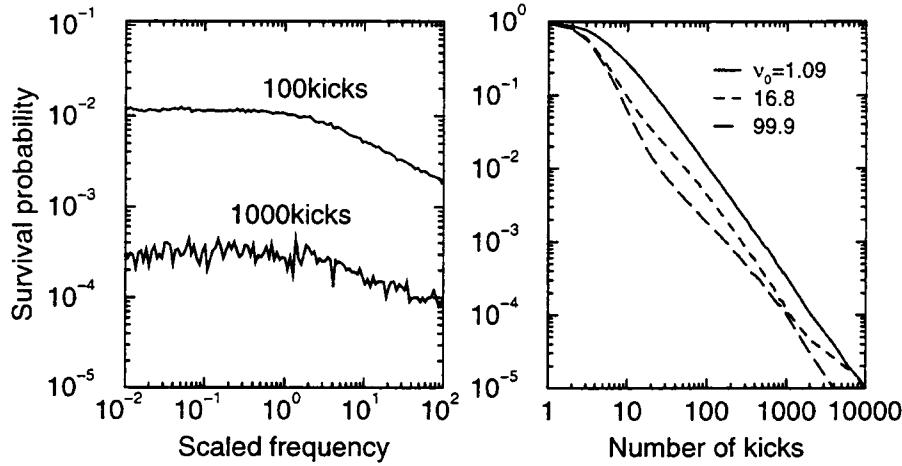


Figure 2.5: Classical survival probability as a function of ν_0 (left) and as a function of K (right). The strength of the kick is $\Delta p_0 = 0.3$. For the right figure, the frequency is set to $\nu_0 = 1.09, 16.8$, and 99.9 .

two degrees of freedom has a four-dimensional phase space and, with one constant of motion such as the energy, the trajectory is confined to a three-dimensional manifold. Fig. 2.6 is a schematic picture of a classical trajectory in this manifold. A trajectory usually becomes quite complex for longer times. The cross section of this trajectory on the $x_1 = 0$ plane, however, exhibits an ensemble of dots (crosses in the figure) which are intersections between the $x_1 = 0$ plane and the trajectory. Whether we can recognize any regular pattern or not in

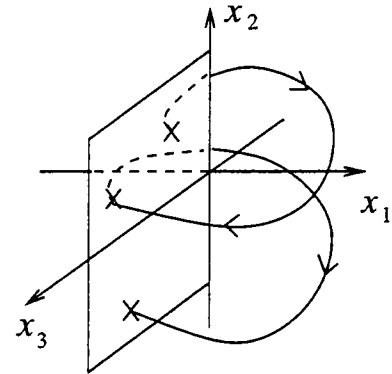


Figure 2.6: Schematic picture of the Poincaré map

this ensemble of dots tells us whether the system is regular or chaotic. For example, if there is an additional constant of motion, $g(x_1, x_2, x_3) = \text{Const}$, in the system (such as in an integrable system), a trajectory is further constrained. As a consequence, the cross section with the $x_1 = 0$ plane displays a regular pattern, $g(x_1 = 0, x_2, x_3) = \text{Const}$ which appears as a line (torus). Alternatively, in the 1-D kicked atom, the ensemble

of dots can be produced by taking stroboscopic snapshots of the phase space during every period T , i.e., $\{(q(t = kT), p(t = kT)) | k = 1, 2, \dots\}$. These snapshots can be interpreted as the Poincaré map for the phase space $(x_1 = t, x_2 = q, x_3 = p)$. Note that, since the kicked atom is a periodic system, the time axis, $x_1 = t$, has a periodic boundary condition, i.e., the $x_1 = t$ plane is identical to the $x_1 = t + T$ plane.

Fig. 2.7 displays Poincaré maps of the kicked 1-D atom for $\Delta p \geq 0$ and $\Delta p \leq 0$. For $\Delta p = 0$ the dynamics is fully regular and forms tori which correspond to different $H_{at} = \text{Const}$ curves. As soon as the perturbation $\Delta p > 0$ is turned on (momentum transfer in the direction of the apocenter, fig. 2.8), the tori are completely destroyed no matter how small Δp is, and the system becomes globally chaotic, in agreement with the predictions of Hillermeier et al [13]. Since chaotic orbits are not confined in any region of phase space, the evolution always results in ionization, as encountered in fig. 2.5. In fig. 2.7, the time evolution is followed only after 500 periods. When a momentum transfer is very small ($\Delta p = 0.001$), trajectories wander around the initial states for long time. Therefore, chaotic regions are not spread over the whole phase space after 500 periods while the fully developed chaotic region is observed for $\Delta p = 0.05$ after the same amount of time. In contrast, for $\Delta p < 0$ (kick towards the Coulomb force center, fig. 2.8), some of the tori (regular motion) survive but become distorted or split into smaller tori. For $\Delta p = -0.001$, the small closed curves appear as dashed lines along the unperturbed tori. As the perturbation increases, they start to grow and become visible occupying a finite area of phase space ($\Delta p = -0.05$). At the same time, many chaotic regions become immediately interconnected forming a so-called “chaotic sea”. This unconstrained chaotic sea leads to ionization of the atom while the regular regions termed stable islands lead to stabilization of the atom. The coexistence of the chaotic sea and stable islands determines the ionization dynamics.

One of the biggest advantages of using the Poincaré map is that any high-dimensional system can be projected onto the lower dimensional phase space. In this way, the 3-D

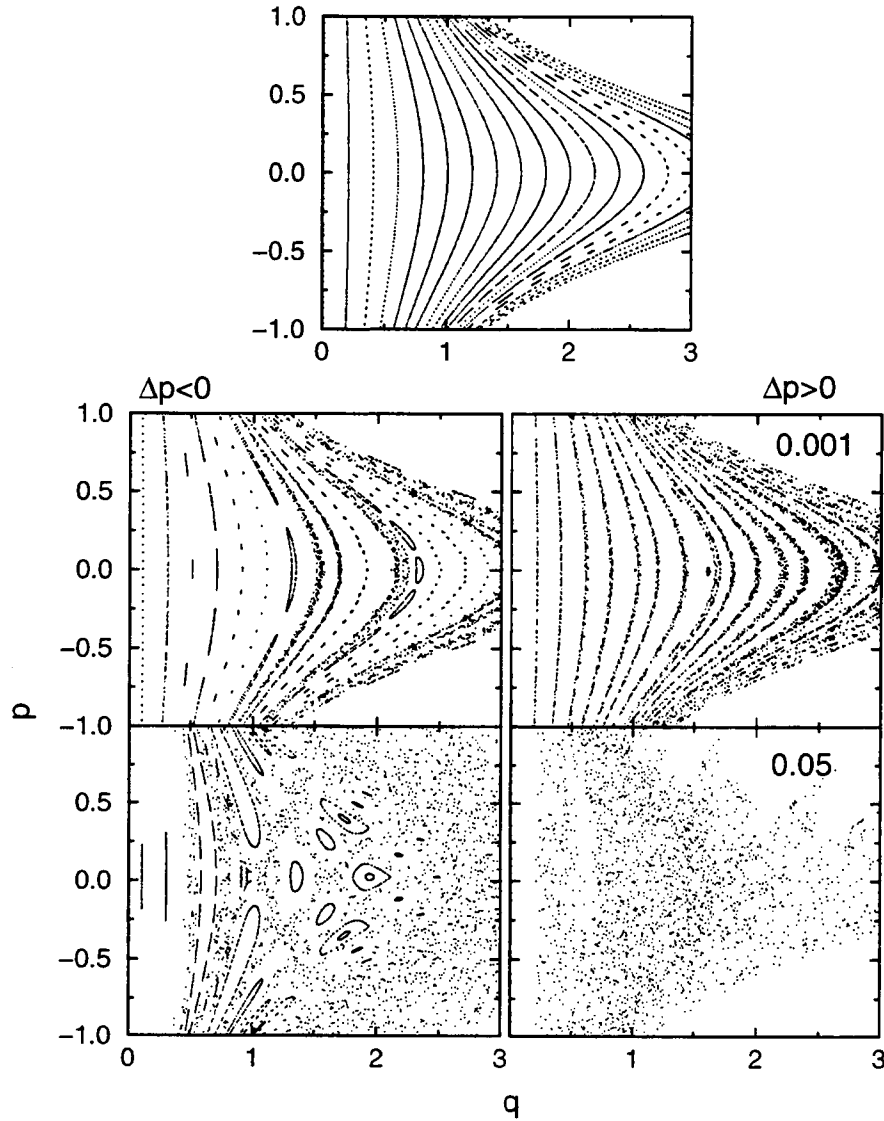


Figure 2.7: Poincaré maps for various cases. Top: $\Delta p = 0$, Left middle: $\Delta p = -0.001$, Left bottom: $\Delta p = -0.05$, Right middle: $\Delta p = 0.001$, Right bottom: $\Delta p = 0.05$. The frequency of the train of kicks is $\nu = 5.55$ for all figures.

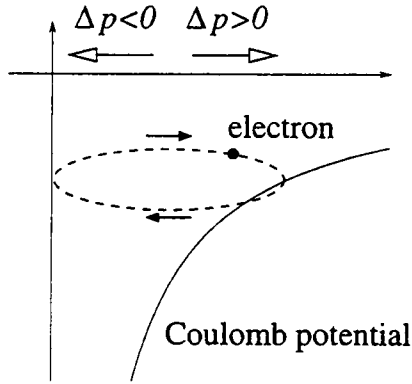


Figure 2.8: Schematic picture of the Coulomb potential and the direction of the kick

and 1-D kicked atoms can be compared on the same level (fig. 2.9). Note that, for the 3-D case, the construction of the Poincaré map requires, in addition to taking stroboscopic pictures, the slicing of phase space, $(\rho \pm \Delta\rho)$, $(p_\rho \pm \Delta p_\rho)$ near $\rho \sim 0.1$, $p_\rho \sim 0$ and $L_z = 0$. Clearly, setting $\rho = 0$, $p_\rho = 0$, and $L_z = 0$ in eq. (2.1) yields a Hamiltonian that is equivalent to the 1-D Hamiltonian. The close correspondence

between the Poincaré maps in 1-D and 3-D in fig. 2.9 is due to the fact that the phase space slice taken near $\rho = 0$, $p_\rho = 0$ corresponds to regions in phase space that have large overlap with the extreme “uphill” or “downhill” parabolic states whose orbits are almost constrained to the one-dimensional straight line parallel to the z -axis. However, because of the larger available phase space, chaotic trajectories in 3-D are unlikely to return to the original slice of the Poincaré section after a finite number of kicks.

2.3.2 Stabilization and Poincaré map

Thus, stabilization and ionization of the atom can be observed in phase space using the Poincaré map. The mixture of a chaotic sea and stable islands explains the pronounced structure which was seen in fig. 2.4. Fig. 2.10 illustrates the Poincaré maps for six different frequencies in fig. 2.4. For the calculation of the survival probability, the initial state has a scaled fixed energy, $E_0 = -0.5$, whose ensemble is depicted as the dashed line in this figure. In the Poincaré map, the initial energy level is defined by the scaling factor n_i by which the set of parameters $(\Delta p, \nu)$ are scaled to $(\Delta p_0, \nu_0)$. The phase space is also scaled using the same factor, i.e., $q_0 = q/n_i^2$ and $p_0 = pn_i$. In this scaled phase space (q_0, p_0) , the Poincaré map becomes invariant under the scaling. For repetition frequencies corresponding to the pronounced peaks, $\nu_0 = 0.616, 1.07, 2.12$, the initial

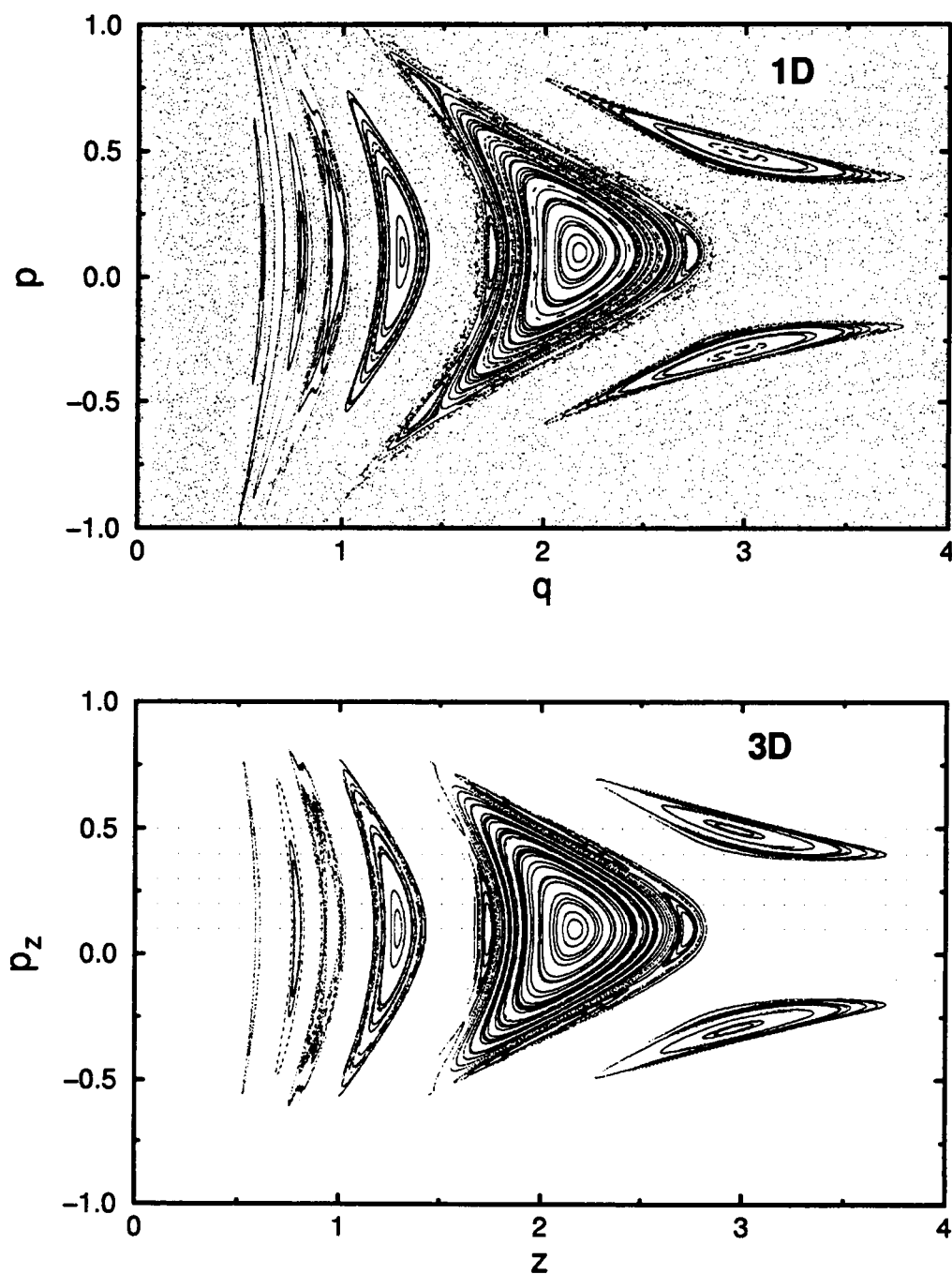


Figure 2.9: Comparison of the Poincaré maps for the 1-D kicked hydrogen atom and the 3-D kicked hydrogen atom ($L_z = 2.5e-4$) subject to a train of pulses with $\Delta p_0 = -0.2$ and $\nu_0 = 1$. The 3-D section corresponds to $\rho = 0.1$ and $p_\rho = 0$.

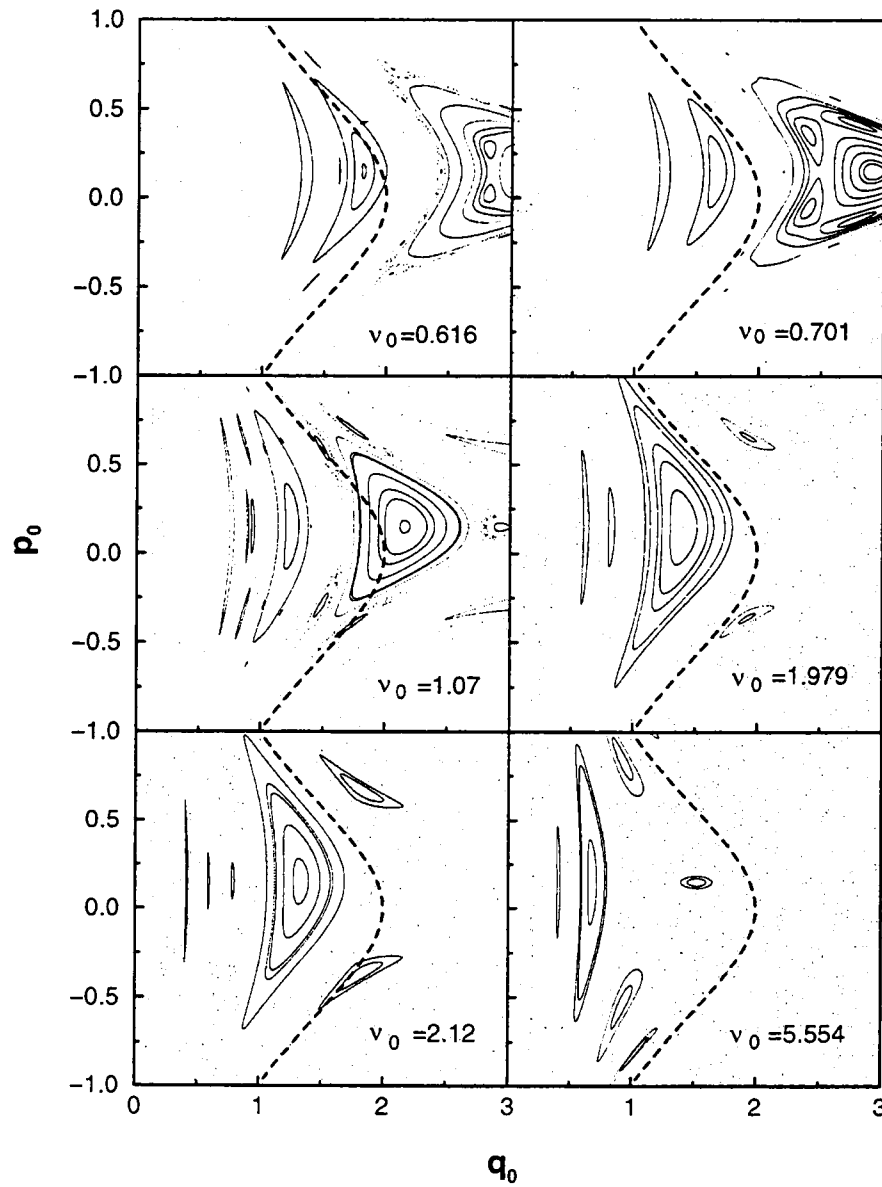


Figure 2.10: Poincaré maps for the 1-D kicked atom for $\Delta p_0 = -0.3$ and various ν_0 values. The dashed line indicates the unperturbed torus associated with the initial state of the atom [16].

unperturbed torus overlaps with different stable islands and, therefore, stabilization is obtained by trapping the phase space trajectories within a given island. In turn, for frequencies corresponding to the valleys, $\nu_0 = 0.701, 1.978, 5.554$, the whole initial torus lies in the chaotic sea and the atom becomes fully ionized.

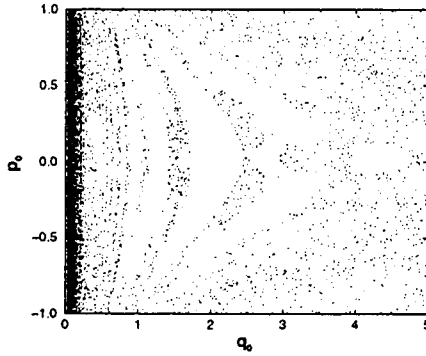


Figure 2.11: Poincaré map of a single trajectory starting in a chaotic region of phase space for the 1-D kicked hydrogen atom for $\Delta p_0 = -0.3$ and $\nu_0 = 1$ [16].

Ionization does not necessarily happen immediately and, in fact, an electron may wander among various regions of phase space before reaching the continuum. This is illustrated in fig. 2.11 where we display a Poincaré map of a single trajectory of an electron which is eventually ionized. The time evolution of the electron displays intermittency, periods of trapping near stable islands. However, since the residual tori are not confining, the trapping is only transient and the trajectory will eventually “jump” to another region of the chaotic sea and escape into the continuum.

The identification of the periodic orbits around which the stable islands are organized proceeds by noting that the binding energy must be unchanged following some integer number j of applied kicks, i.e.

$$E_{k+j} = E_k. \quad (2.11)$$

where E_k is the energy of the electron right before the k -th kick. For a period-one ($j = 1$) fixed point, eq. (2.11) implies

$$E_{k+1} - E_k = \frac{\Delta p^2}{2} + p\Delta p = 0 \quad (2.12)$$

or $p = -\Delta p/2$, which agrees with the p coordinate of the center of the most prominent

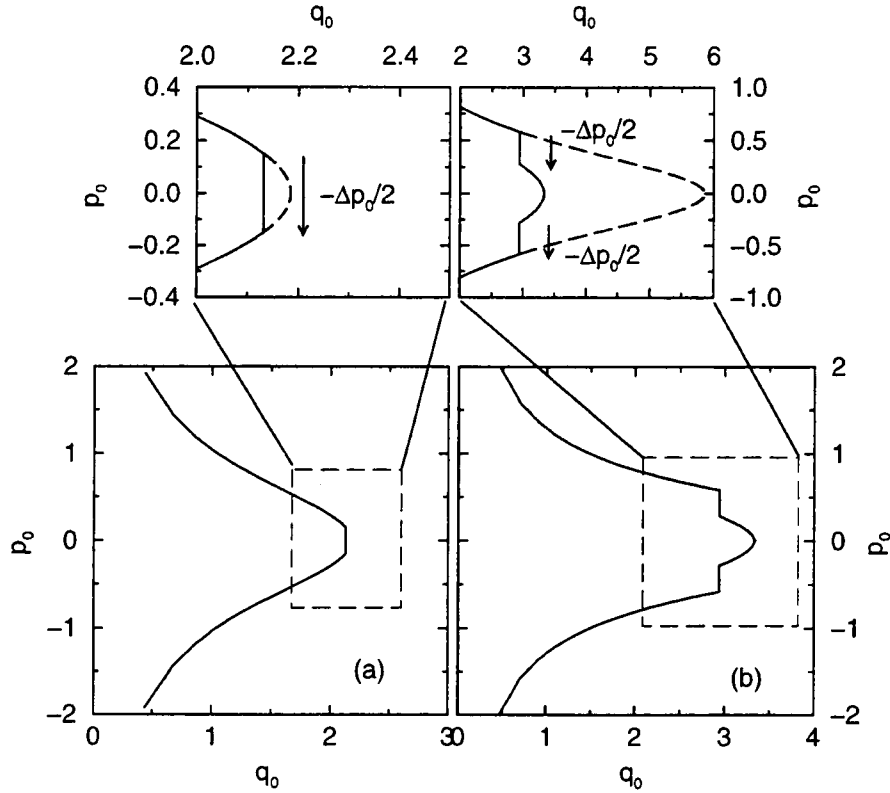


Figure 2.12: Periodic orbits with a period T (a) and with a period $2T$ (b) for $\Delta p_0 = -0.3$ and $\nu_0 = 1.09$. The dashed curves in the enlargements indicate the segments of the Coulomb orbits that are not reached by the electron.

islands in fig. 2.10. The periodic orbit which corresponds to the center of the largest stable island can be identified with the help of its projection onto the (q, p) plane, as shown in fig. 2.12. The trajectory has been followed for several kicks involving segments of several Coulomb orbits having the same binding energy i.e. the same unperturbed period. A period two stable orbit ($j = 2$) is also plotted in this figure. The reason these periodic orbits are found as centers of stable islands only for $\Delta p < 0$ is that the electron is kicked towards the nucleus (fig. 2.8), which can be interpreted as an infinitely high wall, while, for $\Delta p > 0$, the kick points towards the Coulomb barrier (fig. 2.8), which has a finite height and makes all periodic orbits unstable.

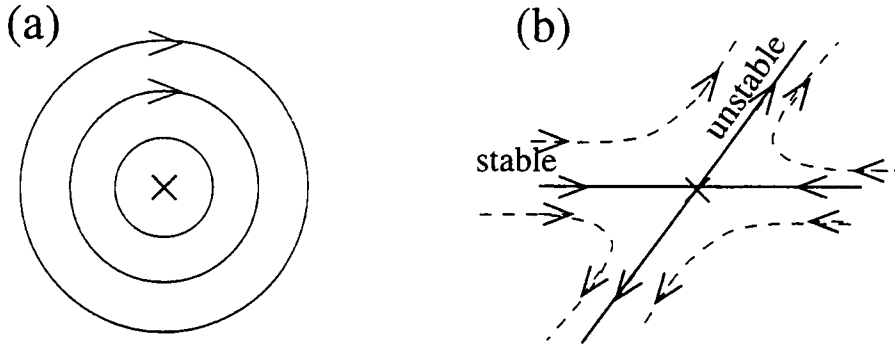


Figure 2.13: (a) stable fixed point (b) unstable fixed point

2.3.3 Unstable periodic orbits and fixed points

Even though the Poincaré map exhibits a fully chaotic phase space for $\Delta p > 0$, a trajectory can be bounded by the Coulomb potential and it may become a periodic orbit. This periodic orbit hidden in the chaotic sea leads to a 'scar' of a wave function for the quantum system (see introduction). Before discussing the quantum system, the classical features of this periodic orbit are analyzed.

Fixed points in the Poincaré map provide the signature of periodic orbits. A period j fixed point, $\mathbf{X} = (X_q, X_p)$, is the point that comes back to itself after the finite period, $\Delta t = jT$, i.e.,

$$M^j(X_q, X_p) = (X_q, X_p). \quad (2.13)$$

Every periodic orbit involves a finite number of fixed points. Since the kicked atom is a conservative system, which means that any area on phase space is preserved during the time evolution (Liouville's theorem [26]), there are possibly two kinds of motions around a fixed point: elliptic or hyperbolic. The former is a rotational motion (fig. 2.13(a)) which is constrained to a finite region of phase space and leads to a stable island. The latter is the combination of stretching and shrinking, which is unconstrained, corresponding to unstable periodic orbits. Note that stability refers here to the stability of the fixed point and not of the atom.

The stability of a fixed point is defined according to the time evolution of $\delta\mathbf{X} = (\delta X_q, \delta X_p)$ which is a displacement vector from the fixed point. When $|\delta\mathbf{X}| \ll 1$, the time evolution (eq. (2.10)) of a point near the fixed point, $\mathbf{X} + \delta\mathbf{X}$, can be expanded around the fixed point,

$$\begin{aligned} (X_q + \delta X_{qj}, X_p + \delta X_{pj}) &\equiv M^j(X_q + \delta X_q, X_p + \delta X_p) \\ &= M^j(X_q, X_p) + \frac{\partial M^j(X_q, X_p)}{\partial(X_q, X_p)} \cdot (\delta X_q, \delta X_p) \\ &\quad + O(\delta\mathbf{X}^2). \end{aligned} \quad (2.14)$$

Because of eq. (2.13),

$$\begin{aligned} (X_q + \delta X_{qj}, X_p + \delta X_{pj}) &\simeq (X_q, X_p) + \frac{\partial M^j(X_q, X_p)}{\partial(X_q, X_p)} \cdot (\delta X_q, \delta X_p), \\ \text{i.e., } (\delta X_{qj}, \delta X_{pj}) &= \frac{\partial M^j(X_q, X_p)}{\partial(X_q, X_p)} \cdot (\delta X_q, \delta X_p). \end{aligned} \quad (2.15)$$

The dynamics of the displacement vector, $(\delta X_q, \delta X_p)$, is governed by the 2×2 Jacobian matrix, $\partial M^j(X_q, X_p)/\partial(X_q, X_p)$. Since this map is area-preserving, i.e.,

$$\det \left(\frac{\partial M^j(X_q, X_p)}{\partial(X_q, X_p)} \right) = 1, \quad (2.16)$$

the product of the eigenvalues of this matrix, λ_1, λ_2 , is always 1. When the eigenvalues are complex numbers, $\lambda_1 = \lambda_2^* = \exp(i\theta)$, the distance, $|\delta\mathbf{X}|$, is preserved and forms the stable islands (fig. 2.13). On the other hand, when they are real, $|\lambda_1| = 1/|\lambda_2| > 1$ and the corresponding eigenvectors form a stable manifold (shrinking) and an unstable manifold (stretching) (fig. 2.13). In this case, the distance, $|\delta\mathbf{X}|$, increases exponentially with time and, therefore, the fixed point appears in the chaotic sea of the Poincaré map.

2.3.4 Layout of the periodic orbits in phase space

A fixed point for the kicked atom can be characterized by two integer numbers (i, j) and the winding number. The winding number is the ratio $R_{fix} \equiv i/j$, where i is the period of the fixed point divided by T and j is the number of times the electron is scattered by the nucleus during the period iT . In the limit $\Delta p \rightarrow 0$, R_{fix} is equivalent to the ratio of the Kepler period to the period of the pulse train, $R_{fix} = T_n/T$ and, therefore, there are an infinite number of tori, termed 'resonant tori', which satisfy the resonant condition, $R_{fix} = i/j$ (a rational number). For a kick of finite strength, a resonant torus is destroyed, and it either creates a chain of stable islands, or yields unstable fixed points which are intermingled into the chaotic sea (KAM theorem [5]).

Fig. 2.14 illustrates various series of periodic orbits: e.g. $1/j$, $j/1$, and j/j ($j = 1, 2, \dots$). Clearly there are an infinite number of periodic orbits belonging to each of the series. Within a given series, the bigger the R_{fix} is, the farther the orbit extends out from the nucleus. Since R_{fix} is roughly the number of kicks that the electron experiences within a Kepler period, a periodic orbit with a big value of R_{fix} involves orbits with large Kepler periods. This is consistent with fig. 2.14 which shows that as $R_{fix} = j/1$ increases with $j = 1, 2, \dots$, the orbit moves farther from the nucleus, and, as $R_{fix} = 1/j$ decreases with $j = 1, 2, \dots$, the outer turning point becomes closer to the nucleus.

This rule for the layout of the periodic orbits is also valid when i' and j' in $R_{fix} = i'/j'$ are commensurable but only on average. That is, a high order resonance with the resonance condition $R_{fix} = i'/j'$ has an orbit which surrounds the periodic orbit with the lowest order resonance, $R_{fix} = i/j = i'/j'$ where i and j are incommensurable. One example is the 5/5 orbit (fig. 2.14(c)) which corresponds to a high order of the 1/1 periodic orbit. In this example, the fixed points are stable and, therefore, the corresponding resonances appear as stable islands in the Poincaré map (fig. 2.15). In the left figure, it is observed that five small islands (5/5 resonant tori) surround the main stable island (1/1 resonant torus). In addition, hints of other higher order resonant tori

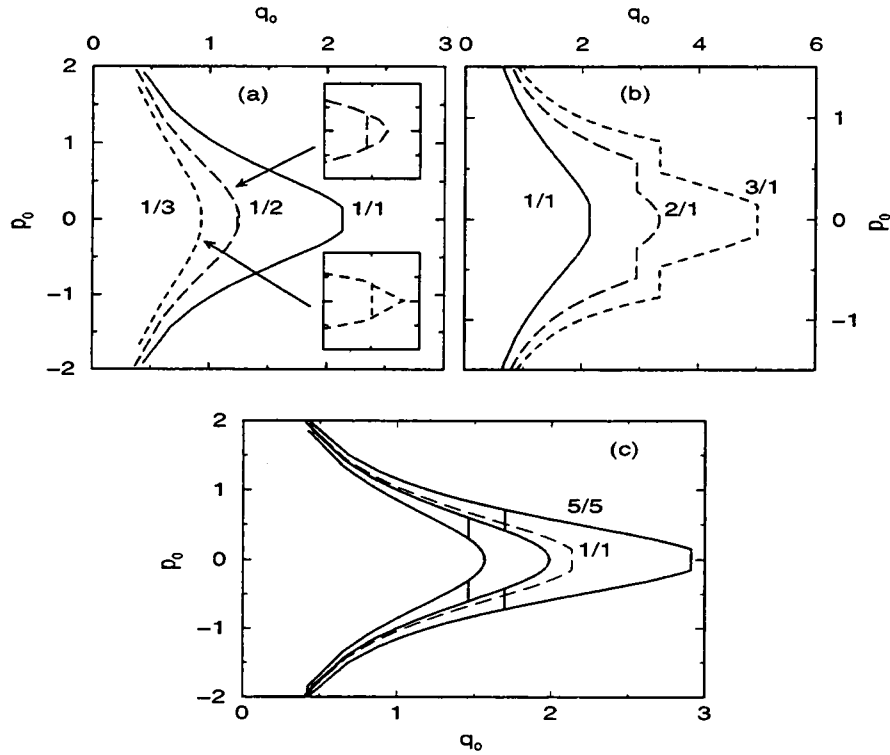


Figure 2.14: Series of periodic orbits : $j/1$ (a), $1/j$ (b), and $1/1$ (thin dashed line) and $5/5$ (thick solid line) (c). The parameters of the perturbation are $\Delta p_0 = -0.3$ and $\nu_0 = 1.09$.

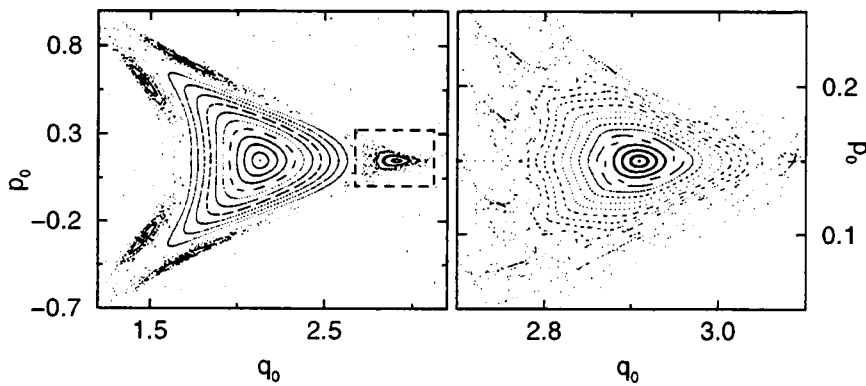


Figure 2.15: Stable island corresponding to the $1/1$ periodic orbit (left) and zoom up of the dashed square area in the left figure (right) corresponding to the $5/5$ periodic orbit. The parameters of the perturbation are $\Delta p_0 = -0.3$ and $\nu_0 = 1.09$.

can be seen as dashed closed lines within the main island. Note that the areas of these islands are so small that they are not visible within the resolution of the Poincaré map. In the enlargement of one of the five small islands (right figure in fig. 2.15), we can also observe the several resonant tori which are higher order resonances of the 5/5 periodic orbit. These resonant tori may form a fractal-like structure of stable islands in phase space. That is, the phase space structure around the stable island associated with the high order of resonance may mimic the structure around the island with the lowest order. These studies are left for future investigations.

One more important aspect about the layout of fixed points is that there are no fixed points in the $H_{at} > 0$ region when $\Delta p_0 > 0$. This is due to the fact that the electron always acquires a positive momentum, when it becomes ionized, and it can no longer turn around, i.e., the position q monotonically increases and there is no chance for the orbit to be periodic.

This fact can be understood visually from another point of view (fig. 2.16). For $\nu_0 = 17$, the unperturbed torus ($\Delta p_0 = 0$) with $E_0 = -0.5$ corresponds to the resonant torus with $R_{fix} = 17/1$. As the perturbation increases, this periodic orbit is distorted and its path becomes longer for $\Delta p < 0$ and shorter for $\Delta p > 0$. Since all periodic orbits originate in bound states of the unperturbed system (continuum states have hyperbolic orbits and, therefore, they cannot be periodic), the positive momentum transfer compresses all periodic orbits into a smaller region of phase space within the ionization threshold. Thus fixed points cannot be in the continuum region of phase space for $\Delta p > 0$ while they exist for $\Delta p < 0$. This is a unique feature of the positively kicked system which plays a very important role in the quantum description of the system.

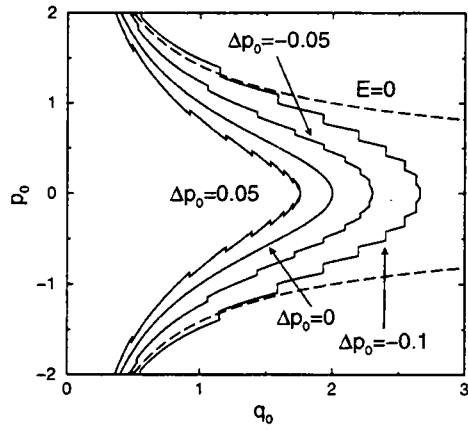


Figure 2.16: Unperturbed orbit and 17/1 periodic orbits for different momentum transfers, $\Delta p_0 = 0, 0.05, -0.05$, and -0.1 . Scaled frequency is $\nu_0 = 17$. Dashed line is an ionization threshold ($H_{at} = 0$).

Chapter 3

Numerical evolution of the quantum system

For a large number of dynamical atomic processes, the numerical solution of the time-dependent Schrödinger equation requires the propagation of “free” wavepackets out to large times and large distances. Only at that point does projection onto asymptotic final states allow the unambiguous determination of transition amplitudes and, hence, of the T or S matrix. These include ionization of atoms by charged particles, photons, and intense electromagnetic fields. In all cases, the non-stationary wavepacket contains a continuum component which will eventually escape the interaction region. Numerical representations of the wavepacket in terms of a finite basis set, either in terms of atomic pseudo-states or lattice-based representations, have the fundamental limitation that they subtend only a finite domain in coordinate space up to a certain distance R . Therefore, any finite basis representation contains a “wall” or boundary at R , either explicitly in box or lattice representations or implicitly in pseudo-state representations, at which the continuum portion of the wavepacket will eventually be reflected and will reenter the interaction region, thereby artificially distorting the bound-state portion of the evolved wavepacket. Depending on the method used, the wall may be hard or soft

and its efficient position may depend on the momentum and energy of the wavepacket. While this problem is ubiquitously present in all numerical propagation schemes, it is of relatively little influence in the study of transitions into low-energy states and short times. It becomes, however, a major hurdle for long interaction times and problems involving highly excited states such as Rydberg states.

Suppression of reflections is particularly important in investigations of the classical-quantum correspondence of Hamiltonian systems with mixed phase space. The “discordance” between the quantum evolution with the corresponding classical system exhibiting “soft chaos” should manifest itself for sufficiently long times of the order of the so-called Heisenberg times $t_H \approx \hbar/\langle\Delta E\rangle$ where $\langle\Delta E\rangle$ is the typical mean level spacing of a system [27]. In order to delineate the breakdown of classical-quantum correspondence, the challenge is to integrate the time-dependent Schrödinger equation (TDSE) out to times longer than t_H . This time typically exceeds the time when the first reflections in the basis set have occurred. The kicked atom system is one of the prototype systems where we encountered this difficulty. It is therefore crucial to control and suppress reflections at the walls without distortion of the wavepacket evolution in the physically relevant region of coordinate space where the classical-quantum correspondence is being investigated.

In the first section of this chapter, the time propagation of a free 1-D particle is discussed. In this simple model, reflections and their suppression can be clearly visualized. Two different methods which can suppress artificial reflections are introduced, and their applicability is discussed. In the second section of this chapter, we discuss the application of one of the methods to the kicked atom. In the last section of this chapter, the convergence of the numerical solution of the TDSE is discussed: whether reflections are really suppressed or their suppression causes any artificial error. A stabilization method is introduced to check for the convergence of the numerical solutions.

3.1 Time propagation of a free 1-D particle

— time-independent Hamiltonian —

3.1.1 Coupled-states method

Consider the dynamics of a particle with coordinate q and Hamiltonian H . One of the most versatile and most frequently employed techniques to numerically solve the time-dependent Schrödinger equation is the coupled-states method. Its core ingredient is a finite basis expansion of the wave function as

$$|\psi(t)\rangle = \sum_{n=1}^N a_n(t) |\phi_n\rangle \quad (3.1)$$

where N is the number of basis states $|\phi_n\rangle$ included in the truncated expression. Eq. (3.1) converts the TDSE into a system of coupled ordinary differential equations of the form

$$i\dot{\mathbf{a}}(t) = \hat{H}(t)\mathbf{a}(t) \quad (3.2)$$

where $\mathbf{a}(t) = (a_1(t), \dots, a_n(t), \dots, a_N(t))$ is the state vector, and $\hat{H}(t)$ is the Hamiltonian matrix with elements $\langle \phi_n | H | \phi_{n'} \rangle$. In eq. (3.2) and in the following we assume that the basis set is orthonormal. If the basis functions $|\tilde{\phi}_n\rangle$ are non-orthogonal, it can be orthogonalized through the transformation

$$|\phi_n\rangle = \sum_{n'=1}^N (\hat{S}^{-1/2})_{nn'} |\tilde{\phi}_{n'}\rangle \quad (3.3)$$

where $\hat{S}$ is the overlap matrix $\hat{S}$ with elements $S_{nn'} = \langle \tilde{\phi}_n | \tilde{\phi}_{n'} \rangle$.

The key point for the following analysis is that in any truncated expansion of the form, eq. (3.1), where N is finite (limited by present computational capabilities) only a finite domain in coordinate space up to a radius $q \lesssim R$ can be adequately represented. Thus, as the wave function expands in time, it becomes reflected as it reaches this

boundary. Here we study a few techniques, old and new, for avoiding these reflections using various square integrable basis functions $|\phi_n\rangle$. For simplicity, these methods are applied to the evolution of a free particle and it is assumed that N refers to the number of basis states in the radial direction, thereby ignoring the basis states required to subtend the angular degrees of freedom. For zero angular momentum, the problem is equivalent to that of a free 1-D particle with the Hamiltonian

$$H_{free} = -\frac{1}{2} \frac{d^2}{dq^2}, \quad (3.4)$$

and boundary condition on the wave function $\psi(0, t) = 0$ for all t . It should be kept in mind, however, that in realistic 3-D calculations a total number of N basis states have to be distributed among all degrees of freedom such that only $\sim N^{1/3}$ states are available in the radial direction. In other words, just increasing N is not a viable option to control the problem of reflections.

It is useful to distinguish two different classes of basis states:

a) Strongly localized basis expansions greatly simplify the evaluation of coordinate operators such as arbitrary potentials or masking functions. They include, among others, lattice expansions [28, 29] and discrete variable representations (DVR) [30]. In each case, $\phi_n^G(q)$ is effectively localized at one grid point q_n of the lattice and the matrix representation of an operator $O(q)$ is diagonal,

$$\langle \phi_m^G | O(q) | \phi_n^G \rangle \propto \delta_{m,n} O(q_n). \quad (3.5)$$

b) Pseudo-state expansions, on the other hand, are delocalized within a finite domain of coordinate space with a variable number of nodes, typically $\phi_n(q)$ contains $n - 1$ radial nodes. A prototype is the set of radial box (B) wave functions for a box of radius R

$$\langle q | \phi_n^B \rangle = \phi_n^B(q) = \sqrt{\frac{2}{R}} \sin(p_n q) \quad (3.6)$$

with $p_n = \pi n/R$. Another example of atomic pseudo-states which we discuss in the following is the Sturmian (S) pseudo-states [31, 32, 33]

$$\langle q | \tilde{\phi}_n^S \rangle = \phi_n^S(q) = \frac{2}{n\sqrt{n_S}} \frac{q}{n_S} e^{-q/n_S} L_{n-1}^1(2q/n_S), \quad (3.7)$$

where n_S is referred to as the Sturmian parameter. Note that the Sturmian wave function is normally used for the 3-D wave function and the 1-D Sturmian wave function corresponds to the radial part of the 3-D Sturmian wave function for s -states. The specific advantage of the Sturmian expansion is that for properly chosen n_S , a single ϕ^S can represent a hydrogenic atomic state for a given quantum number with its nodal structure (for $n_S = n$ the equivalence is exact) and it properly describes a Coulomb singularity for $q \rightarrow 0$. Moreover, for any fixed n_S the discrete set is complete and its truncation at N yields a discrete representation of a portion of the continuum [22, 31, 32, 33] (details are in Appendix E).

One common feature of all these expansions is the presence of a “wall” at some value $q \simeq R$. For lattice-based expansions, reflections occur at or near the outermost grid point, i.e., $q_N = R$. For box wave functions, R is obviously given by the wall of the box, while for atomic pseudo-states of Sturmian type the wall is “soft” and its location is less obvious. It can be estimated from the radial expectation values for Sturmian pseudo-states

$$\langle q \rangle_n = \langle \tilde{\phi}_n^S | q | \tilde{\phi}_n^S \rangle = \frac{3}{2}n \quad n_S \leq \frac{3}{2}Nn_S. \quad (3.8)$$

The position of the wall is therefore of the order of $\langle r \rangle_N$ and scales linearly with n_S . In fact, the effective position of the wall is energy (or momentum) dependent since the local density of states (LDOS) varies with the distance from the origin.

Fig. 3.1 provides an example of reflections at the wall. This figure shows the time propagation of a Gaussian wavepacket. In order to satisfy the boundary condition at $q = 0$ for all t , we choose at $t = 0$ the antisymmetric linear combination of Gaussian

wavepackets

$$\psi(q, 0) = A \left\{ \exp \left[-\frac{(q - q_0)^2}{4\sigma^2} + ik_0 q \right] - \exp \left[-\frac{(q + q_0)^2}{4\sigma^2} - ik_0 q \right] \right\} \quad (3.9)$$

where A is a normalization constant, k_0 is the initial (mean) momentum of the wavepacket, q_0 its mean position, and σ its radial width. While the exact solution,

$$|\psi(q, t)|^2 \simeq \frac{2(A\sigma)^2}{\sqrt{t^2 + 4\sigma^2}} \times \exp \left[-\frac{2\sigma^2 \{q - (q_0 + tk_0)\}^2}{t^2 + 4\sigma^2} \right],$$

continues beyond the wall, $R \sim 100$, the onset of reflections can be observed. As the wavepacket approaches the wall to within its approximate width, oscillations due to interference with the reflected portion become visible. At larger evolution times, the exact solution and the Sturmian pseudo-state expansion have completely diverged from each other. While the wavepacket has moved out to large distances and has completely left the inner region, the pseudo-state expansion describes a unitary transformation within the inner region of the wall subtended by the truncated expansion and retains the whole wavepacket. Now we discuss several alternative methods to avoid reflections and to describe the wavepacket as accurately as possible within the subspace subtended

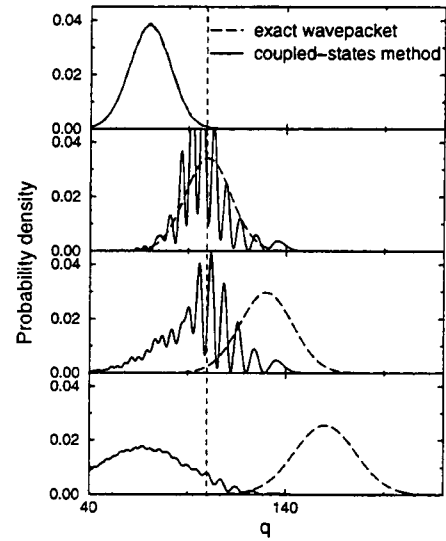


Figure 3.1: Comparison of the exact wavepacket (dashed lines) and the results obtained by the coupled-states method using Sturmian pseudo-states with $N = 70$ and $n_S = 1$ (solid lines). The initial Gaussian wavepacket has a peak at $q_0 = 40$ with a width $\sigma = 10$ and an average momentum $k_0 = 0.5$. Each figure is plotted at $t = 60, 120, 180, 240$ from the top to the bottom, respectively. The vertical dashed line is the approximate position of the reflecting wall.

by the truncated expansion. As a benchmark of the methods, this Gaussian wavepacket propagation will be used.

3.1.2 Suppressing reflections

Suppose that the full Hilbert space of square integrable functions is divided into P and Q subspaces such that $\{P\} = \{\phi_n; n = 1, \dots, N\}$ is the subspace subtended by our finite basis set and

$$1 = |P + Q\rangle\langle P + Q| = |P\rangle\langle P| + |Q\rangle\langle Q| \quad (3.10)$$

$$|P\rangle\langle P| = \sum_{n=1}^N |\phi_n\rangle\langle\phi_n|. \quad (3.11)$$

The task is to find a good approximation for the projection of the wave function onto the subspace P which is given by

$$|\psi(t)\rangle_P = |P\rangle\langle P|\psi(t)\rangle = |P\rangle\langle P|e^{-iHt}|P\rangle\langle P|\psi(0)\rangle, \quad (3.12)$$

where we have assumed that the initial state $|\psi(0)\rangle$ of the wavepacket is well localized in our basis set, i.e.

$$|\psi(0)\rangle \simeq |P\rangle\langle P|\psi(0)\rangle, \quad (3.13)$$

$$\langle Q|\psi(0)\rangle \simeq 0. \quad (3.14)$$

Note that apart from the assumption (eq. (3.14)), the wave function $|\psi(t)\rangle_P$ is exact. It differs from the coupled-states solution of eq. (3.2) which is given by $\mathbf{a}(t) = \exp(-i\hat{H}t)\mathbf{a}(0)$ or, in the present notation, $\mathbf{a}(t) = \langle P|\psi(t)\rangle$, $\hat{H} = \langle P|H|P\rangle$,

$$|\psi^U(t)\rangle_P = |P\rangle e^{-i\langle P|H|P\rangle t} \langle P|\psi(0)\rangle, \quad (3.15)$$

due to the different evolution operators

$$\exp(-i\langle P|H|P\rangle t) \neq \langle P|\exp(-iHt)|P\rangle. \quad (3.16)$$

The matrix representation of the evolution operator within the P space (l.h.s. of inequality (eq. (3.16)) is unitary and does not allow for any flux of probability outside the P space. In turn, the r.h.s., $\langle P|\exp(-iHt)|P\rangle$, is not unitary since it is a representation of the exact evolution operator which allows for coupling to the Q space. The differences between (eq. (3.15)) and (eq. (3.12)) can be made more explicit by expressing the wave function in terms of the eigenvectors of the evolution operators:

$$|\psi(t)\rangle_P = \sum_{k=1}^N b_k(0) e^{-iE_k t} |\chi_k\rangle, \quad (3.17)$$

$$|\psi^U(t)\rangle_P = \sum_{k=1}^N c_k(0) e^{-i\epsilon_k t} |\varphi_k\rangle. \quad (3.18)$$

In (eq. (3.18)), ϵ_k denotes the real eigenvalue of the Hamiltonian $\langle P|H|P\rangle$. In eq. (3.17), on the other hand, E_k is defined through the relation

$$\langle P|\exp(-iHt)|P\rangle \langle P|\chi_k\rangle = \exp(-iE_k t) \langle P|\chi_k\rangle. \quad (3.19)$$

The non-unitarity is reflected in the complex eigenvalues $E_k = E_k^R + iE_k^I$. Suppression of reflections in the exact evolution operator can therefore be attributed to the presence of an imaginary part of the effective spectrum that eliminates probability from the P space. The basic ingredient to all approximate prescriptions for controlling reflections is the introduction of a non-unitary operator whose effect is to eliminate probability flux that is associated with the reflecting portion of the wavepacket. Within a coupled-states approach, for example, a non-Hermitian interaction can be added to the Hamiltonian to induce the non-unitary evolution. Such additional terms are often referred to as “relaxation operators” or “optical potentials”. For a faithful representation of the long-

time evolution, it is essential that the effect of the relaxation operator be confined to the region of the wall and not disturb the evolution in the “inner” region.

Masking method

For lattice-based localized basis expansions (eq. (3.5)), the choice of relaxation operators is straightforward. We briefly discuss their properties before turning to the construction of the corresponding operators for atomic pseudo-state expansions, which is used for the investigation of the kicked atom system. At the most elementary level, a relaxation operator can be constructed by a masking function [28, 29, 34, 35]. Let $\mathcal{M}(q)$ be a masking function so that

$$\mathcal{M}(q) = \begin{cases} 1 & \text{if } q < q_N \\ f(q) < 1 & \text{if } q_{N+1} < q \leq q_M \end{cases}. \quad (3.20)$$

The range of lattice sites, $q_{N+1}, \dots, q_M$ close to the reflecting wall now represents a finite Q' subspace ($Q' \subset Q$) that corresponds to a finite number of lattice sites beyond the P subspace ($q < q_N$). In Q' the wave function is allowed to relax by way of an amplitude-absorbing mask. The masking function $f(q)$ can be chosen to be continuously differentiable at q_N to high order in order to minimize effects of discontinuities. Masking is effected by simply multiplying the state vector after every time interval Δt_j by the masking operator $\mathcal{M}$ which is diagonal in the lattice basis ϕ_k :

$$\begin{aligned} |\psi^{\mathcal{M}}(t)\rangle_P &= |P\rangle\langle P|P+Q'\rangle \\ &\times \left(\prod_{j=1}^J \mathcal{M} e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t_j} \right) \\ &\times \langle P+Q'|\psi(0)\rangle \end{aligned}$$

with

$$t = \sum_{j=1}^J \Delta t_j . \quad (3.21)$$

Using this simple procedure, reflections can be suppressed effectively. This is shown in fig. 3.2 by plotting the propagation of a Gaussian wavepacket. We used here a DVR expansion which belongs to the class of lattice-based expansions. As a masking function in eq. (3.20) we used $f(q) = 0$ if $q > R$, $q_N = R = 100$, and $r_M = 200$ and this masking function is applied every time interval, $\Delta t = 60$ (a.u.). Because of the simple masking function, the hard wall at $q = 100$, which is depicted as a vertical dashed line, can be observed very clearly as a border between P and Q' subspaces, and reflections are suppressed very effectively. We can expect that a smoother masking function suppresses reflections even more effectively with smaller distortion of the wavepacket within a wall. The masking method can be used only for a lattice-based basis. In an atomic system, a pseudo-state basis, such as a Sturmian basis, has the big advantage to describe the Coulomb

wave functions. The extension of this method to a pseudo-state basis is called the repetitive projection method which is the subject of the next subsection.

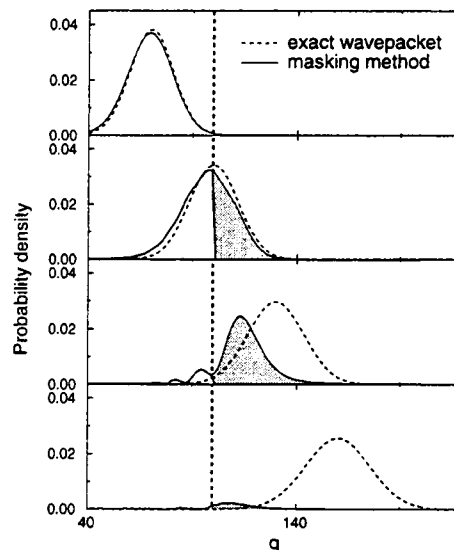


Figure 3.2: Comparison of the exact wavepacket (dashed lines) and the results of the masking method (solid lines) using a masking function $f(q) = 0$ ($q > 100$). The shaded area is a portion of wavepacket belonging to Q' where the probability is projected out. The initial wavepacket and the times of the snapshots are the same as those in Fig. 3.1

Repetitive projection method (RPM)

The implementation of the analogue to masking for atomic pseudo-state expansions is not obvious because of the delocalized nature of the basis states. No particular subset of the basis can be directly associated with the spatial region near the boundary. Consequently, the relaxation operator will be, in general, non-local and non-diagonal with respect to the basis. The construction of such a relaxation operator is clearly not unique. We show in the following that repetitive projection onto a conveniently chosen subspace provides a realization of a relaxation operator. We implement this method for the Sturmian basis set (eq. (3.7)). Many features of this repetitive projection method (RPM) are, however, valid for other basis sets as well [23].

The starting point is the observation that radial expectation values are ordered with quantum numbers (eq. (3.8)). Consequently, despite the delocalized nature and nodal structure of the basis states, one can associate the Sturmian states with the largest quantum numbers with the probability amplitude in the region of coordinate space closest to the effective wall. We therefore decompose the truncated Hilbert space into two finite subspaces

$$\begin{aligned}\{P\} &= \{\phi_n^S\}_{1 \leq n \leq N} \\ \{Q'\} &= \{\phi_n^S\}_{N+1 \leq n \leq M}\end{aligned}\tag{3.22}$$

with the description of the unity within the M dimensional model space (i.e. eq. (3.10) but for a finite Q' space). The P space represents the interaction region or inner region where the initial state $|\psi(0)\rangle$ of the wavepacket is localized (i.e. eq. (3.13)).

After a time step Δt , we project the time evolved wave function in the model space $P + Q'$ onto P ,

$$\begin{aligned}|\psi^{RPM}(\Delta t)\rangle_P &= |P\rangle\langle P|P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t} \\ &\times \langle P + Q'|P\rangle\langle P|\psi(0)\rangle.\end{aligned}\tag{3.23}$$

That is, from the evolved wavepacket we now remove the component that has reached the Q' space, the boundary region, much like for the exact wave function (eq. (3.12)) for which the $P + Q'$ space would be the full Hilbert space of square integrable functions. Repeating this process for a total of J time intervals Δt_j (not necessarily equal) leads to

$$\begin{aligned} |\psi^{RPM}(t)\rangle_P &= |P\rangle \left(\prod_{j=1}^J \langle P|P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t_j} \langle P + Q'|P\rangle \right) \\ &\times \langle P|\psi(0)\rangle. \end{aligned} \quad (3.24)$$

Note that the domain of the Hamiltonian is the full model space $P + Q'$. Moreover, H is not block-diagonal with respect to the $P-Q'$ decomposition, i.e.

$$\begin{aligned} H &= |P\rangle\langle P|H|P\rangle\langle P| + |Q'\rangle\langle Q'|H|P\rangle\langle P| \\ &+ |P\rangle\langle P|H|Q'\rangle\langle Q'| + |Q'\rangle\langle Q'|H|Q'\rangle\langle Q'| \end{aligned}$$

where $\langle P|H|Q'\rangle = \langle Q'|H|P\rangle^*$ because of Hermiticity. Within each time interval, the Hamiltonian couples the wavepacket to the full $P + Q'$ space including the “boundary region” represented by the Q' space. After each projection, only the portion of the wave function remaining in the inner region is kept. Eq. (3.24) is the central result for the RPM.

Figure 3.3 presents an example for the same wavepacket as in Figs. 3.1, but now with repetitive projection applied with $N = 70$, and $M = 270$. Clearly, the projection-induced masking introduces some distortion of the wavepacket similar to the one observed for lattice-based masking method. The distortion is, however, confined to the masking region. Only when $q_0 \approx 100$ and is close to the “wall”, distortions due to interferences become visible while the inner region remains unaffected.

It is now of interest to explore the efficiency of the RPM and its tunability to different wavepackets. Figure 3.4 shows the transmission probability through the wall (i.e. the loss of probability from the “inner” region) as a function of the time interval Δt between successive projections and different k_0 . For different values of k_0 , the transmission probability reaches $\gtrsim 90\%$ for the same range of $\Delta t \approx 5 - 50$. Consequently, for a wide range of k values (variation by a factor 4) and energies (factor 16), a large amount of suppression of reflections can be achieved.

The transmission curves show a rapid fall-off from the maximum towards larger Δt as well as smaller Δt . The reduced transmission through the wall, or equivalently, enhanced reflection for large Δt has a simple “geometric” interpretation. If the time interval exceeds the round trip time through the “masking region” of length ΔR ,

$$\Delta t \geq 2\Delta R/k_0, \quad (3.25)$$

the wavepacket is reflected at the “outer wall” associated with the border of the domain $P+Q'$ to the inner region (states ϕ_n with $n \leq N$) before the next projection takes place. Note that the discontinuous drop-off in Fig. 3.4 for $k_0 = 1$ occurs when Δt changes abruptly from $\Delta t = t$ to $\Delta t = t/2$ corresponding to $J = 1, 2$ (the total propagation time for the smaller momenta is, in turn, outside of the time range in the figure).

The transmission is also reduced when the projection is performed too often, i.e. when Δt is too small. This is nothing but the manifestation of the onset of the quantum

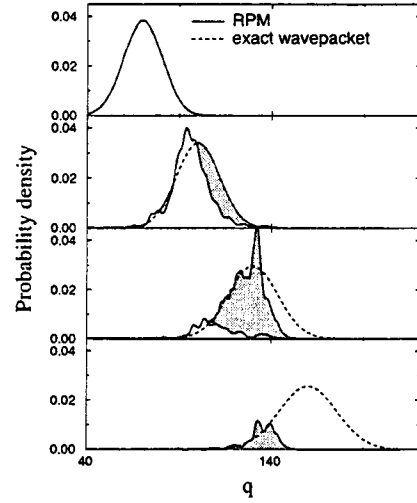


Figure 3.3: Comparison of the exact wavepacket (dashed lines) and the results of the repetitive projection method (RPM) using Sturmian pseudo-states with $N = 70$, $M = 270$, and $n_s = 1$ (solid lines). The shaded area is the portion of the wavepacket belonging to Q' where the probability is projected out. The initial wavepacket and the times of the snapshots are the same as those in Fig. 3.1

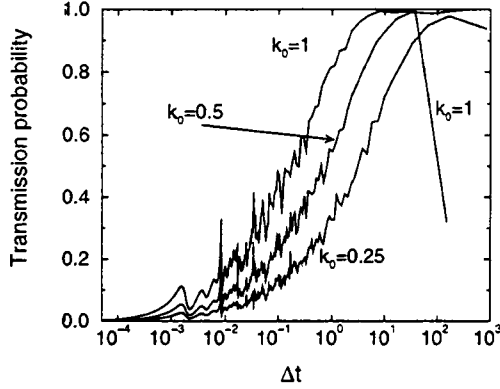


Figure 3.4: Loss of probability generated by the repetitive projection method. Each curve corresponds to a different momentum and total propagation time, t , is such that 99% of the exact wavepacket should have passed through the inner wall. For $k_0 = 0.25$ $t = 830$, for $k_0 = 0.5$ $t = 320$, and for $k_0 = 1$ $t = 150$. The parameters for the initial wavepacket are $\sigma = 10$ and $r_0 = 30$. The parameters for the basis sets used in this calculation are $N = 70$, $M = 120$, and $n_s = 1$ [23].

Zeno effect [36], here observed for the free-particle wavepacket evolution. Its physical interpretation is that by projecting too often, the evolution of the wavepacket is “frozen” inside the P space which prevents the transmission and the leakage out. For the limit $\Delta t \rightarrow 0$ this can be easily shown as follows: Using the decomposition (eq. (3.21)) we find for small Δt

$$\begin{aligned} & |P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t} \langle P + Q'|P\rangle \\ & \simeq |P\rangle (1 - i\langle P|H|P\rangle\Delta t) \\ & + |Q'\rangle (-i\langle Q'|H|P\rangle\Delta t). \end{aligned} \quad (3.26)$$

Therefore,

$$\begin{aligned} & \langle P|P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t} \langle P + Q'|P\rangle \\ & \simeq 1 - i\langle P|H|P\rangle\Delta t - \frac{1}{2}\langle P|H|P\rangle^2\Delta t^2 \\ & - \frac{1}{2}\langle P|H|Q'\rangle\langle Q'|H|P\rangle\Delta t^2. \end{aligned} \quad (3.27)$$

Note that there are no couplings to the Q' space to first order in Δt but only to second order $\sim \Delta t^2$. If we take a fixed evolution time t and J time steps, $\Delta t = t/J$, we find in the limit $J \rightarrow \infty$

$$\begin{aligned} & \langle P|P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle J\Delta t} \langle P + Q'|P\rangle \\ & \simeq \left[\langle P|P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle\Delta t} \langle P + Q'|P\rangle \right]^J \\ & \simeq (1 - i\langle P|H|P\rangle\Delta t)^J - \frac{J\Delta t^2}{2}\langle P|H|Q'\rangle\langle Q'|H|P\rangle \end{aligned}$$

$$\simeq 1 - i\langle P|H|P\rangle t - \frac{t}{2}\langle P|H|Q'\rangle\langle Q'|H|P\rangle\Delta t. \quad (3.28)$$

Therefore, in the limit $J \rightarrow \infty$, $\Delta t \rightarrow 0$, and $J\Delta t = t = \text{const}$, the coupling to the Q' space vanishes. This is the direct analog to the quantum Zeno effect in spin systems. In the present case, it corresponds to the complete eradication of the masking effect and the replacement by a complete reflection at the boundary between the interaction region and the masking region. This – at first counter-intuitive – result is the essence of the quantum Zeno effect. The decrease of transmission in Fig. 3.4 with decreasing Δt can therefore be considered as the onset of this effect which is completely realized at $\Delta t \lesssim 10^{-4}$.

Complex rotation method

As has been pointed out some time ago [37], complex coordinate scaling provides a method to suppress reflections. Complex scaling involves the following canonical transformation in the complex plane [37]. The position q and momentum p are rotated by an angle θ into the complex plane,

$$q \longrightarrow qe^{i\theta}, \quad (3.29)$$

and

$$p \longrightarrow pe^{-i\theta}. \quad (3.30)$$

Correspondingly, the basis functions are rotated as

$$\phi_n(q) \longrightarrow \phi_n^\theta(q) = \phi_n(qe^{i\theta}), \quad (3.31)$$

which are usually referred to as complex basis functions [37]. For Sturmian pseudo-states, the complex rotation of q is equivalent to using a complex Sturmian parameter $n_S^\theta = n_S \exp(-i\theta)$ [38]. It can be shown that the projection of the wave function onto

the P space is equivalent to

$$\begin{aligned} |\psi(t)\rangle_P &= e^{-iHt}|\psi(0)\rangle \\ &= |P(-\theta)\rangle\langle P(-\theta)|e^{-iHt}|P(-\theta)\rangle\langle P(-\theta)|\psi(0)\rangle \end{aligned} \quad (3.32)$$

where the subspace $\{P(\theta)\}$ corresponds to the set $\{\phi_n^\theta\}$. Once the initial wave function is projected to the rotated subspace $\{P(\theta)\}$ i.e. $\langle P(-\theta)|\psi(0)\rangle$, it evolves in this subspace by the evolution operator $\langle P(-\theta)|e^{-iHt}|P(-\theta)\rangle$. Then the final wave function is rotated back to the real P space. Note that we use the notations,

$$\begin{aligned} \langle q|\phi_n^\theta\rangle &= \phi_n(qe^{i\theta}) \\ \langle \phi_n^\theta|q\rangle &= \phi_n^*(qe^{i\theta}) \equiv \left(\phi_n(qe^{-i\theta})\right)^*. \end{aligned} \quad (3.33)$$

In this way, $\langle P(-\theta)|$ projects a wave function from the real to the rotated subspace, and $|P(-\theta)\rangle$ projects it from the rotated to the real subspace.

Using the property

$$\begin{aligned} \langle \phi_n^{-\theta}|H|\phi_m^{-\theta}\rangle &= \int d(qe^{-i\theta})\phi_n^*(qe^{-i\theta})H\phi_m(qe^{-i\theta}) \\ &= \int dq\phi_n^*(q)H(\theta)\phi_m(q) = \langle \phi_n|H(\theta)|\phi_m\rangle, \end{aligned} \quad (3.34)$$

and the approximation, which is the same approximation used for the coupled-states method (eq. (3.15))

$$\langle P(-\theta)|\exp(-iHt)|P(-\theta)\rangle \simeq \exp(-i\langle P(-\theta)|H|P(-\theta)\rangle t), \quad (3.35)$$

one finally arrives at

$$|\psi^{CR}(t)\rangle_P \simeq |P(-\theta)\rangle e^{-i\langle P|H(\theta)|P\rangle t} \langle P(-\theta)|\psi(0)\rangle \quad (3.36)$$

or, equivalently,

$$\psi^{CR}(q, t) = \sum_{n=1}^N c_n^\theta(0) e^{-iE_n t} \varphi_n(qe^{-i\theta}), \quad (3.37)$$

where the initial state is supposed to be contained in the rotated basis and φ_n are the eigenvectors of the Hamiltonian (eq. (3.18)). These equations are seemingly very similar to eqs. (3.15) and (3.18). However, the rotated Hamiltonian $H(\theta)$ is no longer Hermitian. Upon rotation of p

$$H = -\frac{1}{2} \frac{d^2}{dq^2} \longrightarrow H(\theta) = -\frac{1}{2} e^{-2i\theta} \frac{d^2}{dq^2}, \quad (3.38)$$

the solutions $|\varphi_n\rangle$ of the energy eigenvalue equation now yield complex eigenvalues. The free-particle continuum is rotated into the lower half plane,

$$k \longrightarrow k = k_R + ik_I = |k|(\cos \theta - i \sin \theta) \quad (3.39)$$

$$E = \frac{k^2}{2} \longrightarrow \frac{|k|^2}{2} e^{-2i\theta} = E^R + i E^I \quad (3.40)$$

with

$$E^R = \frac{1}{2}(k_R^2 - k_I^2) = \frac{1}{2}|k|^2 \cos 2\theta, \quad (3.41)$$

$$E^I = k_R k_I = -\frac{1}{2}|k|^2 \sin 2\theta. \quad (3.42)$$

All positive-energy discrete eigenvalues of the Hamiltonian in the pseudo-state basis lie on a ray emanating from the origin and making an angle of -2θ with the positive (real) energy axis (fig. 3.5). The free-particle continuum states are square-integrable and satisfy, apart from exponential damping at large distances, outgoing boundary conditions $\sim e^{ir k_R} e^{-r|k_I|}$. This property suggests that complex rotation may also be well suited for describing the reflection-free propagation of the wavepacket.

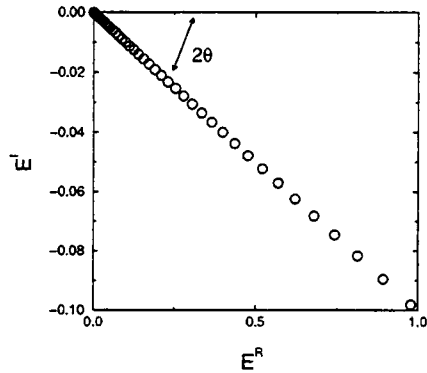


Figure 3.5: Energy spectrum of the free-particle Hamiltonian calculated with the complex rotation method using $N = 70$ Sturmian functions (circles). The rotation angle for the complex rotation method is $\theta = 0.05 \text{ rad}$ and the Sturmian parameter is $n_s = 1$.

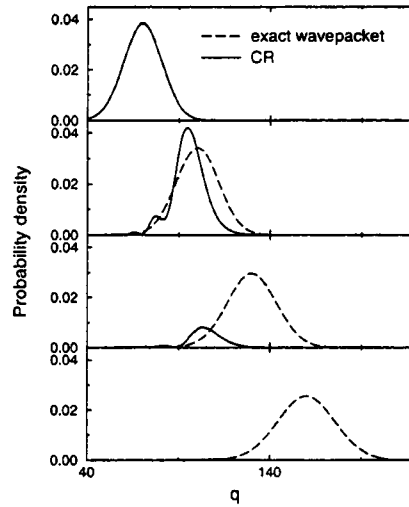


Figure 3.6: Comparison of the exact wavepacket (dashed lines) and the complex rotation results using a Sturmian basis with $n_s = 1$, $N = 70$, and an angle $\theta = 0.05$ (solid lines). The initial wavepacket and the times of the snapshots are the same as those in Fig. 3.1.

Figure 3.6 illustrates that evolution of the Gaussian wavepacket in a complex-rotated basis also provides for a non-unitary evolution and an approximate suppression of reflection. The origin of the loss of probability is damping due to the complex energy spectrum (eq. (3.40)). An optimization at a high level of transmission through the wall (i.e. absorption) without significant distortion in the inner region could be accomplished by tuning to a small rotation angle of $\theta = 0.05 \text{ rad} = 2.86 \text{ deg}$. For such small rotation angles, the effective region of phase space that can be represented by the rotated basis is very similar to that of the unrotated basis.

3.2 Application to the kicked atom system

— time-dependent Hamiltonian —

The methods for suppressing reflections discussed above will now be applied to the time-dependent Schrödinger equation for the kicked atom. First, the application of the RPM to the system with delta-shaped pulses is discussed. Subsequently, it is shown how this method can also be applied to HCPs of finite widths using the split operator method.

Kicked atom

For periodic systems, the time evolution

$$|\psi(t)\rangle = U(t, 0)|\psi(0)\rangle \quad (3.43)$$

is reduced to the evaluation of the period-one evolution operator, $U(T, 0)$, since $U(KT, 0) = [U(T, 0)]^K$. In the kicked atom system (eqs. 2.8 and (2.9)), one period extends from right before the k th kick to right before the $(k + 1)$ th kick, i.e.

$$\begin{aligned} U(T, 0) &= U(kT, (k-1)T) \\ &= \lim_{\epsilon \rightarrow 0} U(kT - \epsilon, (k-1)T + \epsilon) U((k-1)T + \epsilon, (k-1)T - \epsilon) \\ &= \lim_{\epsilon \rightarrow 0} e^{-iH_{at}(T-2\epsilon)} e^{-2iH_{at}\epsilon + iq\Delta p} \\ &= e^{-iH_{at}T} e^{iq\Delta p}. \end{aligned} \quad (3.44)$$

Since we can work only in a finite Hilbert space $\{P\} = \{|\phi_n\rangle | n = 1, \dots, N\}$, the objective of our calculation is to find a good approximation for the non-unitary projection of $U(T, 0)$ onto the subspace P ,

$$\begin{aligned} \langle P | U(T, 0) | P \rangle &\simeq \sum_{m,l,n}^N \langle P | \phi_l \rangle \langle \phi_l | e^{-iH_{at}T} | \phi_m \rangle \\ &\quad \times \langle \phi_m | e^{iq\Delta p} | \phi_n \rangle \langle \phi_n | P \rangle \end{aligned} \quad (3.45)$$

with an orthonormal basis set, $|\phi_n\rangle$. A unitary method cannot be applied for the evaluation of the free evolution operator, $\exp(-iH_{at}T)$, and the boost operator, $\exp(iq\Delta p)$, within a subspace P since there is strong coupling to the complement Q of the full Hilbert space. To avoid reflections, two different schemes are used, one for each operator. First, the exact matrix elements of $\exp(iq\Delta p)$ are calculated. Detailed evaluation is discussed in Appendix G. Second, one of the methods discussed in the last section has to be applied to evaluate the operator $\exp(-iH_{at}t)$.

As basis functions, Sturmian pseudo-states (eq. (3.7)) are chosen in our calculations, since they properly describe Coulomb wave functions (Appendix E) and the Hamiltonian or the dipole matrix elements can be easily evaluated using recursion relations of Laguerre polynomials (Appendix F). Using this basis set, we can apply the complex rotation method (eq. (3.37)) or the RPM (eq. (3.24)) for the evaluation of a free evolution or a boost operator matrix. However, the application of the complex rotation method is not so obvious. Since the Stark field is not dilatation analytic [32, 33], the corresponding quasi-energy in the complex rotation method, E^I in eq. (3.40), can be positive and reflections may be enhanced by exponentially growing, $\exp(E^I t)$, rather than exponentially decreasing, $\exp(-E^I t)$, terms. This applies to the kicked atom, where the perturbation is a Stark field multiplied by a sum of delta functions. Therefore, the RPM is utilized.

In the present scheme, the free evolution operator and the boost operator are evaluated separately using different basis sizes N and M ($N < M$) (eq. (3.24) and Appendix F). The boost operator can be evaluated analytically as a sum of hypergeometric functions [39] (an asymptotic expansion [40] must be used for very high quantum numbers). For large values of the momentum transfer, the numerical evaluation of those hypergeometric functions is relatively stable. Therefore, we use the analytical form of the boost operator. Alternatively, one can evaluate the boost operator using the RPM (e.g. for

small momentum transfers)¹. Thus, our numerical solution of the TDSE is in fact a generalized RPM. The exact form is basically equivalent to the limit $M \rightarrow \infty$ in the RPM evaluation of the operator.

Pulses with a finite width

In this subsection, we discuss the numerical treatment of experimental pulse profiles, i.e., with a finite width T_p and a time varying field $F(t)$. Note that the 3-D system is discussed in this part for the purpose of simulating the experimental data². To this end the split operator method is introduced [22, 41]. In this method, the time evolution operator from $t = 0$ to $t = T_p$ is broken down into a product of K evolution operators for time intervals $\Delta t = T_p/K$,

$$U(T_p, 0) = \prod_{k=0}^{K-1} U((k+1)\Delta t, k\Delta t). \quad (3.46)$$

In each step the evolution operator is split at the midpoint.

$$\begin{aligned} U((k+1)\Delta t, k\Delta t) &\simeq \exp\left(-\frac{i}{2}H_{at}\Delta t\right) \exp(iz\delta p_k) \\ &\quad \times \exp\left(-\frac{i}{2}H_{at}\Delta t\right) \end{aligned} \quad (3.47)$$

$$\delta p_k = - \int_{k\Delta t}^{(k+1)\Delta t} F(t) dt \quad (3.48)$$

which has an $O((\Delta t)^3)$ error. The error arises from the fact that the commutators $[H_{at}, z] \neq 0$ and, in general, $[H(t), H(t')] \neq 0$. The resulting evolution operator becomes

$$U(T_p, 0) = \exp\left(-\frac{i}{2}H_{at}\Delta t\right)$$

¹Detailed evaluation is in Appendix F

²Comparison between the experimental and theoretical results is seen in Appendix D.

$$\times \left[\prod_{k=0}^{K-1} \exp(iz\delta p_k) \exp(-iH_{at}\Delta t) \right] \\ \times \exp\left(\frac{i}{2}H_{at}\Delta t\right)$$

which is identical to the delta-shaped kicked atom system with a time varying momentum transfer, δp_k .

Because of the $O(\Delta t^3)$ error, the split operator method is accurate only in the limit $K \rightarrow \infty$. However, if a large enough value of K is used, the error becomes negligible and converged results can be obtained. Fig. 3.7 illustrates the convergence of the split operator method for different scaled pulse durations $T_{p0} = T_p/2\pi n_i^3$ as a function of the number of splits (kicks). Since the field strength F_p is kept constant during T_p in this simulation, the exact ionization probability (solid line) can be calculated by diagonalizing the Hamiltonian, which is time-independent in this case. Clearly, the longer the pulse, the larger number of splits required to reach convergence.

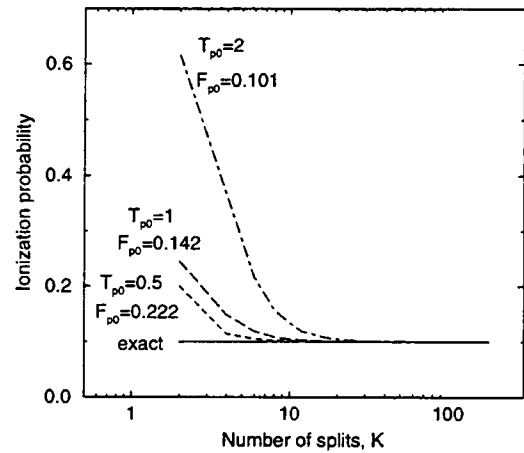


Figure 3.7: Probability of ionization of $H(n_1 = 4, n_2 = 0, m = 0)$ atoms by rectangular HCPs of various scaled durations, T_{p0} , as a function of the number of splits of the evolution operator. For each value of T_{p0} the scaled field strengths F_{p0} have been chosen such that the ionization probability is ten percent. The basis size is set to $N = 1035$ and the Sturmian parameter to $n_S = 5$ [22].

3.3 Stabilization method

Since the RPM neglects the coupling from the Q space to the interaction region P , important questions arise: does this affect the numerical solution? Is back-coupling from Q to P negligible? And, as a practical problem, what value should the Sturmian parameter have in order to get an accurate result with the smallest basis set?

In order to answer these questions, the so-called stabilization method is applied to the time-dependent Schrödinger equation. The time-dependent stabilization method [22] can be viewed as an extension of the time-dependent variational principle, very much like the case of the stationary Schrödinger equation [42]. While the variational principle assures that the solution of the form (eq. (3.2)) is the best result within the given basis, the stabilization method goes beyond that by providing information as to how accurate the solution is within the whole Hilbert space. The standard form of stabilization is associated with the convergence of a given transition probability $P_{i,f} = \langle \phi_f | U(t, 0) | \phi_i \rangle$ with respect to the basis size N (in the limit $N \rightarrow \infty$, $P_{i,f}$ stabilizes).

A more useful stabilization property also exists with respect to the parameter n_S which defines the basis set for a fixed value of N . This fact can be understood using the very schematic picture in fig. 3.8. Suppose that the full Hilbert space is represented by the plane such that the "exact" evolution of the wave function is given by a trajectory in the plane (e.g. trajectories A, B, and C). Two finite Hilbert subspaces, P_1 and P_2 , generated by bases with parameters n_{S_1} and n_{S_2} are represented in the figure by triangular regions. These regions can be chosen to provide a good representation of the initial wave function (open circle) but may not always contain the exact final wave function (solid circles). If a trajectory such as A is contained in the overlap of both triangular regions, the calculation of the evolution of the wave function should be stable with respect to a change from P_1 to P_2 , i.e., the solution should be

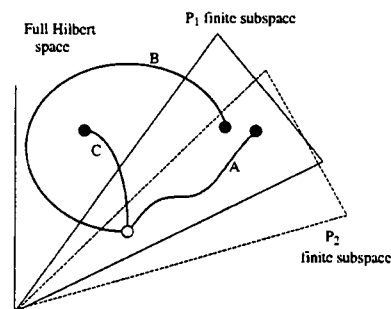


Figure 3.8: Schematic picture of the full Hilbert space. The trajectories A, B, and C represent different exact solutions of the time-dependent Schrödinger equation starting from the same initial state (represented by an open circle) but with different final wave functions (represented by solid circles). The triangular regions denote two finite Hilbert spaces. See text. [22]

"exact". In turn, if a trajectory such as B or C leaves the finite subspaces subtended, the

approximate calculations in each basis set will yield, in general, different non-converged results. There could be, of course, exceptions such that convergence is reached (not necessarily to the correct limit) even if trajectories corresponding to these results leave the finite subspace. Thus, an accurate calculation of a transition probability should be stable with respect to all variations of the basis set, e.g., n_S . The larger the basis, the larger the range of n_S parameters for which the calculations should be stable. Note, however, that stabilization of a given transition probability does not imply stabilization for other transition probabilities (i.e., some trajectories may leave the domain subtended).

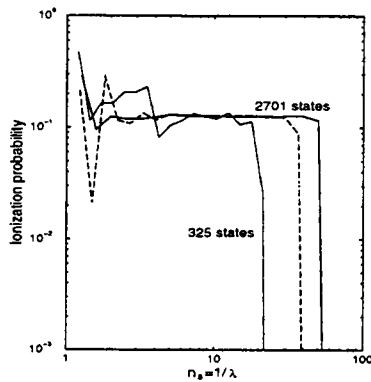


Figure 3.9: Ionization probability of $H(n_1 = 9, n_2 = 0, m = 0)$ subject to a rectangular HCP with $F_{P0} = 0.3$ and $T_{P0} = 0.5$ as a function of n_S . The various curves in the figure correspond to basis sizes of $N = 325, 1035, 2701$. The larger the basis, the broader the stabilization plateau. [22]

Fig. 3.9 demonstrates the application and significance of the stabilization method for calculating the ionization probability of 3-D hydrogen atoms in the $|n_1 = 9, n_2 = 0, m = 0\rangle$ parabolic state subject to a rectangular HCP, i.e., $F(t) = F_p$ ($0 < t < T_p$). For a fixed value of N , the calculated ionization probability as a function of the Sturman parameter exhibits a characteristic plateau. Moreover, the size of the plateau increases for increasing values of N . This is precisely the behavior expected: if N is large enough, the calculation must be stable with respect to variations of the basis set. Therefore, the value of the plateau corresponds to a converged ionization probability. The results in fig. 3.9 can be

compared with the work of Schwartz [43] who un-

dertook the first accurate time-independent calculations for $e - H$ scattering employing a similar method. However, because of limited computing power available at that time, the plateaus appeared as shallow minima. The stabilization method can not only pro-

vide accurate results but also furnish a tool that can be used to learn how to choose the most appropriate Sturmian parameter. The stabilization plateau starts to develop at $n_S \lesssim 10$ even for a small basis size. This is partly due to the fact that a basis set with $n_S \simeq 10$ can provide a very good representation of the initial electronic state. However, for the finite subspace to cover the entire time development of the wave function it must also be able to provide a good description of the intermediate and final states. The smaller n_S , the better the representation of continuum states (Appendix E). This is the reason why the optimum Sturmian parameter is slightly smaller than 10.

For simplicity, fig. 3.9 shows the simplest convergence test, i.e., we set $M = N$ in the RPM, therefore, one only needs to check the convergence with respect to n_S and N while it is normally necessary to check the convergence with respect to M and Δt as well.

Chapter 4

Quantum analysis of the stable islands

In the reminder of this thesis, the quantum mechanics of the kicked atom is discussed. The validity of the 1-D kicked atom system to analyze the stabilization or the ionization mechanisms of the 3-D system has already been discussed in chapter 2. Thus, we focus on the quantum dynamics of the 1-D kicked atom. This 1-D system has the additional advantage that accurate quantum simulations can be performed for higher quantum levels, bigger momentum transfers, and longer times. Note that all quantum calculations in this and the next chapter are performed using the RPM and the convergence of the results is checked by the stabilization method.

Fig. 4.1 shows the survival probability of the kicked atom after $K = 200$ impulses as a function of scaled frequency ν_0 of the train of pulses. The initial state is chosen as $n_i = 50$. The scaled momentum transfer $\Delta p_0 = -0.3$ is chosen so that the classical phase space for this system contains sizable stable islands (fig. 2.10). In this figure, we can make three different observations for different frequency regions;

- low frequency ($\nu_0 \lesssim 0.8$): the quantum results are much smaller than

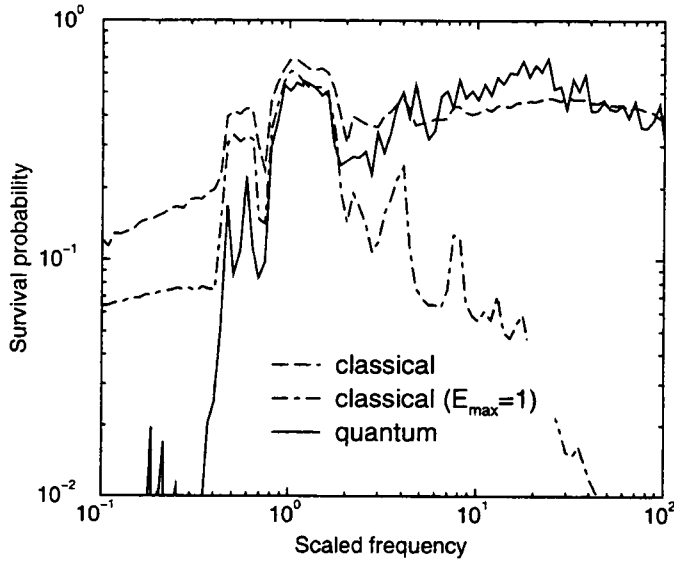


Figure 4.1: Survival probability of the kicked 1-D hydrogen atom as a function of scaled frequency ν_0 for a fixed scaled momentum transfer $\Delta p_0 = -0.3$ after $K = 200$ kicks. The initial quantum level of the atom is $n_i = 50$ and the quantum calculations have been performed using a Sturmian parameter $n_S = 60$ and basis sizes $N = 800$ and $M = 1000$. See text for the definition of E_{max} .

the classical ones.

- intermediate region ($\nu_0 \sim 1$): both results show stabilization peaks and good classical-quantum correspondence is seen.
- high frequency ($\nu_0 \gtrsim 8$): the quantum results are larger than the classical ones.

In the low frequency region, the system evolves for a longer time evolution for a fixed number of kicks and, therefore, there are bigger chances to lose a larger portion of probability because of the finite domain of the basis. This is partly the reason why the quantum survival probability is smaller than the classical one. The stabilization method confirms this non-convergence of the result in the low frequency regime.

On the other hand, the survival probability for high frequencies is larger for the

quantum result than for the classical one. This may be due to reflections associated with the quantum Zeno effect. According to the stabilization method, when the basis sizes N and M are increased, subspaces P and Q' are enlarged and smaller reflections are expected. However, the numerical calculation shows that the survival probability increases as the basis sizes become bigger, which indicates that the larger survival probability for the quantum result is not caused by reflections due to the finite basis size. Thus, this can be considered as the onset of quantum stabilization (or localization) and this stabilization is discussed in detail in the next chapter.

In the intermediate frequency, the classical and the quantum results are, overall, in good qualitative agreement. Note, however, that the quantum survival probability underestimates the classical probability. This is due to the non-unitary time evolution associated with the RPM. Classical calculations show a similar tendency when the classical simulation mimics the RPM, i.e., neglects the coupling from energy levels beyond E_{max} to lower energy levels. The result with $E_{max} = 1$, which is also plotted in fig. 4.1, proves that the underestimation of the quantum survival probability is not a real quantum effect but the artificial error due to the finite basis size.

This is also illustrated in fig. 4.2 which shows the survival probability as a function of K . For $n_i = 5$, the survival probability oscillates with large fluctuations around the classical result but, on average, both results are in good agreement. As n_i is increased ($n_i = 50, 100$), these quantum fluctuations disappear and the quantum survival probabilities follow the classical scaling invariant result reasonably well for short times. After 50 kicks, however, the quantum results depart from the exact classical result. In turn, the quantum results agree with the classical one for $E_{max} = 1$. Clearly, the quantum underestimation is due to the non-unitary time evolution of the RPM. Because of limited computing power, it is not feasible to perform the quantum calculation for much longer duration, therefore, the stability of the system is not yet verified from these results. Using the periodic nature of the system, however, quantum stabilization can be analyzed without the long time propagation. In this chapter, we focus on the interme-

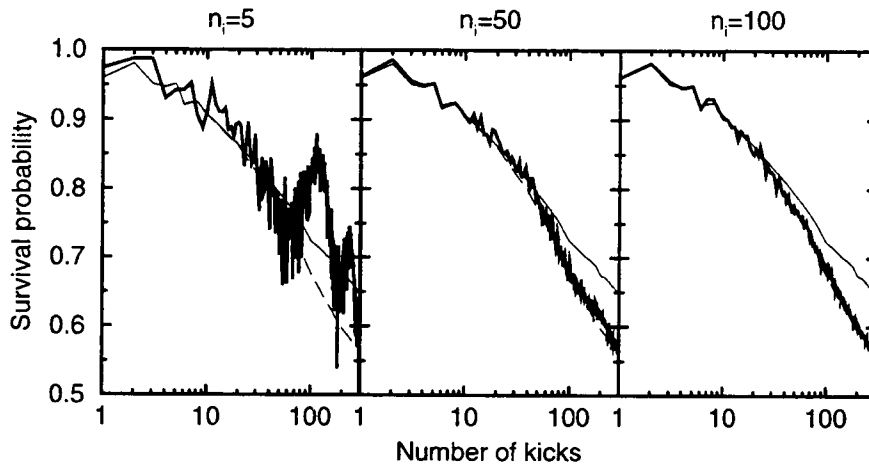


Figure 4.2: Survival probability as a function of K for different initial states $n_i = 5, 50$, and 100 together with classical results. Quantum results (thick solid line) are calculated with the RPM using $N = 200$ and $M = 300$ for $n_i = 5$ and $N = 1500$ and $M = 1800$ for $n_i = 50$ and 100 . Note that various Sturmian parameters are chosen to check the convergence of the calculations. Classical results (thin solid line) are the same for different initial states because of the scaling invariance. The thin dashed line, which agrees with quantum results and is almost invisible, is the classical result for $E_{max} = 1$ (see text). The parameters for the train of kicks are $\Delta p_0 = -0.3$ and $\nu_0 = 1.09$.

diate regime of frequencies, especially a scaled frequency $\nu_0 = 1.09$ which resides in the middle of the main stabilization peak, and discuss the stabilization mechanism in terms of classical-quantum correspondence.

4.1 Manifestation of classical-quantum correspondence in phase space

In classical mechanics, the stability of the system could be understood using a Poincaré map as a mixture of stable islands and chaotic seas. In the quantum system, however, the position and the momentum of the electron cannot be defined at the same time because of the quantum uncertainty principle. Therefore, there is no unique way to

visualize the quantum phase space of the system. A quantum wave function $\psi(q)$ can be projected onto phase space [44, 45, 46] using Wigner and Husimi distributions. Both distributions are briefly introduced here, and some of their properties are discussed.

The Wigner distribution,

$$P_w(q, p) = \frac{1}{\pi} \int_{-\infty}^{\infty} dy \psi^*(q + y) \psi(q - y) e^{2ipy} \quad (4.1)$$

was proposed by Wigner [44] as a phase space distribution function which preserves all the quantum properties of the system. For example, the Wigner distribution still recovers the information of the density distribution of the system in both q and p spaces, i.e.,

$$\begin{aligned} \frac{1}{2\pi} \int dp P_w(q, p) &= |\psi(q)|^2 \\ \frac{1}{2\pi} \int dq P_w(q, p) &= |\bar{\psi}(p)|^2 \end{aligned} \quad (4.2)$$

where $\bar{\psi}(p)$ is the Fourier transform of a wave function $\psi(q)$. The classical limit of quantum mechanics becomes very transparent in this approach since the Wigner function satisfies a dynamical equation whose classical limit converges to the classical Liouville equation [26]. However, since the Wigner distribution is a pure quantum distribution, it has the same oscillatory structures as the quantum wave function. In addition, P_w can acquire negative values and it is therefore referred to as a pseudo probability density. Those features are big disadvantages for the study of classical-quantum correspondence.

In order to study the classical limit, Husimi [45] introduced the positive definite distribution defined by

$$\begin{aligned} P_H(q, p) &= \int dq' \int dp' P_{q,p}(q', p') P_w(q', p') \\ &= \frac{1}{2\pi} \left| \int dr \varphi_{q,p}^*(r) \psi(r) \right|^2, \end{aligned} \quad (4.3)$$

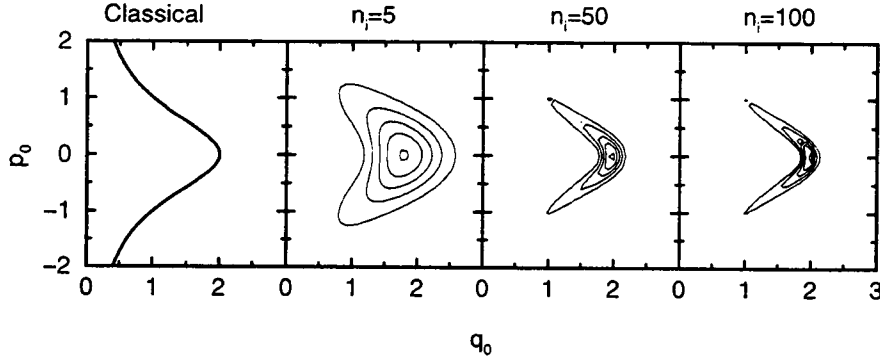


Figure 4.3: Classical and quantum scaled phase-space distributions of a unperturbed hydrogen atom. Husimi distributions are plotted for $n = 5$ and $n = 50$ using $n_S = 60$ and $N = 300$ and for $n = 100$ using $n_S = 120$ and $N = 300$.

with

$$\varphi_{q,p}(r) = (\pi\alpha)^{-\frac{1}{4}} \exp[-(q-r)^2/2\alpha] \exp(ipr), \quad (4.4)$$

where $P_{q,p}$ and P_w are the Wigner distributions of $\varphi_{q,p}$ and ψ , respectively. The Husimi distribution is simply a convolution of the Wigner phase-space distribution with a minimum uncertainty Gaussian wavepacket that contains the “squeezing” parameter α which can be adjusted to improve the resolution in either q or p . We set $\alpha = n_i^3$ so as to render the width of the Gaussian wavepacket invariant under classical scaling (eq. (2.5)), and this value of α is used throughout the remaining thesis. The effect of the Gaussian averaging is to remove the short-wavelength oscillatory structure of the wave function and clarify the correspondence to the classical phase space distribution.

In the kicked atom, the classical initial state of the electron is given by a microcanonical ensemble of points with $H_{at}(q,p) = -1/2n_i^2$, which corresponds to a line in phase space. This line is depicted in fig. 4.3 in scaled units $q_0 = q/n_i^2$ and $p_0 = pn_i$. Because of the classical scaling invariance, this line, $p_0^2/2 - 1/q_0 = -0.5$, is independent of n_i . The corresponding Husimi distributions for $n_i = 5, 50, 100$ are also plotted in fig. 4.3. Remarkably, the Husimi distributions closely resemble the classical distribution except for the finite width due to the quantum uncertainty which is given by

$\Delta q_0 \Delta p_0 = \Delta q \Delta p / n_i \approx 1/n_i$. We can observe that the width becomes narrower as n_i increases.

Snapshots of the classical distribution after 1, 2, and 3 kicks with a frequency $\nu_0 = 1.09$ and a strength $\Delta p_0 = -0.3$ show that the ensemble of points undergoes a deformation (fig. 4.4), and a fraction of the ensemble starts to become organized around classical stable islands. Fig. 4.4 also displays Husimi distributions for the evolved states after 1, 2, and 3 kicks for different initial states. Similar to fig. 4.3, the Husimi distributions resemble the deformation of the classical ensemble with the uncertainty, i.e., the larger the n_i , the better the correspondence. These results are consistent with the fact that classical-quantum correspondence for a short time is reasonably good in fig. 4.2.

Remarkably, a similar degree of correspondence between classical and quantum results is also seen for the long time propagation. This is illustrated in fig. 4.5 where the classical and quantum phase space distributions are plotted after 200 kicks. Thus, classical-quantum correspondence can be reflected in phase space distributions. For $n_i = 50$ and 100, the only discordance which has been seen in fig. 4.2 is due to the non-unitarity of the RPM when the quantum state is distributed widely beyond the finite subspace P . Since the quantum system is mainly localized around a classical stable island which resides within the subspace P , most of the wave function is not affected by this error, and the Husimi distributions (fig. 4.5) can show remarkably similar features to those displayed by the classical distribution. The initial distribution for $n_i = 5$ is relatively broad (fig. 4.3) and has a big overlap with the chaotic sea as well as with stable islands. Thus, the correspondence for this level is not as clear as for $n_i = 50, 100$.

4.2 Stabilization analysis using Floquet theory

In this section, the wave function of the electron is expanded in a set of periodic basis functions termed Floquet states. Because of the periodicity of the basis functions, the information of the long time propagation can be deduced from the information of the

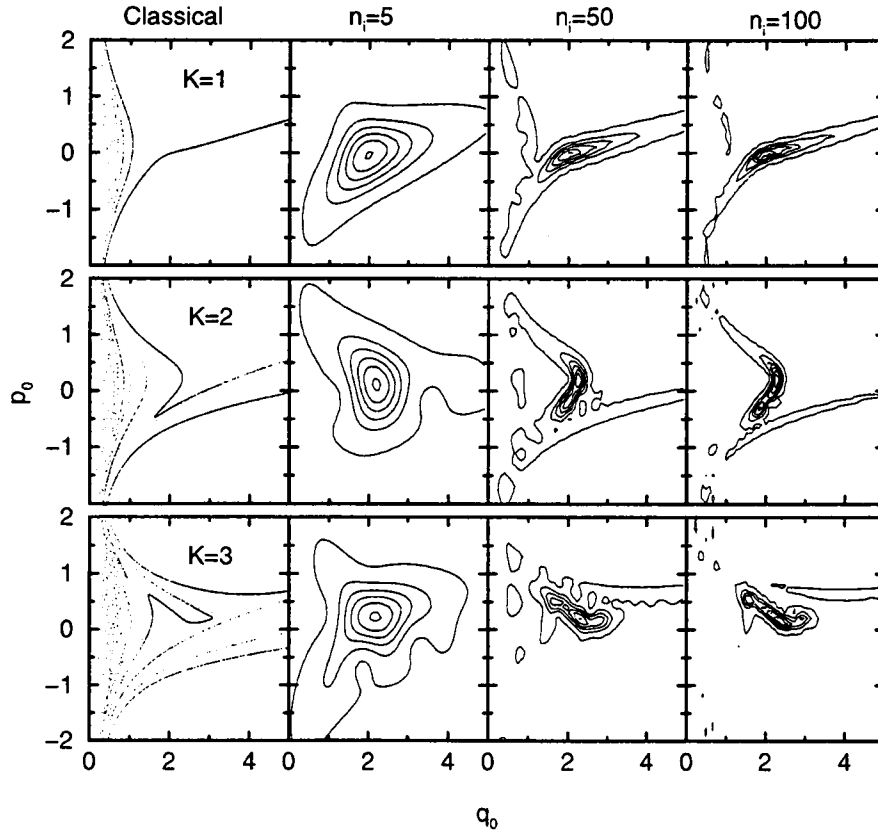


Figure 4.4: Time evolution of the classical and quantum scaled phase-space distributions of a hydrogen atom following application of 1, 2, and 3 kicks with a scaled momentum transfer $\Delta p_0 = -0.3$ and a scaled repetition frequency $\nu_0 = 1.09$. All classical results are represented by an ensemble of 10000 points. Quantum results are plotted for different initial states $n_i = 5, 50$, and 100 using sets of parameters $(n_S, N, M) = (6, 200, 300), (60, 500, 700)$, and $(100, 800, 1000)$, respectively.

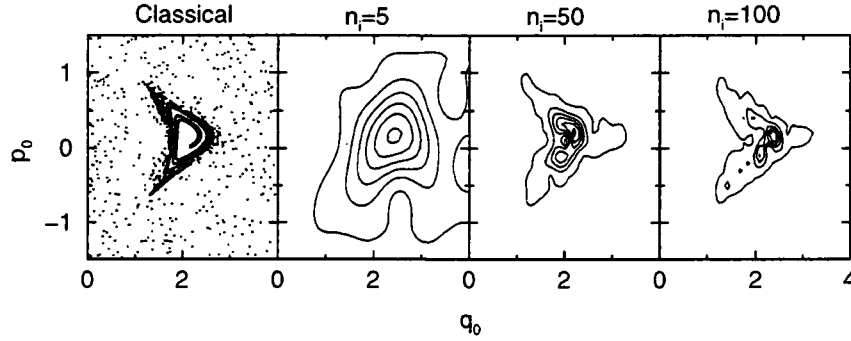


Figure 4.5: Same as fig. 4.4 but after 200 kicks.

short time propagation of the system. Thus, the dynamical stability of the kicked atom system can be confirmed.

Floquet states [47] are defined through the eigenvalue equation

$$U(T, 0)|\phi_n^F\rangle = e^{-i\mathcal{E}_n T}|\phi_n^F\rangle \quad (4.5)$$

with a period-one evolution operator $U(T, 0)$ and a quasi-eigenenergy $\mathcal{E}_n = \mathcal{E}_n^R - i\mathcal{E}_n^I$. After K kicks, the propagated wave function becomes

$$|\psi(KT)\rangle = \sum_{n=1}^N c_n e^{-\mathcal{E}_n^I KT} e^{-i\mathcal{E}_n^R KT} |\phi_n^F\rangle, \quad (4.6)$$

where c_n are the expansion coefficients of the initial state $|\psi(0)\rangle$ in the Floquet basis set. The key point for the stability analysis is that, due to the non-unitarity of the evolution operator, the quasi-eigenenergies of $U(T, 0)$ are complex. The imaginary part $\mathcal{E}_n^I \geq 0$ corresponds to a decay probability within the P space. Therefore, in the limit $K \rightarrow \infty$ the expansion coefficients, $c_n e^{-\mathcal{E}_n^I KT} e^{-i\mathcal{E}_n^R KT}$, of the wave function vanish unless $\mathcal{E}_n^I = 0$. That is,

$$|\psi(KT)\rangle \xrightarrow{K \rightarrow \infty} \sum_{\phi_n^F \in P_s} c_n e^{-i\mathcal{E}_n^R KT} |\phi_n^F\rangle, \quad (4.7)$$

where P_s is the subset of P defined by $P_s = \{|\phi_n^F\rangle | \mathcal{E}_n^I = 0\}$. Thus, stabilization within the P space is one-to-one associated with the subspace P_s .

It is important to note that eq. (4.7) is only necessary but not sufficient to identify stabilization and ionization. Within any N -dimensional representation of the P space, quantum trajectories which perform excursions into the Q space are eliminated from the quantum phase flow due to the RPM. In other words, any Floquet state with $\mathcal{E}_n^I > 0$ has not converged as a function of basis size. This non-convergence within P is either due to phase space flux associated with proper ionization, i.e., it is of physical origin, or due to the fact that stabilized motion with quantum trajectories wandering intermittently into the Q space and returning later into the P space cannot be properly represented, causing an underestimation of the survival probability as seen in fig. 4.2. Likewise, Floquet states of the subspace P_s with $\mathcal{E}_n^I = 0$ are not necessarily converged. If the suppression of reflections is not complete and outbound probability flux is partially returned back into the "inner region", this could provide an artificial contribution to the set P_s . In order to assure that the decomposition of eq. (4.6) into proper ionization and stabilization is realistic, the stabilization method is applied (see previous chapter). Thus, we can identify a Floquet state with $\mathcal{E}_n^I = 0$ as a localized state within the subspace P .

If classical-quantum correspondence exists, the Husimi distributions of the dominant Floquet states leading to stabilization should be localized in phase space around the dominant classical stable islands in a Poincaré map. In fig. 4.6 the Poincaré map, together with the initial classical torus with a scaled energy $E_0 = -1/2$, is displayed featuring several pronounced stable islands. The Husimi distributions of the stable Floquet states, $\mathcal{E}_n^I \simeq 0$, with different initial states are also presented. Figures (a) and (b) for each initial state are the dominant Floquet states among the stable ones: i.e., such that the overlap between the Floquet state and the initial state, $|c_n|^2$, where

$$c_n = \langle \phi_n^F | \phi_{n_i} \rangle, \quad (4.8)$$

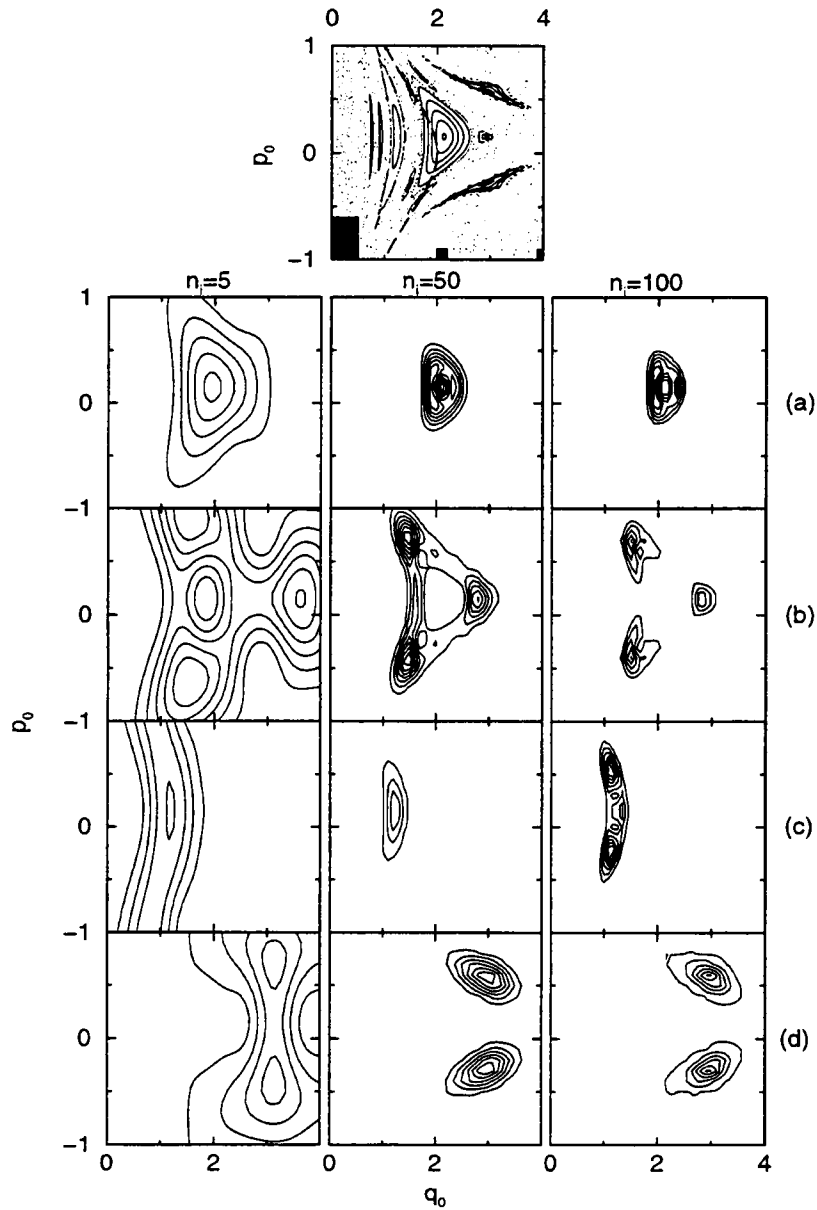


Figure 4.6: Poincaré map in scaled units (top) and Husimi distributions (other 12 graphs) of the stable Floquet states of the kicked atom system with $\Delta p_0 = -0.3$ and $\nu_0 = 1.09$. The dashed line and the three black squares at the bottom of the Poincaré map are the initial torus and the quantum uncertainties corresponding to $n_i = 5$ (lower left corner), $n_i = 50$ (at $(q_0, p_0) = (2, -1)$), and $n_i = 100$ (lower right corner), respectively. Husimi distributions corresponding to different stable islands are plotted for different initial states.

is the biggest one. Since there is always a numerical error in the calculation of quasi-eigenenergies of the order of $O(10^{-5})$ associated with the numerical diagonalization of $U(T, 0)$, those Floquet states with an imaginary part $\mathcal{E}_n^I$ of that order are either stable or very slightly unstable. Among the dominant Floquet states in fig. 4.6, the distribution is relatively broad for $n_i = 5$ because of the quantum uncertainty $\Delta q_0 \Delta p_0 \simeq 1/n_i$ which is represented by black squares in fig. 4.6. When the uncertainty is of the same size as the area of a given classical stable island, the quantum distribution cannot resolve it and becomes rather broader than the classical island. As a consequence, the corresponding Floquet state tends to have a small but finite value of $\mathcal{E}_n^I$ and becomes slightly unstable. This fact can be seen in the table 4.1 where the values of $\exp(-\mathcal{E}_n^I T)$ for each Floquet state are listed.

Table 4.1: Survival probability per period, $\exp(-\mathcal{E}_n^I T)$, of the Floquet states which are plotted in fig. 4.6. The labels of the Floquet states are same as in fig. 4.6

	$n_i = 5$	$n_i = 50$	$n_i = 100$
(a)	0.9997	1.000	1.000
(b)	0.9997	0.9998	0.9998
(c)	0.9998	0.99997	0.99995
(d)	0.9995	0.9997	0.9995

The Floquet state (b) for each initial state corresponds to the period-five island chain, $R_{fix} = 5/5$. Since each island is very small, the Husimi distribution even with $n_i = 100$ cannot fully resolve all five islands and appears as three pronounced peaks. This tendency also appears in the survival probability per period of these Floquet states, which are all slightly unstable (table 4.1). The stable islands with $R_{fix} = 1/2$ and $2/1$, which do not overlap with the initial unperturbed torus, can also be found as the stable Floquet states which are plotted in fig. 4.6 (c) and (d). However, the overlap $|c_n|$ is very

small and, therefore, they do not have a significant contribution to the time evolution of the system. Likewise, those islands are small and the Floquet states become slightly unstable (table 4.1). Note that the island with $R_{fix} = 2/1$ is located in a region of phase space with a relatively high energy which is closer to the boundary of the subspace P . Therefore, the survival probability per period is smaller than the other Floquet states even though the area of the island is bigger than the period-five island chain.

Thus, there exists a very close correspondence between classical stable islands and stable Floquet states. Because of the quantum uncertainty, the corresponding Floquet state becomes slightly unstable as the classical island becomes smaller. In the next chapter we show that classical-quantum correspondence is not completely lost when the classical islands are infinitely small. In this limit, classical signatures appear as scars of wave functions which lead to the quantum localization of the system.

Chapter 5

Quantum localization

Since quantum localization has been already found for the Rydberg atom subject to a microwave field, the kicked Rydberg atom appears to be a promising candidate to study this phenomenon. However, unlike a microwave oscillating field, a unidirectional train of impulses,

$$V(t) = -\frac{q\Delta p}{T} - \frac{2q\Delta p}{T} \sum_{m=1}^{\infty} \cos(2\pi\nu_m t), \quad (0 \leq t \leq (K-1)T) \quad (5.1)$$

has a finite average field, $F_{av} = -\Delta p/T$, and all high harmonics ($\nu_m = m\nu$) with equal strength (i.e. eq. (5.1) is the Fourier expansion of eq. (2.9)). In contrast, $F_{av} = 0$ for a microwave field. For high frequencies, the Stark field becomes so large that it induces transitions among bound and continuum hydrogenic states. This complicates the quantum description of this system since any realistic calculation must involve a large number of continuum hydrogenic states. In fact, the kicked atom can be better viewed as a Rydberg atom plus a DC field subject to a superposition of various harmonics, i.e.,

$$H(t) = H_{Stark} + V'(t), \quad (5.2)$$

$$H_{Stark} = H_{at} + qF_{av}, \quad V'(t) = 2qF_{av} \sum_{m=1}^{\infty} \cos(2\pi\nu_m t). \quad (5.3)$$

For $F_{av} > 0$ ($\Delta p < 0$), the quantum spectrum of H_{Stark} is discrete (i.e. no continuum). On the contrary, for $F_{av} < 0$ ($\Delta p > 0$) the quantum spectrum is only continuous and involves a finite number of well defined resonances whose energy levels are below or near the top of the potential barrier $E_{barrier} = -2\sqrt{\Delta p/T}$ (fig. 5.1). The high harmonics of the perturbation directly couple a bound state to higher energy levels. Thus, the kicked atom is more unstable than the atom in a microwave field. Whether or not quantum localization can be observed is not a priori clear.

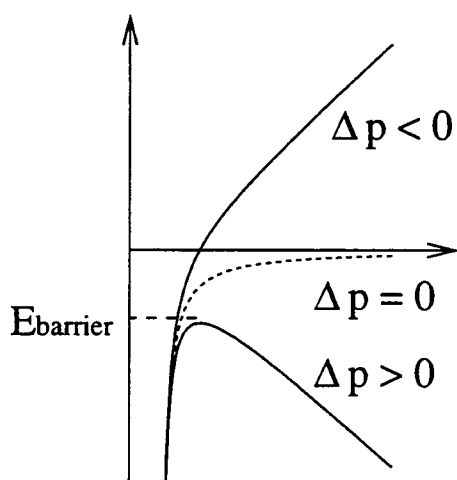


Figure 5.1: Potential curves for the Stark problem, $V_{total}(q) = -1/q + qF_{av}$.

In the first section of this chapter, the existence of quantum localization in phase space is analyzed and its relation to scars of the wave function is examined. In the second section of this chapter, the mechanism of quantum localization is discussed using the ideas introduced by other authors to interpret the quantum localization of other systems, such as, the kicked rotor system or the microwave driven atom. Because of the quantum uncertainty, quantum dynamics is shown to dramatically suppress classical diffusion in the chaotic sea. Surprisingly, quantum localization can still be found even though the high harmonic terms in the perturbation make the system more unstable.

5.1 Unstable fixed points and quantum localization

Negatively kicked atom

For the negatively kicked atom, we could observe that a high frequency train of pulses seemingly makes the quantum system less unstable than the classical system (fig. 4.1).

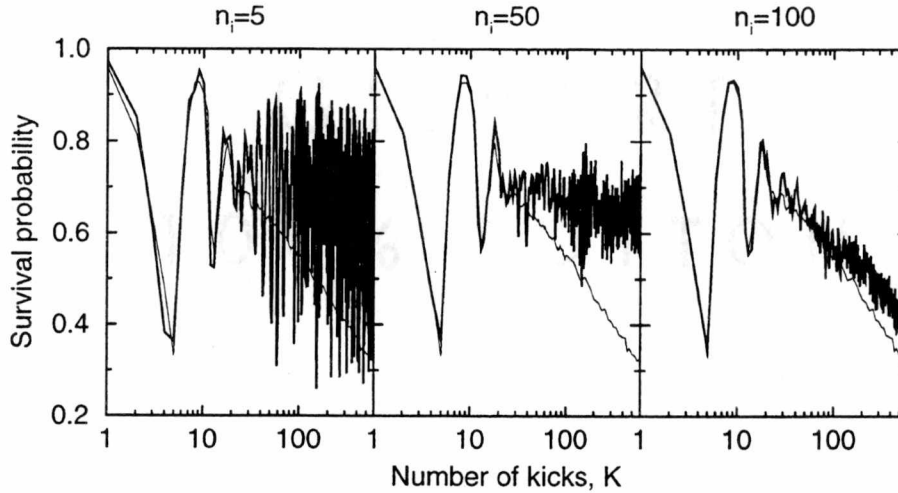


Figure 5.2: Survival probability as a function of the number of kicks K for three different initial states ($n_i = 5, 50$, and 100). Thick lines are quantum results and thin ones are classical results. The parameters for the train of kicks are $\Delta p_0 = -0.3, \nu_0 = 16.8$.

This is analyzed in more detail in fig. 5.2 where the time evolution of the survival probability for a high scaled frequency regime, $\nu_0 = 16.8$, is plotted. Remarkably, the quantum survival probabilities become vastly larger than the classical system and, therefore, providing a clear evidence of quantum localization. Note that, for $n_i = 100$, the quantum calculation is not converged for $K > 200$, therefore, quantum localization is not observed clearly. By definition, a system exhibits quantum localization if its quantum decay rate is slower than the classical one. In this sense, quantum localization is observed in fig. 5.2 for all n_i values.

The classical system decays rapidly as a function of time since the initial state is in the chaotic sea and very far away from any stable island (fig. 5.3). As discussed in chapter 2, the unstable fixed points for this system are densely distributed in the chaotic sea, but their measure is zero. Remarkably, however, the quantum phase space distributions of the stable Floquet states (fig. 5.3) can recollect this classical dynamical property hidden in the chaotic sea, and tend to have enhanced amplitudes around the unstable fixed points. These larger than expected densities are called “scars” of the

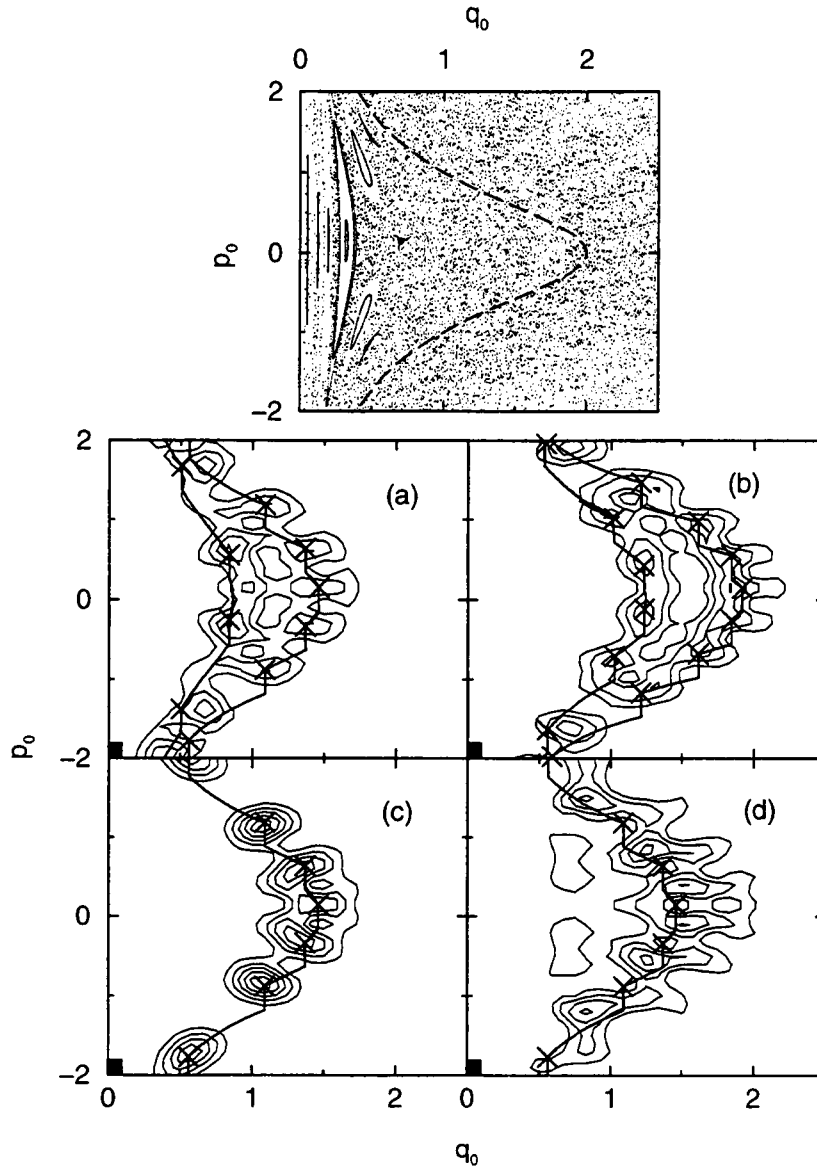


Figure 5.3: Poincaré map for $\Delta p_0 = -0.3$ and $\nu_0 = 16.8$ along with the initial manifold (dashed line) and Husimi distributions of the four dominant Floquet states of the same system with $n_i = 50$. Crosses are the unstable fixed points and the lines connecting them are the periodic orbits. For each figure, (a): Floquet state with $W_1(1000T) \simeq 0.0646$ and periodic orbit with $R_{fix} = 4/1$ and $7/1$, (b): $W_2(1000T) \simeq 0.0589$ and $R_{fix} = 6/1, 9/1$, (c): $W_2(1000T) \simeq 0.0507$ and $R_{fix} = 7/1$, and (d): $W_2(1000T) \simeq 0.0397$ and $R_{fix} = 7/1$ are plotted. Black squares at the lower left corner of each figure illustrates an area corresponding to the uncertainty $\hbar = 1/n_i$.

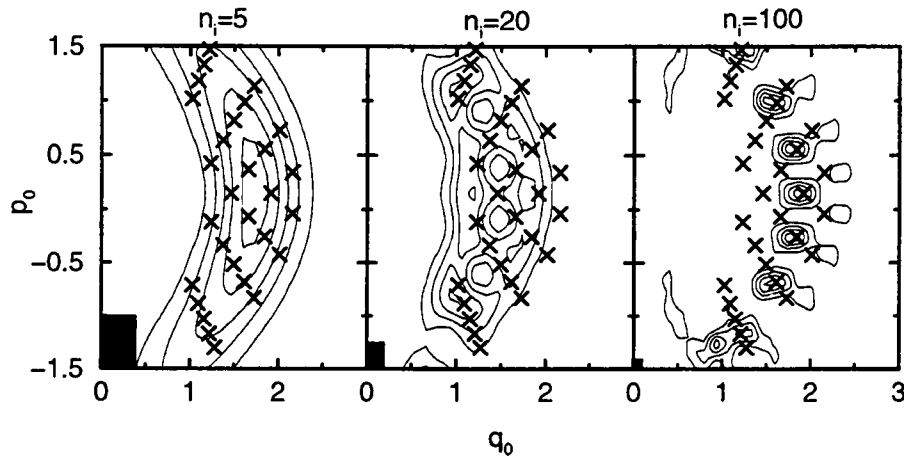


Figure 5.4: Husimi distributions of the dominant Floquet state for $\Delta p_0 = -0.3$, $\nu_0 = 16.8$, and different initial levels, $n_i = 5, 20$, and 100 . Crosses are unstable fixed points belonging to $R_{fix} = 6/1, 7/1, 8/1, 9/1$, and $10/1$. Black squares at the lower left corner of each figure illustrate an area corresponding to the uncertainty $\hbar = 1/n_i$.

wave functions or, in other words, each of these quantum states is called a “scarred wave function” [1]. In this figure, four Floquet states are chosen according to their expansion coefficients in the Floquet basis after $K = 1000$ kicks,

$$W_n(t = KT) = \left| c_n \exp \left(-\mathcal{E}_n^I KT \right) \right|^2. \quad (5.4)$$

When several fixed points are located within the quantum uncertainty, $\Delta r_0 \Delta p_0 \sim 1/n_i$, which is shown as a black square at the lower left corner of fig. 5.3, the Husimi distribution cannot resolve different fixed points belonging to different periodic orbits. This is the reason why different periodic orbits are visible in the same Floquet state ((a) and (b) in the figure). As n_i increases, each peak becomes more pronounced, and, finally, the different periodic orbits can be distinguished as the different Floquet state (fig. 5.4). Most of the stable Floquet states of the system correspond to the unstable periodic orbits which can be classified according to R_{fix} (chapter 2). However, there exists a rare kind of Floquet states which may or may not correspond to those classical

periodic orbits (see fig. 5.3 (d)). Instead of maximizing at the fixed points, these states are localized between the fixed points. At present, this type of localization is not fully understood.

The classical origin of the quantum localization of the system provides us with a useful tool for understanding some of the underlying physics. For example, the oscillatory behavior of the survival probability can be understood from the time evolution of the scarred wave function. During the time evolution, the electron hops around the fixed points, some of which have positive energy values (i.e. $H_{at} > 0$): e.g., three fixed points on the period-9 orbit have positive energy values. Initially, the electron has a large probability to be found near the outer turning point of the orbit at $p_0 \sim 0, q_0 \sim 2$ and acquires a negative average momentum due to the first kick. Every additional kick speeds up the electron and, therefore, excites it to a higher energy level even beyond the hydrogenic continuum threshold, i.e., $H_{at} = 0$. Eventually, the electron is scattered at the nucleus and acquires a positive momentum. Subsequently, each kick slows down the electron deexciting it to a lower energy level and eventually becoming a bound hydrogenic state once again. This hopping can be clearly observed in fig. 5.5, where the time evolution of the Husimi distribution is plotted for $n_i = 50$. Since the time evolution involves a coherent superposition of a few “stationary” Floquet states which are localized around several unstable periodic orbits, different frequencies are involved leading to spreading over phase space as seen in the figure for $K = 10$.

Positively kicked atom

As discussed before, the classical system becomes fully chaotic even for a small strength of the kick and, therefore, this is another interesting test case to examine quantum localization. Quantum localization for the positively kicked atom was found by Blümel for a small momentum transfer and a low frequency [14]. However, the origin of the localization was not understood. In the following, the case of a small positive Δp_0 and relatively high frequency $\nu_0 = 16.8$ is examined. The high frequency lowers the potential

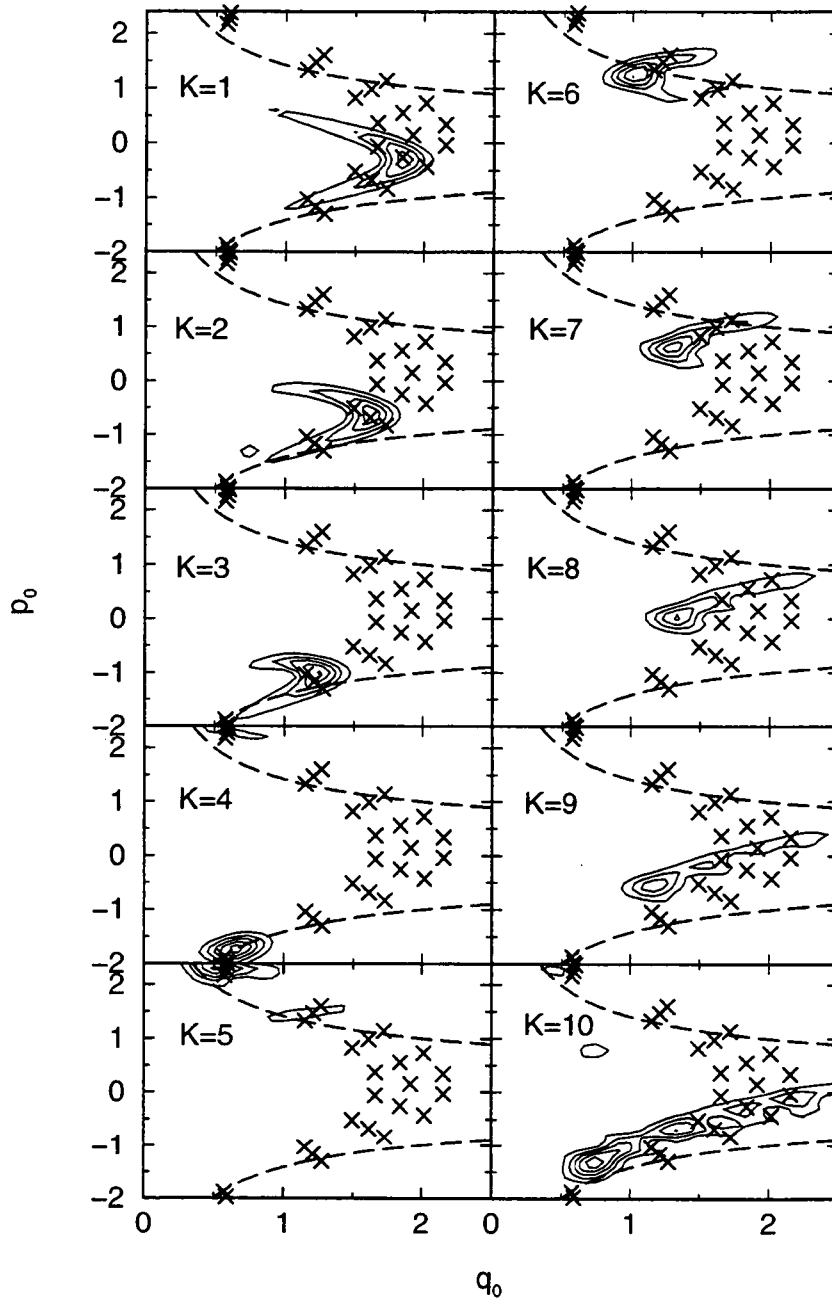


Figure 5.5: Time evolution of the Husimi distribution of the kicked atom system with $n_i = 50$, $\Delta p_0 = -0.3$, and $\nu_0 = 16.8$. Each figure is plotted right before the kick at $t = KT$. Crosses are the unstable fixed points belonging to $R_{fix} = 8/1, 9/1$ and $10/1$ and the dashed lines denote the ionization threshold, $H_{at} = 0$.

barrier $E_{\text{barrier}} = -2\sqrt{\Delta p/T} = -2\sqrt{\Delta p\nu}$ and makes the system even more unstable. In such a situation, however, it is shown that quantum localization can still be observed.

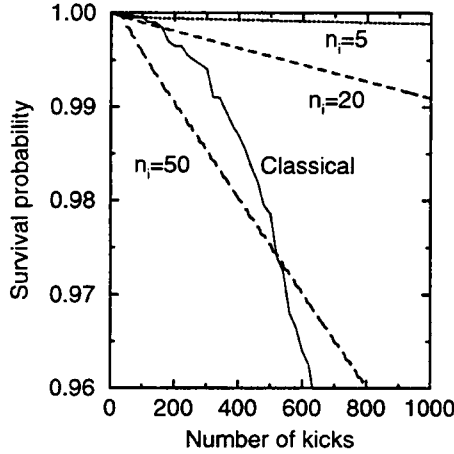


Figure 5.6: Survival probability of the kicked atom system with $\Delta p_0 = 0.01$ and $\nu_0 = 16.8$ as a function of K .

Fig. 5.6 shows the quantum survival probabilities as a function of K for $\Delta p_0 = 0.01$, $\nu_0 = 16.8$ and $n_i = 5, 20$, and 50 together with the classical result. All survival probabilities decay as a function of time but the quantum decay rates eventually become smaller than the classical one. This is considered as the onset of quantum localization. In contrast to the results for $\Delta p_0 < 0$ (fig. 5.2), the survival probability for $\Delta p_0 > 0$ does not exhibit any oscillatory structure. For $\Delta p < 0$, the oscillatory structure is caused by the hopping of the probability among the fixed points which are located in both hydrogenic bound and continuum states. As discussed in the section 2.3.4, however,

fixed points for $\Delta p > 0$ involve only bound states. Thus, even if the quantum probability hops among the fixed points, it is not expected to cause an oscillatory structure in the survival probability.

A more sensitive probe of the underlying dynamics is given by the recurrence probability, $P_{\text{rec}}(t)$, or self correlation function defined by the probability to be in the initial n_i level, e.g., quantum mechanically,

$$P_{\text{rec}}(t) = |\langle \psi(t=0) | \psi(t) \rangle|^2, \quad (5.5)$$

and classically,

$$P_{\text{rec}}^{\text{cl}}(t) = \int_{E_i - \Delta_i}^{E_i + \Delta_{i+1}} dE f(q, p, t) \quad (5.6)$$

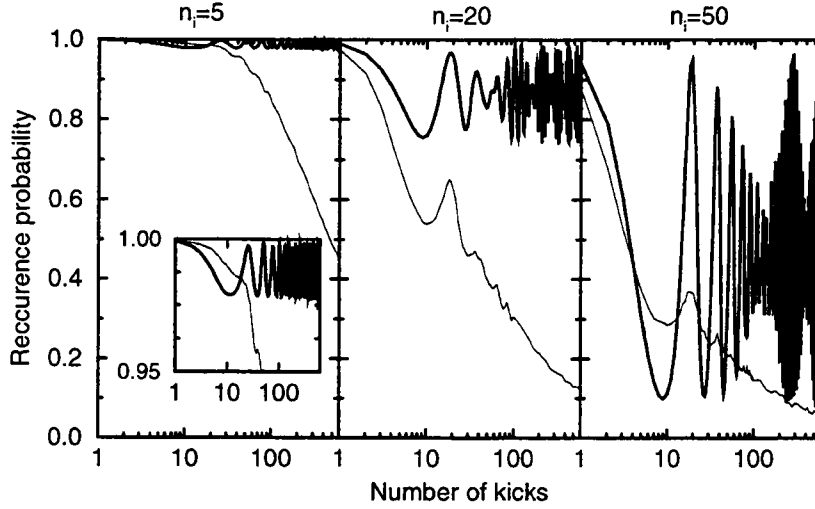


Figure 5.7: Recurrence probability as a function of K for $\Delta p_0 = 0.01$ and $\nu_0 = 16.8$. Thick lines are quantum results and thin ones are classical results.

where $f(q, p, t)$ is the classical state of the system (appendix A), $E_i = -1/2n_i^2$, and $\Delta_i = 1/4(n_{i-1})^2 - 1/4n_i^2$. Note that the recurrence probability is not classically scaling invariant because the quantum energy level spacing is taken into account. Remarkably, the quantum recurrence probability (fig. 5.7) is very large for long times compared with the classical probability. The correspondence between the frequency of the quantum recurrence probability and the frequency of unstable periodic orbits suggests that the latter could be the origin of the observed quantum localization phenomenon. This is confirmed in fig. 5.8 by the Husimi distributions of the dominant Floquet states which are localized around the unstable fixed points of the system. In this case, like in the case of the negatively kicked atom with $n_i = 5$, the fixed points are distributed very densely in phase space (fixed points with $R_{fix} = 15/1, 17/1$ and $19/1$ are plotted in the figure) compared to the uncertainty $1/n_i$ (black square at the lower left corner), and quantum mechanics cannot resolve all fixed points individually. Interestingly, different Floquet states are shifted from the initial torus in the same way as the periodic orbits.

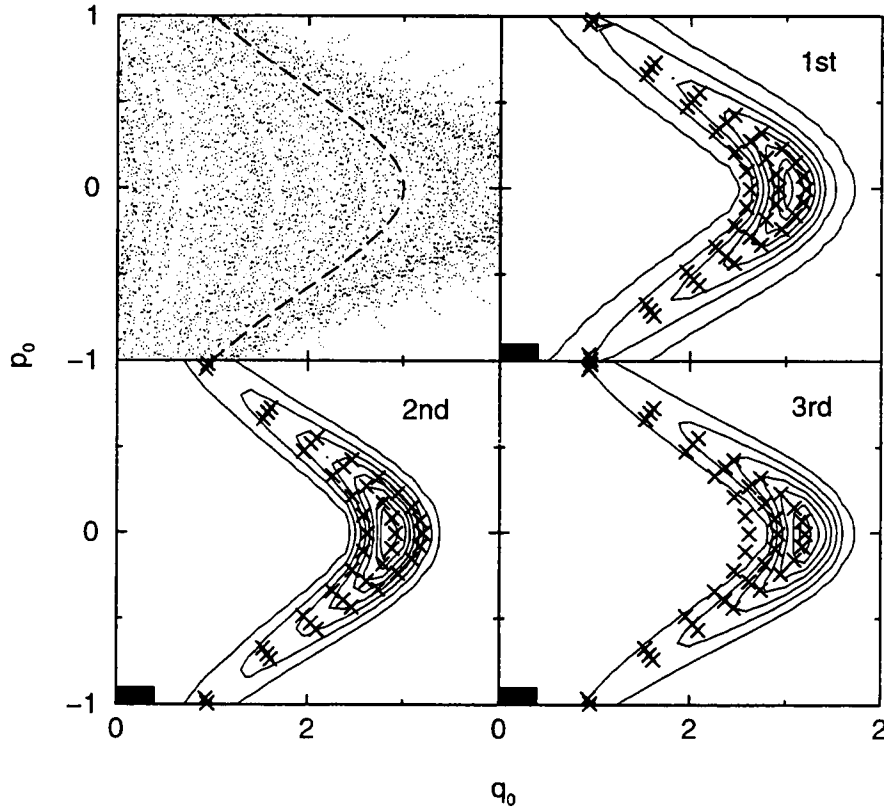


Figure 5.8: Poincaré map along with the initial torus (dashed line) and Husimi distributions of the three dominant Floquet states for the kicked atom with $n_i = 50$, $\Delta p_0 = 0.01$, and $\nu_0 = 16.8$. Crosses are the unstable fixed points with $R_{fix} = 15/1, 17/1$, and $19/1$.

Stark orbit and periodic orbit

Further analysis of the unstable periodic orbits for the present system indicates that they are in fact very similar to stable orbits of the Stark Hamiltonian (eq. (5.3)). Classically, the period of a Stark orbit which resembles a given periodic orbit is found to be very similar to the period of the unstable periodic orbit (fig. 5.9). Quantum mechanically, a great deal of the time evolution can be understood in terms of the Stark eigenvalues and eigenstates of the Stark Hamiltonian (eq. (5.3)). For example, the period of the unstable periodic orbit corresponds to the adjacent Stark level spacings near the Stark state, i.e. eigenstates of H_{Stark} (eq. (5.3)), that has the biggest overlap with a given Floquet state. Thus, the average field of the perturbation is found to play a very important role in the localization of the quantum system and unstable periodic orbits correspond to slightly perturbed Stark orbits.

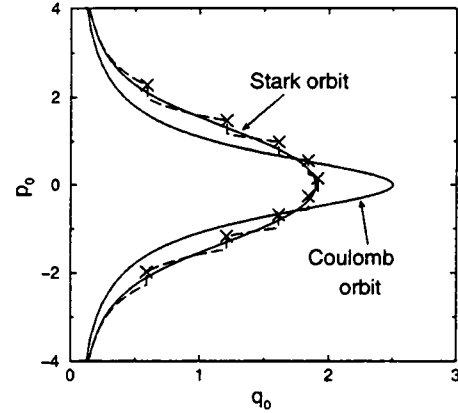


Figure 5.9: Stark orbit and Coulomb orbit together with the unstable periodic orbit (dashed line) and fixed points (crosses) with $R_{fix} = 9/1$. The parameters of the perturbation are $\Delta p_0 = -0.3$ and $\nu_0 = 16.8$. The energies of the Stark state and hydrogenic state are set to $E_0 = -2$ and $E_0 = -0.8$, respectively.

5.2 Localization in energy space

The periodically kicked atom shows two kinds of diffusive motion: "nonresonant diffusion" which is caused by the transition between neighboring states and is associated with classically chaotic diffusion, and "resonant diffusion" which is due to the transition between states whose energies are separated by the angular frequency of the perturbation. The suppression of these diffusion processes for the kicked rotor system and the microwave ionization problem has already been studied. These studies are introduced

in the next two subsections and the applicability to the kicked atom is discussed.

5.2.1 Suppression of nonresonant diffusion

In general, the suppression of classically chaotic nonresonant diffusion is associated with the discreteness of quasi-eigenenergy levels in quantum mechanics. An explanation of this suppression for the kicked rotor (eq. (1.3)) has been suggested by Fishman et al. [4] mathematically reducing the problem to the tight binding Anderson model.

The key point is that, since the sequence of kick strengths can be random, all the Floquet states $|\phi_{\mathcal{E}}^F\rangle$ with quasi-energies $\mathcal{E}$ become exponentially localized around some angular momentum $l_{\mathcal{E}}$ with the same localization length Δ_L [7],

$$\langle l|\phi_{\mathcal{E}}^F\rangle \sim \exp\left(-\frac{\tilde{\hbar}|l-l_{\mathcal{E}}|}{\Delta_L}\right). \quad (5.7)$$

Note that p_{θ} is quantized and it only takes values $p_{\theta} = \tilde{\hbar}l$, ($l = 0, 1, 2, \dots$). Floquet states with nearly identical quasi-energies are generally localized around centers which are far apart. On the other hand, two Floquet states localized at centers close compared with Δ_L have a quasi-energy separated by the spacing proportional to Δ_L^{-1} [7].

Using Floquet states, the time evolution of the kicked rotor can be expressed as

$$\langle l|\psi(t)\rangle = \sum_{\mathcal{E}} \langle \phi_{\mathcal{E}}^F|\psi(t=0)\rangle e^{-i\mathcal{E}t} \langle l|\phi_{\mathcal{E}}^F\rangle \quad (5.8)$$

If, for simplicity, we start with a well-localized state, $\langle l|\psi(t=0)\rangle = \delta_{l, l_{ini}}$, only Floquet states whose centers $l_{\mathcal{E}}$ are within an angular momentum range Δ_L of the initial level $\tilde{\hbar}l_{ini}$ contribute to the time evolution. Hence, the expected value of $(p_{\theta} - \tilde{\hbar}l_{ini})^2$ cannot become much larger than Δ_L^2 (fig. 1.2). The effective number of Floquet states contributing to the time evolution is $\Delta_L/\tilde{\hbar}$ and the corresponding quasi-energies are distributed in $[-\pi, \pi]$ since the eigenvalue of a Floquet state is $\exp(-i\mathcal{E})$ (note that in this units $T = 1$). Thus, the typical energy spacing becomes $\delta\mathcal{E} \sim 2\pi/(\Delta_L/\tilde{\hbar})$,

and the momentum diffuses until the uncertainty principle resolves this energy spacing at $t \simeq 2\pi/\delta\mathcal{E}$. In other words, the discrete quasi-energy spectrum makes the system quasi-periodic and suppresses the classical diffusion at the time $t \simeq 2\pi/\delta\mathcal{E}$ when the periodicity appears in the dynamics of the system. In the classical limit, i.e., $\hbar \rightarrow 0$, the time evolution involves an infinite number of Floquet states and the recurrence of the system never happens.

Much like for the kicked rotor, the numerical calculations for the kicked atom (fig. 5.10) show that the dominant Floquet states are localized (with some structures for $\Delta p_0 = -0.1$) in energy space with almost the same localization length but with different centers of localization. Note that the distributions in the figure are displayed in Stark energy space rather than in hydrogenic because more pronounced localization is observed, i.e., the unstable fixed points, which are the classical representation of a Floquet state, are located along one Stark state while they overlap with several Coulomb orbits (fig. 5.9). Because of the nature of the RPM, all dominant Floquet states are always localized in the finite basis set (P space). Floquet states which are not localized have finite imaginary parts of their quasi-energies and don't contribute to the long time evolution within the P space.

Fig. 5.11 displays the weighted probability density of the difference between an arbitrary pair of quasi-energies, $\delta\mathcal{E}_{ij}^R \equiv |\mathcal{E}_i^R - \mathcal{E}_j^R|$, i.e.

$$\frac{dP}{d(\delta\epsilon^R T)} = \frac{1}{\Delta\epsilon} \int_{\delta\epsilon^R}^{\delta\epsilon^R + \Delta\epsilon} \sum_{i \neq j}^N W_i(t) W_j(t) \delta(\delta\epsilon' - \delta\epsilon_{ij}^R) d(\delta\epsilon') \quad (5.9)$$

The quasi-energy spectrum of the kicked atom exhibits similar features to those of the kick rotor, i.e., the spectrum is discrete and quasi-periodic. Because of the quasi-periodicity, the probability density of $\delta\mathcal{E}^R T$ peaks at incommensurate frequencies and the peaks have a finite width. For $n_i = 1$, the probability density is well localized at $\delta\mathcal{E}^R T \simeq 2\pi/9$. In this case, one or two Floquet states mainly contribute to the time evolution and the system is periodic. As n_i increases, more peaks are visible and each

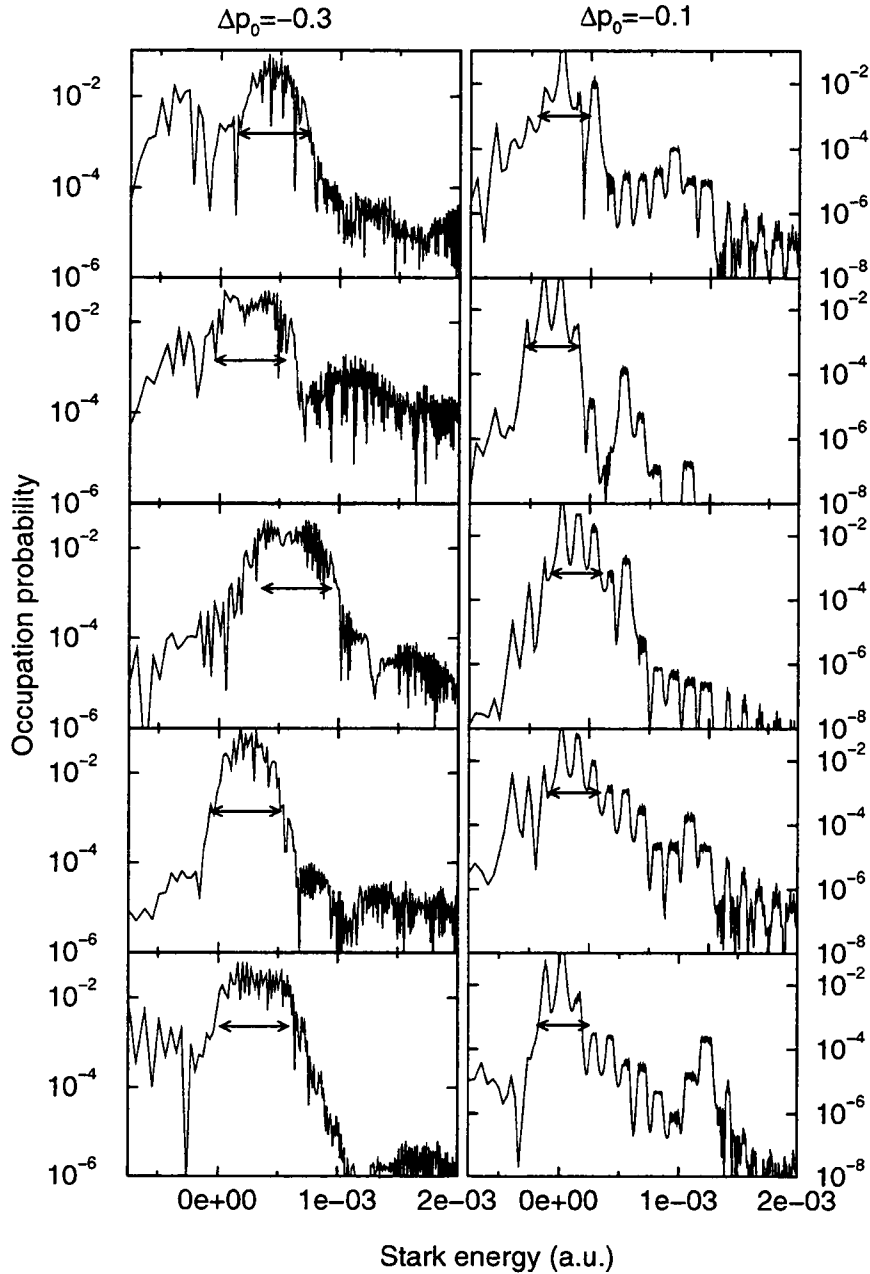


Figure 5.10: Stark energy distributions of the five dominant Floquet states of the kicked atom for $\Delta p_0 = -0.3$ and -0.1 , $\nu_0 = 16.8$, and $n_i = 50$. The figures are ordered according to the relative weight $W_n(t = 1000T)$ of the Floquet states from the top (most important) to the bottom (least important). Roughly estimated localization lengths are plotted as arrows (the length of the arrow is about $10\Delta_L$).

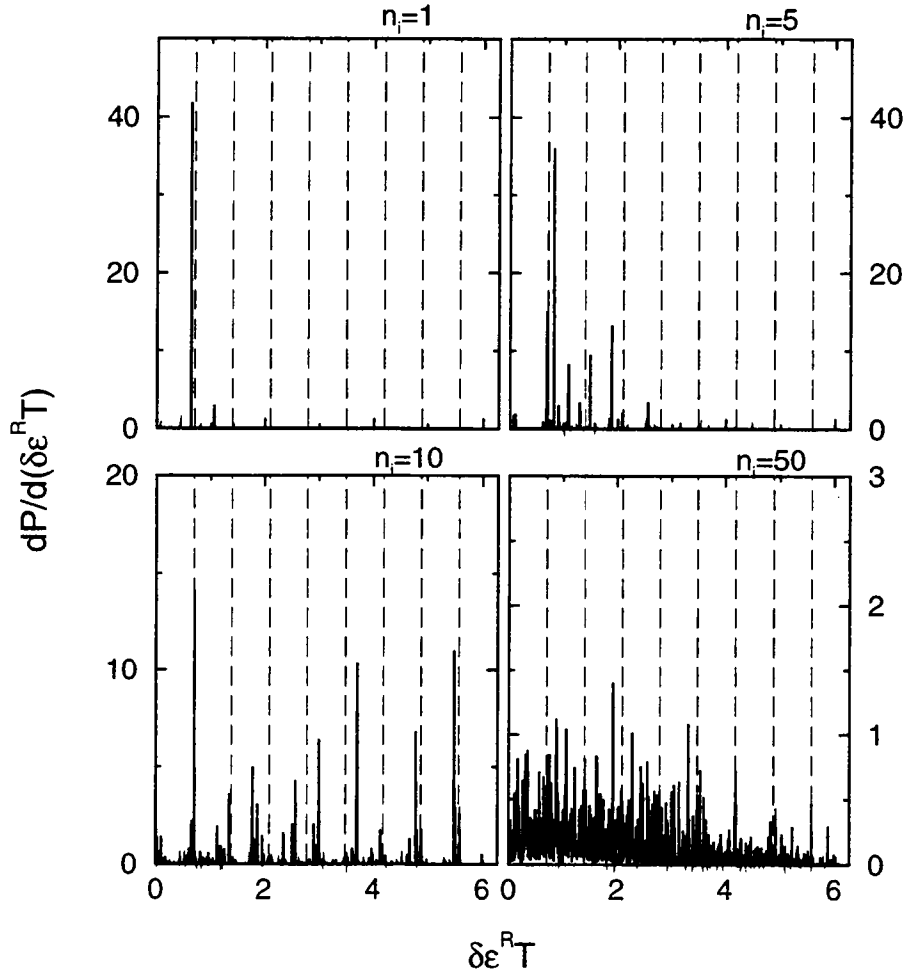


Figure 5.11: Weighted probability density $dP/d(\delta\mathcal{E}^R T)$ of the difference between an arbitrary pair of quasi-energies, $\delta\mathcal{E}^R T$ for the kicked atom system with $\Delta p_0 = -0.3$, $\nu_0 = 16.8$, and different initial states. Vertical dashed lines correspond to $\delta\mathcal{E}^R T = 2\pi m'/9$ ($m' = 1, 2, \dots, 8$).

peak acquires a width. In order to show the incommensurate nature of the spectrum, vertical lines are drawn at $\delta\mathcal{E}^RT = 2\pi m'/9$ ($m' = 1, 2, \dots, 8$). Clearly, more Floquet states contribute to the time evolution for increasing n_i and quantum dynamics starts to resolve several frequencies. As predicted for the kicked rotor, the typical quasi-energy difference $\delta\mathcal{E}^RT$ becomes smaller as $\hbar$ decreases, i.e., n_i increases in the kicked atom. This is consistent with the results in this figure.

Thus, we can apply the ideas for explaining the localization of the kicked rotor system to the kicked atom. Note, however, that we have not proven that the mathematical properties of the Floquet states are identical for both systems. For example, we have not provided a strict proof that all Floquet states are localized with the same localization length. This is beyond the scope of this thesis.

5.2.2 Suppression of resonant diffusion

When the frequency of the perturbation matches the energy difference between two levels, the transition probability becomes enhanced. Such resonant transitions could lead the diffusion in energy space. However, the non-linear behavior of energy levels (e.g. $E \sim n^{-2}$) leads to dephasing and suppresses resonant diffusion. A simple picture along these lines and based on a two-state model was introduced by Jensen et al. [10] to explain quantum localization for the Rydberg atom driven by a weak microwave field. The basic idea is that excitation occurs predominantly between resonant energy levels separated by one-photon energy ω , where $\omega = 2\pi\nu$ is the angular frequency of the perturbation. However, since quantum energy levels of the atom are discrete and their level spacing is not equidistant, the atom is excited to energy levels which are nearby the resonant energy levels. This quantum “detuning” suppresses the resonant excitation process and causes the quantum localization.

Assuming that the quantum detuning is randomly distributed around the resonant energy and in an interval given by the adjacent level spacing around the excited state, δE_1 , the average quasi-resonant excitation induced by a single harmonic with frequency

ω from a state $|0\rangle$ to a state $|1\rangle$, is given by [10]

$$P_{0 \rightarrow 1}^\omega = \frac{|F_{av}\langle 0|q|1\rangle|}{\delta E_1} \tan^{-1} \left[\frac{\delta E_1}{2|F_{av}\langle 0|q|1\rangle|} \right]. \quad (5.10)$$

For Rydberg atoms in a microwave field, this probability defines the localization length since it approximately acquires the same numerical value for different energy levels (e.g. $P_{0 \rightarrow 1}^\omega \sim P_{1 \rightarrow 2}^\omega$). Thus, the final energy distribution $\mathcal{D}(E)$ for that problem becomes exponentially localized in energy space, i.e.,

$$\mathcal{D}(E) \sim \exp \left(-2 \frac{|E - E_i|}{\omega l_{loc}} \right) \quad (5.11)$$

where E_i is the initial energy and l_{loc} is the localization length defined by

$$l_{loc} = -2 / \ln P_{0 \rightarrow 1}^\omega. \quad (5.12)$$

For the kicked atom, however, the resonant diffusion process is different. As mentioned before, the kicked atom is equivalent to the system of an atom in a DC field perturbed by a superposition of all higher harmonics (eq. (5.3)). Each harmonic term $\cos(2\pi m \nu t)$ induces resonant excitation from $|0\rangle$ to $|m\rangle$ ($m = 1, 2, \dots$). When this direct excitation becomes significant compared to the successive resonant excitation, $|0\rangle \rightarrow |1\rangle \rightarrow \dots \rightarrow |m\rangle$, the energy distribution is not exponentially localized.

5.2.3 Localization of the kicked atom

In the kicked atom, both resonant and nonresonant diffusions are clearly observed. In energy space, “nonresonant diffusion” appears as the diffusion around the initial state, and “resonant diffusion” copies the structure around the initial state onto states which are separated from the initial state in multiples of one-photon energy ω . The energy distribution of the system shows the mixture of these two effects in different ways depending on the control parameters, Δp_0 and ν_0 . Since the quantum localization was

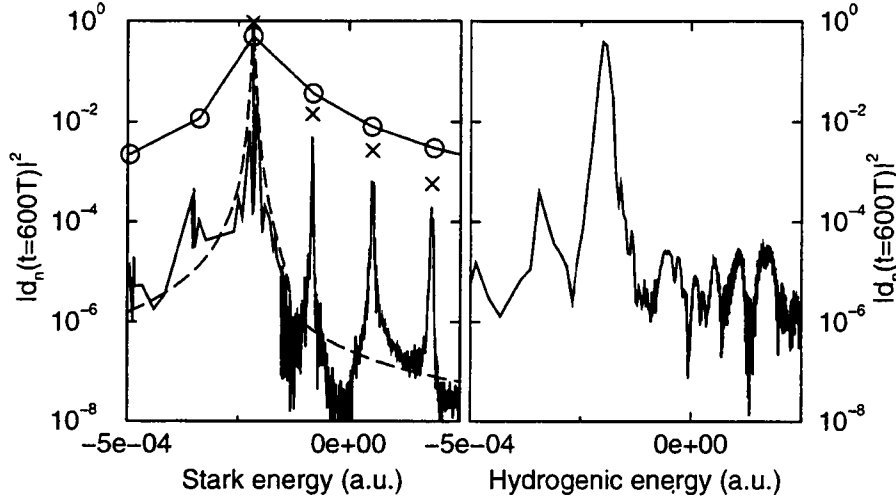


Figure 5.12: Energy distributions of the final state of the atom after application of 600 kicks with $n_i = 50$, $\nu_0 = 16.8$ and $\Delta p_0 = 0.01$. In the left graph, the atom is initially prepared in the Stark state $|0\rangle$ which has the largest overlap with the n_i hydrogenic level. The crosses are the time-averaged integrated probabilities of the resonant peaks. The solid lines with circles are the average excitation probabilities given by $P_{0 \rightarrow m}^{m\omega}$ such that the adjacent energy difference between circles is equal to ω . The dashed line is the dipole coupling strength $|\langle 0|q|\phi_n^{Stark}\rangle|^2$ in arbitrary units. In the right figure, the same energy distribution is plotted as a function of hydrogenic energy but with a hydrogenic initial state.

found for high scaled frequencies earlier in this chapter, we fix the scaled frequency to $\nu_0 = 16.8$ and focus on the dependence on the strength of the kicks.

Numerical results

Fig. 5.12 illustrates how the quantum kicked atom becomes localized in energy space. This figure displays the probability distribution of Stark (left) and hydrogenic (right) states which become populated after 600 kicks. That is, the square of the expansion coefficients $|d_n(t = 600T)|^2$ of the wave function in the Stark basis $|\phi_n^{Stark}\rangle$ or the

hydrogenic basis $|\phi_n^{hyd}\rangle$

$$|\psi(t = 600T)\rangle = \sum_{n=1}^{N_{max}} d_n(t = 600T) |\phi_n^\beta\rangle \quad (\beta = Stark \text{ or } hyd). \quad (5.13)$$

In order to obtain easily recognized structures, the initial distribution is chosen to be a well-localized distribution, i.e., the initial state is set to the hydrogenic state $n_i = 50$ for the hydrogenic basis, and, for the Stark basis, to the Stark state $|0\rangle$ which has the biggest overlap with the hydrogenic state with $n_i = 50$. In the left figure, the energy of the initial state can be recognized by the maximum of the dipole coupling strength, $|\langle 0|q|\phi_n^{Stark}\rangle|^2$, which is also depicted as a dashed line in the figure. Choosing a Stark basis has the effect of sharpening the observed structures since unstable periodic orbits which closely resemble Stark states (fig. 5.9). This can be confirmed by comparing the two energy distributions in the figure.

For this small momentum transfer, the energy distribution exhibits clear resonant excitation peaks at the Stark states $|m\rangle$ which are separated from the initial state, $|0\rangle$, in a multiple of the driving frequency, $E_m - E_0 = m\omega$. In the case of strong perturbations (fig. 5.13), on the other hand, nonresonant diffusion dominates the dynamics of the system and each peak has a very broad width. Therefore, the resonant peaks merge and well defined structures are destroyed. Moreover, an additional quasi-regular pattern with an energy spacing that is smaller than the resonant spacing appears. This pattern is associated with the hopping of the probability among the Stark energy levels associated with the unstable fixed points which overlap the initial state (i.e., much like for the oscillatory behavior of the survival probability in fig. 5.2). The correspondence between the quasi-regular pattern and the Stark energy levels is more clearly observed in the energy distribution of the Floquet state since all peaks in this quasi-regular pattern have almost the same probability (fig. 5.14).

To numerically evaluate the suppression of classical diffusion, it is necessary to define the localization length of the energy distribution. As discussed before, the localization

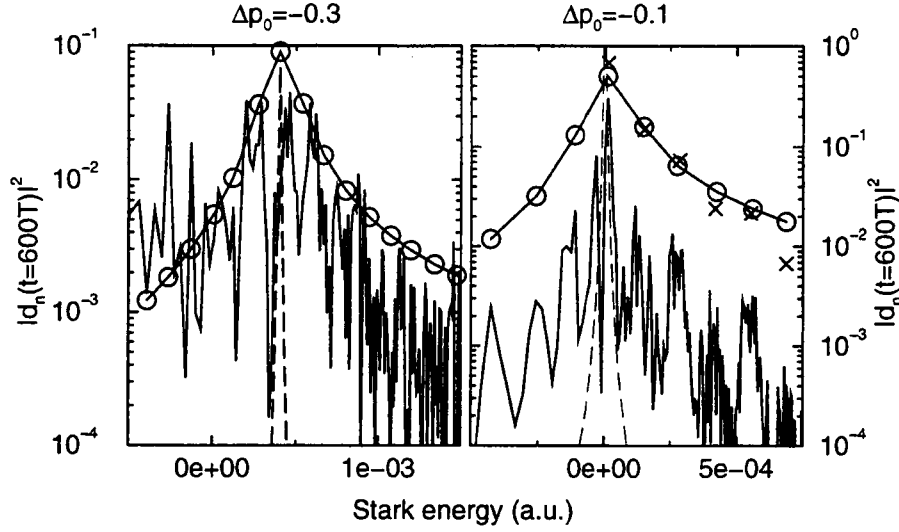


Figure 5.13: Same as fig. 5.12 but with momentum transfers $\Delta p_0 = -0.3$ (left) and -0.1 (right).

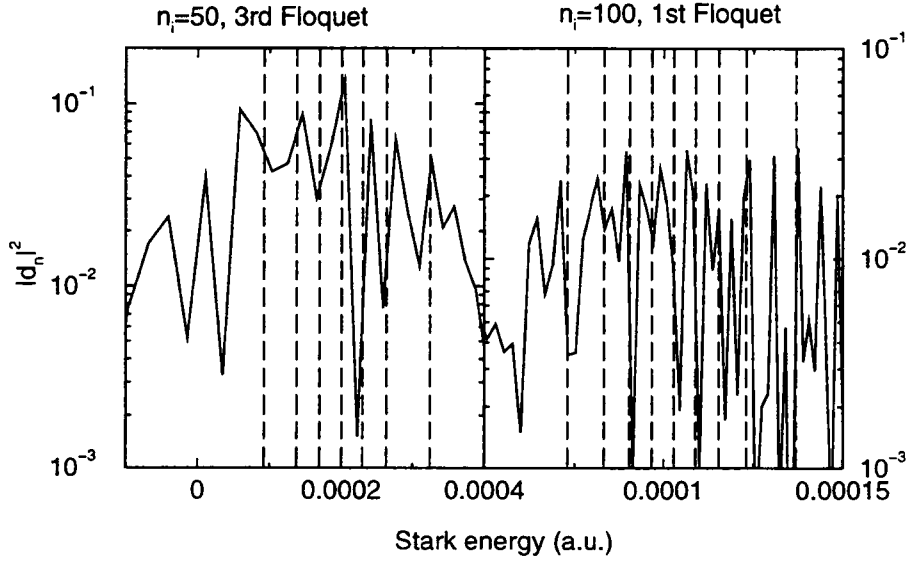


Figure 5.14: Energy distributions of the Floquet states (solid line) and energy levels of the unstable fixed points (vertical dashed line). The strength of the kicks is $\Delta p_0 = -0.3$ and the frequency is $\nu_0 = 16.8$. For $n_i = 50$, the corresponding unstable fixed points belongs to the periodic orbit with $R_{fix} = 7/1$ (fig. 5.3(c)) and, for $n_i = 100$, with $R_{fix} = 9/1$ (fig. 5.4).

length is related to the number of effective Floquet states contributing to the time evolution. Therefore, the localization length plays a very important role for the suppression of classical diffusion. Since there are two kinds of diffusion observed in the kicked atom, two localization lengths are defined, one for each diffusion; the localization length within the dominant peak (nonresonant diffusion) and the one involving all resonant peaks (resonant diffusion). In the following the main factors which define these two localization lengths is discussed.

Decay rate of nonresonant diffusion

Since nonresonant diffusion is the result of the transition to the neighboring energy levels, the dipole coupling $\langle \phi_n^{Stark} | q | \phi_{init}^{Stark} \rangle$ controls the localization length within a peak. For $\Delta p_0 = 0.01$, resonant peaks are well-separated from another, and the localization structure within a peak is clearly displayed. In fig. 5.12, we can see that the distribution almost mimics the decay rate of the direct dipole coupling strength (dashed line). As Δp_0 increases, the quasi-regular pattern associated with unstable fixed points (fig. 5.14) starts to appear, and the structure within one resonant peak is divided into several peaks. For $\Delta p_0 = -0.1$ (the right figure in fig. 5.13), we can still see one main peak whose localization length agrees with the dipole coupling strength. However, for $\Delta p_0 = -0.3$, several peaks appear clearly and different localization structures cannot be distinguished. Note that each peak in this quasi-regular pattern may mimic the dipole coupling strength but, since there are not enough energy levels within a peak, the localization length cannot be defined in this case.

Decay rate of the resonant peaks

In the microwave system with a weak field, it was reported that the energy distribution of the final state became stationary and the height of each resonant peak was exponentially decaying with energy from the initial energy level [10]. In the kicked atom, however, an

infinite number of harmonic terms (eq. (5.1)) change the resonant excitation mechanism, and different localization structures in the final energy distribution can be expected.

The field F_{av} used in the kicked atom is so strong compared to the field in the microwave problem [10] that it induces relatively strong couplings between neighboring states. As a result, it accelerates the nonresonant diffusion and broadens each peak. This nonresonant diffusion and the quantum suppression of this diffusion deform the structure within a peak and the height of the peak is not stationary. The height of the main peak at the initial energy level is in fact identical to the recurrence probability (eq. (5.5)) depicted in fig. 5.7. Note, however, that for a Stark initial state, the amplitude of the oscillation becomes much smaller than that in fig. 5.7 but the oscillation can still be observed.

Thus, it is necessary to introduce some form of time averaging to measure the localization length of the system. The integrated probability within each peak, i.e., the area of the peak, is plotted as a function of K in fig. 5.15. For $\Delta p_0 = 0.01$, a relatively stable distribution as a function of time is obtained. However, for $\Delta p_0 = -0.1$, an oscillatory structure is clearly visible. Thus, in order to obtain a stationary result for the calculation of the localization length, we take the time average over a period of the oscillation.

The averaged peak areas, which are depicted as crosses in fig. 5.12 and 5.13, are seen to decay less rapidly than exponentially with increasing Stark energy. This happens because the peaks are predominantly due to a direct coupling from the initial state through the high harmonics of the perturbation: e.g. $P_{0 \rightarrow 2}^{2\omega} \gg P_{0 \rightarrow 1}^{\omega} P_{1 \rightarrow 2}^{\omega}$. This is confirmed by the fact that the resonant peak structure appears even after two kicks, which is much shorter than the time for which significant successive transitions from $|0\rangle$ to $|m\rangle$ levels are expected (fig. 5.16). In addition, even when the resonant structure disappears for strong momentum transfers ($\Delta p_0 = -0.3$) the overall structure still follows the averaged two-state excitation probabilities (fig. 5.13).

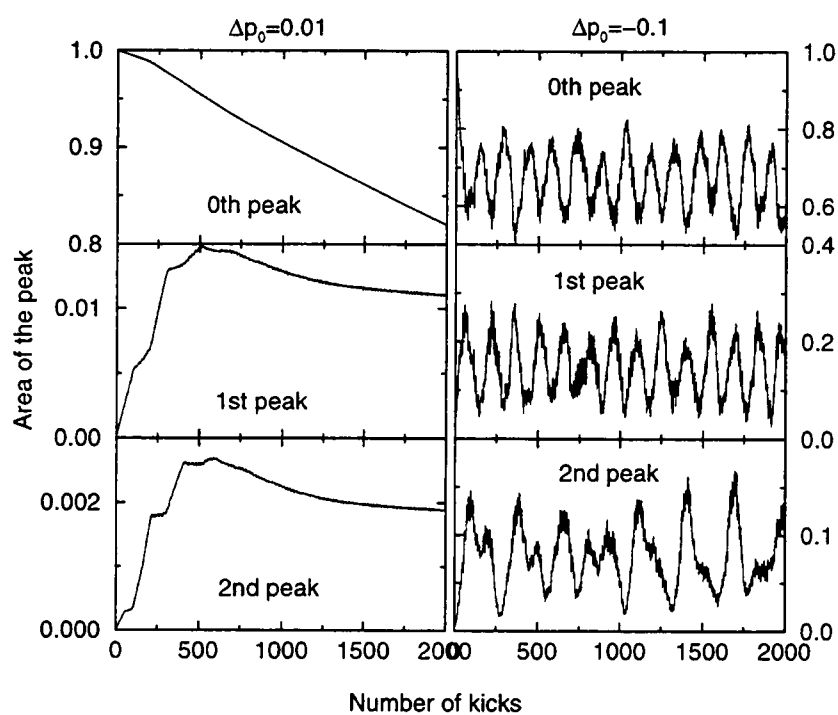


Figure 5.15: Integrated probability within a peak as a function of K . The frequency of the perturbation is $\nu_0 = 16.8$ and the initial state is a Stark state which has the largest overlap with a hydrogenic state $n_i = 50$.

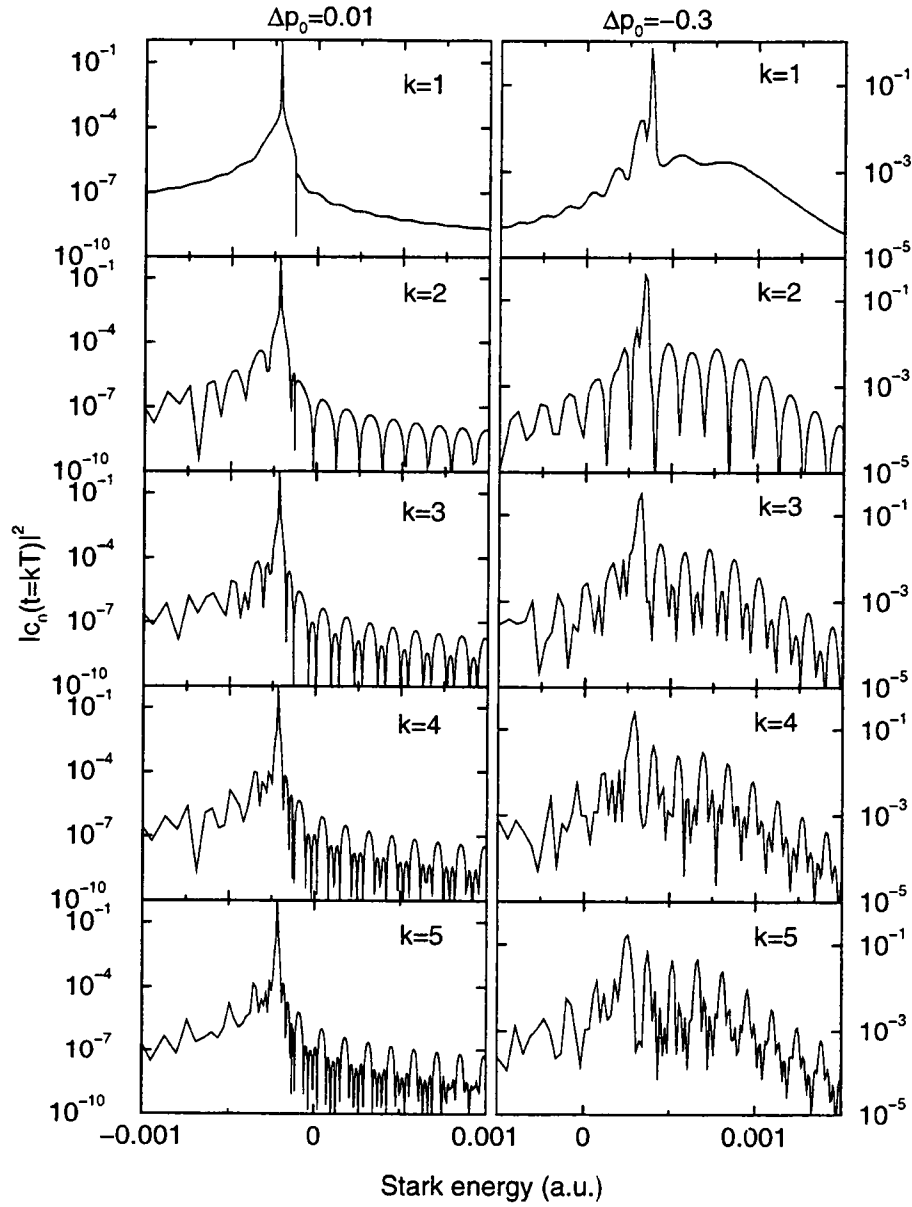


Figure 5.16: Time evolution of the Stark energy distribution with $n_i = 50$, $\nu_0 = 16.8$ and different strengths of the kicks.

Chapter 6

Conclusions and outlook

In this thesis, the dynamical properties of the periodically kicked atom have been analyzed focusing on classical-quantum correspondence. In the limit of large quantum numbers, a very clear correspondence between the classical and the quantum phase space properties of the system has been established. When the classical phase space is characterized by sizeable stable islands, the quantum system has been found to be localized within these islands. In turn, when the classical phase space is chaotic, the quantum system has been found to be localized around the unstable periodic orbits of the system (i.e. scarred wave functions). Still, many technical and fundamental questions remain unresolved.

A numerical method to solve the Schrödinger equation called the “RPM” has been developed by adapting the idea of the masking method to a pseudo-atomic basis of Sturmian wave functions. This method has played a crucial role in the determination of the localized nature of the quantum system. However, the finiteness of the basis size sets a limit for this method. The subspace P is expanded very slowly even when the basis size increases by a big amount: e.g., the limit in the energy space is $E_{max} = 0.8$ (scaled units) with basis sizes $N = 500$ and $M = 700$, and $E_{max} = 1$ with $N = 1500$ and $M = 1800$. Clearly, in order to study quantum stabilization for longer times, the

dynamics for lower frequencies, or the 3D kicked atom, a new method needs to be developed. Semiclassical methods may be useful for these purposes.

The Floquet states of the kicked atom have been shown to have similar properties to those of the kicked rotor system. Thus, an analogy between the quantum localization of the kicked atom and the Anderson localization model has been drawn. However, further work is needed to fully understand this quantum localization phenomenon. One possible avenue would be to establish a precise relation between the quantum localization of the kicked atom and the Anderson localization model. Alternatively, a different approach can be suggested based on classically chaotic orbits and the quantum uncertainty in the following way.

Consider a system whose Poincaré map shows a fully developed chaotic sea (fig. 6.1). Suppose that we take an initial condition, point A , in this chaotic sea. The sequence of points associated with the classical time evolution of the particle are distributed randomly in phase space. Because of this randomness, there is a possibility that, after a time period jT , the particle comes back to a point B which is within an area of the size of the quantum uncertainty $\hbar$ from the initial condition A (if the system is ergodic, this surely happens after a long enough period of time). In quantum

mechanics, the difference between A and B cannot be distinguished because of the uncertainty principle. Therefore, the time evolution following B becomes identical to the trajectory that originated from A . If a measurable area of points comes back to the initial “quantum” location at the same time, the quantum system acquires a quasi-periodicity which is not seen in the classical system.

When the point A is near the unstable manifold of a fixed point (fig. 2.13), the particle quickly goes away from the fixed point but may be trapped and returned to the

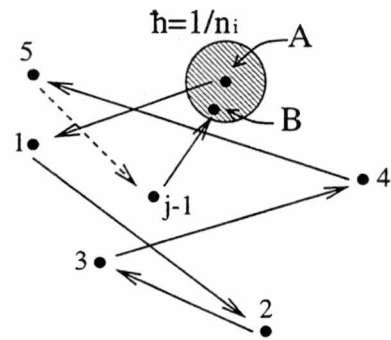


Figure 6.1: Schematic picture of a trajectory with the non-classical periodicity

original location at a later time by the stable manifold. More importantly, if A is close to the fixed point, the particle hops around in close proximity to a periodic orbit. In fact, a measurable area of points which are near the fixed point come back to its original location (within the quantum uncertainty) after the period of the periodic orbit. The value of this area of recurring initial points is determined by the decay rate (Lyapunov exponent) at the fixed point. This is the reason why the existence of scarred wave functions depends on the ratio of the classical decay rate to the quantum uncertainty [1].

It would be interesting to confront this intuitive picture of quantum localization with results of numerical simulations. One possibility would be to follow "quantum trajectories" in phase space as has recently been proposed by L. Kaplan et al. [48] to understand scarred wave functions for the billiard problem. The basic idea would be to follow the time evolution of a minimum uncertainty Gaussian wavepacket which is initially localized at a fixed point in phase space.

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Appendix

Appendix A

Classical trajectory Monte Carlo method

In the classical limit, the time evolution of the electronic wave function is modeled using an ensemble of classical particles that mimics the initial quantum state. That is, the quantum wave function, $\psi(\mathbf{r}, t)$, is replaced by a classical probability density in phase space, $f(\mathbf{r}, \mathbf{p}, t)$. Formally, the time evolution of this density is governed by the classical Liouville equation for the Hamiltonian $H(t)$,

$$\frac{\partial f}{\partial t} = [H, f] \quad (\text{A.1})$$

with the boundary condition

$$f(\mathbf{r}, \mathbf{p}, t) \xrightarrow[t \rightarrow 0]{} f_i(\mathbf{r}, \mathbf{p}) . \quad (\text{A.2})$$

where $[,]$ denotes a Poisson bracket and f_i is the initial state. Since phase space points evolve in time independently, the Liouville equation can be easily solved using a Monte Carlo technique which calculates the time evolution of a randomly chosen sample of the initial state. This method is usually referred to as the classical trajectory Monte Carlo

(CTMC) approach [49].

There exists no unique way of determining an initial phase space state that exactly mimics the initial quantum state. The most common choice of initial states, which we adopt here, is a subset of a microcanonical ensemble

$$f_i(\mathbf{r}, \mathbf{p}) = C_i \delta \left[E_i - \frac{p^2}{2} - V_{at}(r) \right] \mathcal{U}_i \quad (\text{A.3})$$

where C_i is a normalization constant, E_i is the initial quantum mechanical binding energy, and $\mathcal{U}_i$ is a characteristic function representing the other quantum numbers of the initial state. This type of initial state yields the exact quantum mechanical probability density of the momentum for a statistical average of states within a given n manifold.

For a 3-D hydrogenic initial spherical state $|n_i, l_i, m_i\rangle$,

$$\mathcal{U}_{l_i, m_i} = \Theta(L - l_i) \Theta(l_i + 1 - L) \Theta \left(L_z - \frac{L(2m_i - 1)}{2l_i + 1} \right) \Theta \left(\frac{L(2m_i + 1)}{2l_i + 1} - L_z \right) \quad (\text{A.4})$$

where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the classical angular momentum and Θ denotes a step function. In turn, for a hydrogenic parabolic state with quantum numbers n_i, n_{1i}, n_{2i} , we use

$$\begin{aligned} \mathcal{U}_{n_{1i}, n_{2i}} &= \Theta \left(N_1^c - n_{1i} + \frac{1}{2} \right) \Theta \left(-N_1^c + n_{1i} - \frac{1}{2} \right) \\ &\quad \times \Theta \left(N_2^c - n_{2i} + \frac{1}{2} \right) \Theta \left(-N_2^c + n_{2i} - \frac{1}{2} \right) \end{aligned} \quad (\text{A.5})$$

$$N_{1,2}^c = \frac{1}{2} [n_i (1 \mp A_z) - (|L_z| + 1)] \quad (\text{A.6})$$

where $\mathbf{A} = \mathbf{p} \times \mathbf{L} - \hat{\mathbf{r}}$ is the Runge-Lenz vector.

For the 1-D atom, $\mathcal{U}_i = 1$, i.e.,

$$f_i(q, p) = C_i \delta \left[E_i - \frac{p^2}{2} - V_{at}(q) \right]. \quad (\text{A.7})$$

Appendix B

Classical scaling invariance

In classical mechanics, the motion of the planet around the sun and the motion of an electron around the nucleus have same dynamical properties and, by proper scaling, both motions become identical. This is called scaling invariance which is a unique feature of classical mechanics for a particular group of interactions and one of the measures which distinguishes classical mechanics from quantum mechanics.

The dynamics of a classical particle is governed by the Hamilton's equations,

$$\begin{aligned}\frac{d\mathbf{r}}{dt} &= \frac{\partial H(\mathbf{r}, \mathbf{p}, t)}{\partial \mathbf{p}} \\ \frac{d\mathbf{p}}{dt} &= -\frac{\partial H(\mathbf{r}, \mathbf{p}, t)}{\partial \mathbf{r}}\end{aligned}\tag{B.1}$$

Using the scaling transformation

$$\begin{aligned}r_0 &= \frac{r}{n_i^2} \\ p_0 &= p n_i \\ t_0 &= \frac{t}{n_i^3},\end{aligned}\tag{B.2}$$

the Hamiltonian for the kicked atom is scaled into

$$\begin{aligned}
 H(\mathbf{r}, \mathbf{p}, t) &= \frac{p^2}{2} - \frac{1}{r} - z\Delta p \sum_k \delta(t - kT) \\
 &= \frac{p_0^2}{2n^2} - \frac{1}{r_0 n^2} - n^2 z_0 \frac{\Delta p_0}{n} \sum_k \frac{1}{n^3} \delta(t_0 - kT_0) \\
 &= \frac{1}{n^2} H(\mathbf{r}_0, \mathbf{p}_0, t_0).
 \end{aligned} \tag{B.3}$$

Therefore, the Hamilton's equations become

$$\begin{aligned}
 \frac{d\mathbf{r}}{dt} &= \frac{1}{n} \frac{\partial H(\mathbf{r}_0, \mathbf{p}_0, t_0)}{\partial \mathbf{p}_0} \\
 &= \frac{d\mathbf{r}_0}{dt_0} \frac{n^2}{n^3} \\
 \frac{d\mathbf{p}}{dt} &= -\frac{1}{n^4} \frac{\partial H(\mathbf{r}_0, \mathbf{p}_0, t_0)}{\partial \mathbf{r}_0} \\
 &= \frac{d\mathbf{p}_0}{dt_0} \frac{n}{n^3}.
 \end{aligned} \tag{B.4}$$

Since these dynamical equations are also scaled by the time-independent factor, the solution $(\mathbf{r}(t), \mathbf{p}(t))$ can be scaled into $(n^2 \mathbf{r}_0(t_0), n^{-1} \mathbf{p}_0(t_0))$. Thus the classical dynamics of two different initial conditions, $(\mathbf{r}_1(0), \mathbf{p}_1(0))$ and $(\mathbf{r}_2(0), \mathbf{p}_2(0))$, become identical after scaling.

In this thesis, the scaling parameter n is chosen as the initial n level of the electron ($n = 1/\sqrt{-2E}$). The following scaled variables are used throughout

$$\begin{aligned}
 \mathbf{r}_0 &= \frac{\mathbf{r}}{n^2} \quad (q_0 = \frac{q}{n^2}, \text{ for the 1-D system}) \\
 \mathbf{p}_0 &= \mathbf{p}n \quad (p_0 = pn, \text{ for the 1-D system}) \\
 \Delta \mathbf{p}_0 &= \Delta \mathbf{p}n \quad (\Delta p_0 = \Delta pn, \text{ for the 1-D system}) \\
 t_0 &= \frac{t}{2\pi n^3} \\
 T_0 &= \frac{T}{2\pi n^3}
 \end{aligned}$$

$$\begin{aligned}\nu_0 &= \nu 2\pi n^3 = \frac{1}{T_0} \\ \omega_0 &= \omega n^3 \\ E_0 &= E n^2.\end{aligned}$$

Note that an irrelevant factor of 2π has been added to the time scaling. For the kicked atom, the scaling invariance implies, for example, that 1-D Poincaré maps are only a function of the variables Δp_0 , ν_0 , p_0 , and q_0 (i.e. they are independent of n). Similarly the ionization probability of an atom in a give n level is only a function of ν_0 and Δp_0 . In turn, quantum mechanics is not scaling invariant. Thus, departures from this scaling provide a clear evidence of quantum dynamics.

Appendix C

Classical Coulomb map

Consider the initial phase space coordinates (q_{k-1}, p_{k-1}) which become (q_k, p_k) after the time evolution in a period T . Using the parametric form of Coulomb orbits [50] the Coulomb mapping M_{Coul} for $E_k = H_{at}(q_k, p_k) < 0$ is given by a set of implicit equations:

$$\begin{aligned} q_{k-1} &= n_k^2(1 - \epsilon_k \cos \xi_{k-1}) \\ p_{k-1} &= \frac{n_k}{q_{k-1}} \epsilon_k \sin \xi_{k-1} \\ t_{k-1} &= n_k^3 \xi_{k-1} - \epsilon_k \sin \xi_{k-1} \\ t_k &= t_{k-1} + T = n_k^3 \xi_k - \epsilon_k \sin \xi_k \\ q_k &= n_k^2(1 - \epsilon_k \cos \xi_k) \\ p_k &= \frac{n_k}{q_k} \epsilon_k \sin \xi_k \end{aligned} \tag{C.1}$$

where $n_k = (2|E_k|)^{-1/2}$ is the classical principal action (directly related to the principal quantum number) and $\epsilon_k = \sqrt{1 + 2E_k\Lambda^2} = 1$ is the eccentricity. For $E_k > 0$, M_{Coul} becomes correspondingly

$$q_{k-1} = n_k^2(\epsilon_k \cosh \xi_{k-1} - 1)$$

$$\begin{aligned}p_{k-1} &= \frac{n_k}{q_{k-1}} \epsilon_k \sinh \xi_{k-1} \\t_{k-1} &= n_k^3 \epsilon_k \sinh \xi_{k-1} - \xi_{k-1} \\t_k &= t_{k-1} + T = n_k^3 \epsilon_k \sinh \xi_k - \xi_k \\q_k &= n_k^2 (\epsilon_k \cosh \xi_k - 1) \\p_k &= \frac{n_k}{q_k} \epsilon_k \sinh \xi_k\end{aligned}\tag{C.2}$$

Appendix D

Kicked atom with a finite width HCP

It has been observed in fig. 2.2 that the finite width of a HCP enhances the stability of the kicked atom. In addition, it has been already proved that the stability of the kicked atom is also sensitive to the shape of each HCP [22]. This pulse shape dependence of the stability of the atom is critical when the theoretical and the experimental results are compared especially for $T_{p0} \gtrsim 1$. These facts are in this appendix explained by looking at the 10% ionization threshold of the 3-D atom subject to one HCP with different pulse shapes. Note that all calculations are performed for relatively low quantum numbers and short interaction times, which makes 3-D calculations possible.

Fig. D.1 displays the scaled momentum transfer (left) and the scaled peak field (right) for 10% ionization of Rydberg atoms as a function of the scaled pulse width T_{p0} . This figure shows that a HCP becomes equivalent to a kick when $T_{p0} \lesssim 0.1$ and that the ionization threshold is scaling invariant. Moreover, it is clearly observed that a small momentum transfer is necessary for ionizing the atom in the short pulse limit, $T_{p0} \rightarrow 0$. This indicates that the kicked atom subject to a delta-shaped pulse is more unstable than the one subject to a finite width pulse. For $T_{p0} > 1$, i.e., when the

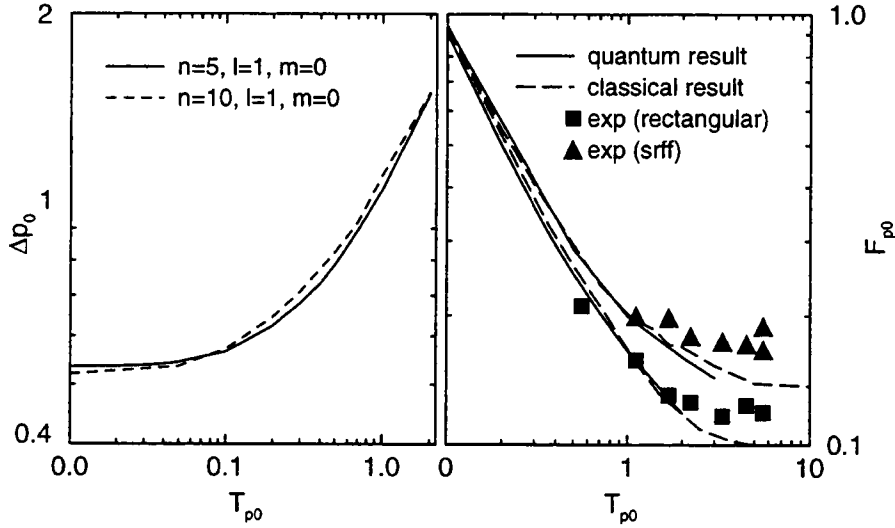


Figure D.1: Scaled momentum transfer (left) and scaled peak field (right) for 10% ionization of Rydberg atoms as a function of the scaled pulse width. In the right figure, different pulse shapes are used, which are illustrated in fig. D.2 [22].

rise time is large compared to the orbital period, quantum states evolve approximately adiabatically, which leads to an increased stability against stabilization. In contrast, a HCP with a sudden turn-on dynamically couples the initial state to other n levels, which can be ionized more easily than the adiabatically shifted state. The pulse shape dependence of the ionization threshold can be seen in the right figure. The rectangular pulse has a short rise time and a fast fall-off (left figure in fig. D.2). In turn, the chirped pulse has a slow rise and a fast fall-off (srff). This difference of the rise time changes the ionization process of the atom. Note that the momentum transfers for different pulse shapes are identical with a fixed T_{p0} and F_{p0} . Obviously, for a fixed T_{p0} , the atom subject to a rectangular pulse is more unstable than the one subject to a srff pulse. The narrow avoided crossing between different Stark states due to the nonhydrogenic core in the alkali-metal atoms do not play a significant role when $T_{p0} \sim 1$. This is verified by the fact that the hydrogen and alkali-metal atoms indicate the same rise-time dependence [22]. However, there is another type of avoided crossing, sometimes termed “hidden”

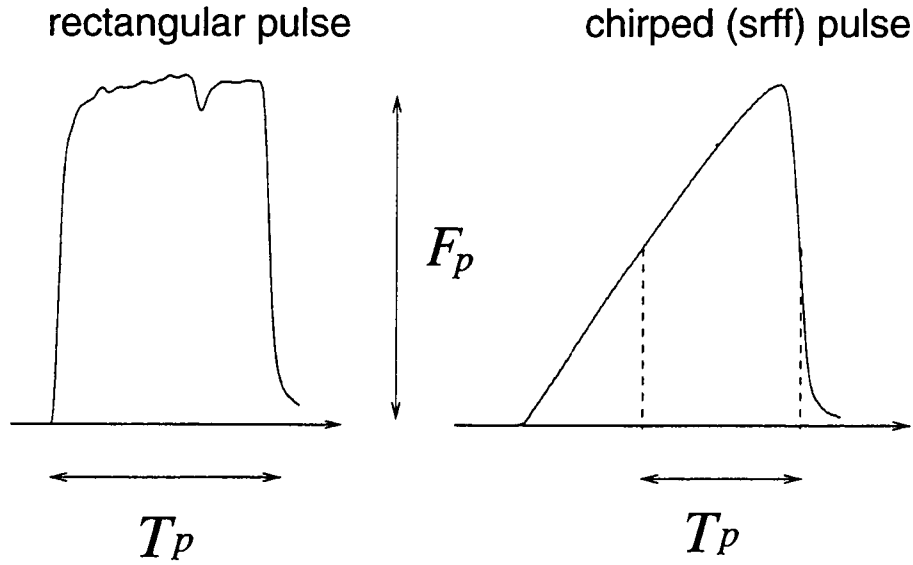


Figure D.2: HCP with two different pulse shapes.

crossing [51]. It corresponds to an interaction between the most red-shifted Stark states of adjacent manifolds and is characterized by a width that is a considerable fraction of the zero-field level spacing. Translated into classical dynamics, this amounts to a time scale of a few zero-field orbital periods. The observed rise-time dependence is related to the inverse level density of resonances near and above the ionization threshold.

Appendix E

Sturmian wave functions

A Sturmian basis set [31] is defined by the complete set of functions obeying

$$\left(\frac{p^2}{2} - \frac{n/n_S}{r}\right) |\tilde{\phi}^S\rangle = -\frac{1}{2n_S^2} |\tilde{\phi}^S\rangle \quad (\text{E.1})$$

where $n = 1, 2, \dots, \infty$ and n_S is a Sturmian parameter. In general, this parameter can be taken to be a complex number [32, 33]. Eq. (E.1) is identical to the eigenvalue equation for a 3-D hydrogenic atom in a quantum level n for an effective nuclear charge $Z_{eff} = n/n_S$. Thus, this equation can be easily solved using standard methods for separation of variables in either spherical ($r = \sqrt{x^2 + y^2 + z^2}$, $\theta = \cos^{-1}(z/r)$, $\varphi = \tan^{-1}(y/x)$), or parabolic ($\xi = r + z$, $\eta = r - z$, z) coordinates. The solutions of eq. (E.1), in spherical and parabolic coordinates, are given by

$$\begin{aligned} \langle \mathbf{r} | \tilde{\phi}_{n,l,m}^S(n_S) \rangle &= \frac{2}{n_S \sqrt{n n_S}} \left(\frac{(n-l-1)!}{(n+l)!} \right)^{\frac{1}{2}} \left(2 \frac{r}{n_S} \right)^l \\ &\times e^{-r/n_S} L_{n-l-1}^{2l+1} \left(2 \frac{r}{n_S} \right) Y_l^m(\theta, \varphi) \end{aligned} \quad (\text{E.2})$$

$$\begin{aligned} \langle \mathbf{r} | \tilde{\phi}_{n_1, n_2, m}^S(n_S) \rangle &= \frac{e^{m\phi}}{\sqrt{\pi n}} \left(\frac{n_1! n_2!}{(n_1 + m)!(n_2 + m)!} \right)^{\frac{1}{2}} n_S^{-(m+\frac{3}{2})} \\ &\times e^{-(\xi+\eta)/2n_S} (\xi\eta)^{\frac{m}{2}} L_{n_1}^m \left(\frac{\xi}{n_S} \right) L_{n_2}^m \left(\frac{\eta}{n_S} \right) \end{aligned} \quad (\text{E.3})$$

where n, l, m are spherical quantum numbers, n_1, n_2, m are parabolic quantum numbers ($n = n_1 + n_2 + m + 1$, $n_{1,2} = 0, 1, \dots, (n - |m| - 1)$), L_n^m denotes a Laguerre polynomial, and Y_l^m is a spherical harmonic. In eq. (E.3), $m \geq 0$ is assumed. For negative m , we have $\langle \mathbf{r} | \tilde{\phi}_{n_1, n_2, m}^S(n_S) \rangle = (-1)^m \langle \mathbf{r} | \tilde{\phi}_{n_1, n_2, -m}^S \rangle^*$. A complete and countable basis set for the full Hilbert space is generated by changing n, l, m (or n_1, n_2, m). Because the Hamiltonian in eq. (2.1) has cylindrical symmetry, m is a constant of motion. In practice, we use $1 \leq n \leq n_{max}$ which, for $m = 0$, corresponds to the number of states $N = n_{max}(n_{max} + 1)/2$. For the 1-D system, Sturmian wave functions are generated using the radial part of eq. (E.2) and setting $l = m = 0$.

E.1 Sturmian basis set and hydrogenic bound states

In this section, we discuss how effectively a finite Sturmian basis set can represent bound states.

Fig. E.1 shows the norm of the projection of a hydrogenic bound state $\langle n_1, n_2, m |$ on a finite subspace,

$$\sum_{n_1, n_2, m}^N \left| \langle n_1, n_2, m | \phi_{n_1, n_2, m}^S \rangle \right|^2, \quad (\text{E.4})$$

for different values of n_s and n_{max} . A basis set that provides a good representation of the bound state should yield a norm very close to unity. This is an obvious prerequisite for calculating the evolution in the presence of the field. As expected,

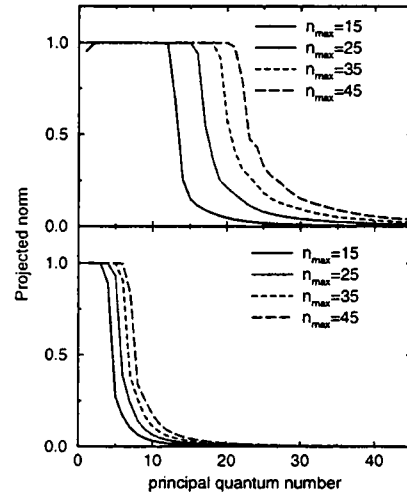


Figure E.1: Norm of the projection of a hydrogenic state with $n_1 = m = 0$ onto different Sturmian basis sets as a function of the principal quantum number of the hydrogenic state. The different Sturmian basis sets are characterized by $n_{max} = 15, 25, 35, 45$ and $n_s = 10$ (top) or $n_s = 1$ (bottom).

the norm becomes closer to unity for a larger range of n levels, as the basis size increases. Note, however, that the n levels which are well represented strongly depend on the value of n_s . High n levels are clearly described better using higher values of n_s (here $n_s = 10$) rather than lower values (here $n_s = 1$) and vice versa. Since both basis sets contain the same number of states, this indicates that the basis with lower value of n_s involves a larger number of continuum states ($E_k > 0$) and, hence, provides a more suitable representation of the continuum.

E.2 Sturmian basis set and hydrogenic continuum states

Because Sturmian functions decay exponentially in the limit $r \rightarrow \infty$ (see eq. (E.3)), continuum states cannot be exactly reproduced. It is, however, possible to find a good representation of continuum wave functions in a limited range $r \lesssim R$ which is proportional to the maximum average radius of a Sturmian function with $n = n_{max}$, i.e. $R \propto r_{max} = n_s n_{max}$. An accurate solution of the Schrödinger equation can be obtained as long as the wave function is localized in this region of coordinate space. Fig. E.2 shows a comparison of a spherical continuum state calculated from a finite Sturmian basis set with the exact continuum state given by

$$\begin{aligned} \langle r | K, l, m \rangle &= \sqrt{\frac{2}{\pi}} e^{\pi \frac{\eta}{2}} \frac{|\Gamma(1 + l + i\eta)|}{(2l + 1)!} (2Kr)^l e^{-iKr} \\ &\times {}_1F_1[1 + l + i\eta, 2l + 2, 2iKr] Y_l^m(\theta, \varphi) \end{aligned} \quad (\text{E.5})$$

where $\eta = Z/K$ and ${}_1F_1$ is a confluent hypergeometric function. The wave function in the left figure has an energy $E = K^2/2 = 0.0032a.u.$, $m = 0$, and $l = 0$. The approximate wave functions have been calculated using $n_s = 5$ and therefore $r_{max} = 75, 125, 275a.u.$ for $n_{max} = 15, 25, 55$, respectively, which contains the range of r values in the figure. The larger the basis size, the larger the range of radii for which the approximate wave function agrees with the exact one. Note that the precise radius up

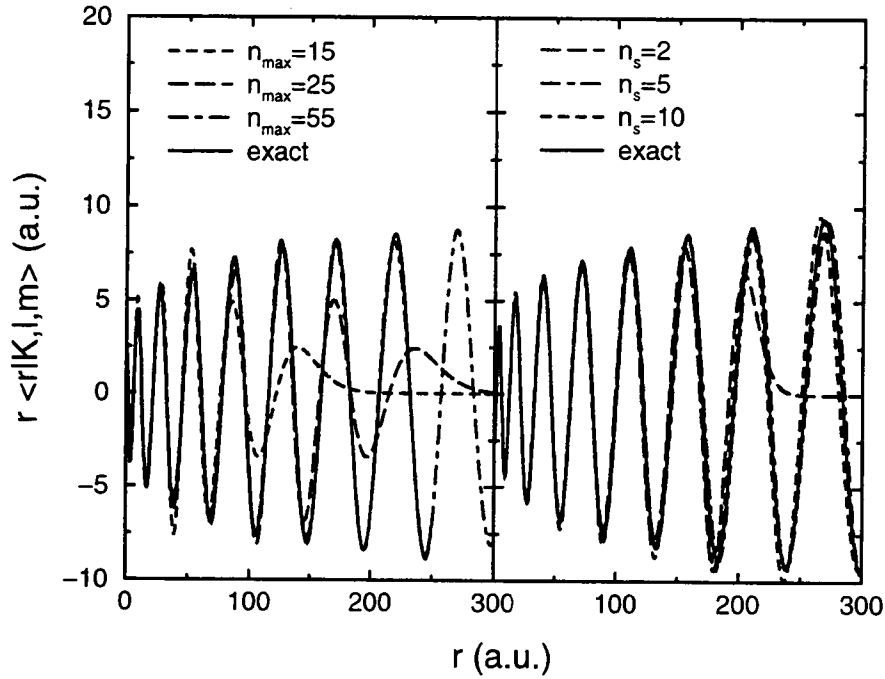


Figure E.2: Comparison of the exact and approximate continuum wave function times the radius using different basis sizes for a spherical continuum state with $E = 0.0032 a.u.$, $l = m = 0$ (left) and using various Sturmiian parameters, n_s , for a spherical continuum state with $E = 0.0016 a.u.$, $l = m = 0$ (right).

to which a basis set can reproduce a continuum state is a function of not only r_{max} but also the wavenumber, K . The maximum wave vector that can be represented properly in a finite Sturmiian basis is proportional to $\sim n_s^{-1}$. This is illustrated in fig. E.2 (right) which shows a spherical continuum state with $E = 0.0016 a.u.$, $l = m = 0$, obtained as the Sturmiian parameter is changed while maintaining the basis size fixed. As expected, the smaller n_s , the better the agreement between the approximate and the exact wave functions. Thus, a finite Sturmiian basis set can approximate continuum wave functions within certain ranges of both wavenumber and radius which depend on n_s and n_{max} .

Alternatively, the limitation of the finite Sturmiian basis set in phase space can be

evaluated by the deviation function Δ_g ,

$$\Delta_g = \int_0^\infty dr |\varphi(r) - \varphi_{app}(r)|^2 \quad (\text{E.6})$$

with

$$|\varphi_{app}\rangle = \sum_{n=0}^N \langle \phi_n^S | \varphi \rangle |\phi_n^S\rangle. \quad (\text{E.7})$$

where $\varphi(r)$ is a Gaussian wavepacket localized at (r_g, p_g) with a width σ in coordinate space. $\Delta_g = 0$ indicates that the finite Sturmian basis set represents the wavepacket at (r_g, p_g) accurately and $\Delta_g = 2$ indicates that the error is maximum.

For simplicity, we used a spherical symmetric Gaussian wavepacket for this test, therefore, we only need Sturmian wave functions with $l = 0$ as basis functions and the problem becomes identical to the 1-D problem. Fig. E.3 displays lines of constant Δ_g for different values of the Sturmian parameter n_S and a fixed width of the wavepacket $\sigma = 10$ in coordinate space. The contours are given for the value $\Delta_g = 0.1$ such that the wavepacket is well localized in the basis set. We can simply estimate this boundary in phase space using the asymptotic expression of $\phi_n^S(r)$ for large r and n [52],

$$\lim_{r,n \rightarrow \infty} \phi_n^S(r) \propto \cos\left(\sqrt{8nr/n_S} - 3\pi/4\right). \quad (\text{E.8})$$

Near $r = n_S n$ the local wavelength is approximately given by

$$\lambda \simeq \sqrt{2\pi n_S} \quad (\text{E.9})$$

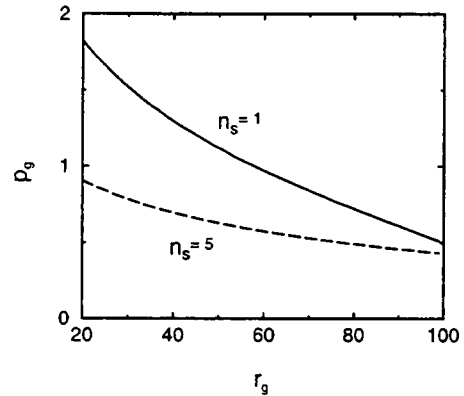


Figure E.3: Lines of constant Δ_g , i.e., deviation of the approximate from the exact wave function, for two different Sturmian parameters ($n_S = 1$ or 5). Above (below) each curve Δ_g is bigger (smaller) than 0.1 . $N = 70$ is used as a basis size.

corresponding to an n -independent local momentum

$$\langle p \rangle \approx \sqrt{2}/n_S. \quad (\text{E.10})$$

Thus we can approximate this contour lines by hyperbolas $r_g p_g \approx \text{constant}$. Moreover, from eq. (3.8), the range of p_g for a given r_g supported by the basis set increases with decreasing n_S . Note, however, that $n_S \rightarrow 0$ is not a viable strategy to increase the least error region of phase space since for small n_S the error Δ_g for representing well-localized atomic initial states will eventually increase.

Appendix F

Matrix elements

F.1 Matrix elements for a unitary calculation

The matrix elements of the 3-D atomic Hamiltonian (eq. (2.1)) and the dipole operator z in the non-orthogonal Sturmian basis are

$$\begin{aligned} \langle \tilde{\phi}_{n',l',m'}^S | H_{at}^{3D} | \tilde{\phi}_{n,l,m}^S \rangle &= -\frac{1}{2n_S^2} \langle \tilde{\phi}_{n',l',m'}^S | \tilde{\phi}_{n,l,m}^S \rangle \\ &+ \left(\frac{n}{n_S} - 1 \right) \langle \tilde{\phi}_{n',l',m'}^S | \frac{1}{r} | \tilde{\phi}_{n,l,m}^S \rangle \end{aligned} \quad (\text{F.1})$$

$$\begin{aligned} \langle \tilde{\phi}_{n',l',m'}^S | z | \tilde{\phi}_{n,l,m}^S \rangle &= \langle \tilde{\phi}_{n',l',m'}^S | r | \tilde{\phi}_{n,l,m}^S \rangle \\ &\times \left[\sqrt{\frac{l^2 - m^2}{4l^2 - 1}} \delta_{l',l-1} \delta_{m',m} \right. \\ &\left. + \sqrt{\frac{l'^2 - m^2}{4l'^2 - 1}} \delta_{l',l+1} \delta_{m',m} \right] \end{aligned} \quad (\text{F.2})$$

Thus all matrix elements are reduced to the evaluation of the integral, $\langle \tilde{\phi}_{n',l',m'}^S | r^p | \tilde{\phi}_{n,l,m}^S \rangle$ (p is an integer). Note that, for the 1-D kicked atom, the matrix elements of the atomic Hamiltonian are identical to this 3-D Hamiltonian with $l = 0$ and the “dipole” matrix

elements correspond to the radial part of the 3-D dipole matrix.

This integral is easily evaluated using the recursion relation of Laguerre polynomials

$$xL_i^j(x) = (2i + j + 1)L_i^j(x) - (i + 1)L_{i+1}^j(x) - (i + j)L_{i-1}^j(x). \quad (\text{F.3})$$

Suppose we define $I(n', n, l, n_S)$ such that

$$\langle \tilde{\phi}_{n', l', m'}^S | r^p | \tilde{\phi}_{n, l, m}^S \rangle = C(n', n_S) C(n, n_S) I(n', n, l, n_S) \delta_{l, l'} \delta_{m, m'}, \quad (\text{F.4})$$

or, equivalently,

$$\begin{aligned} I(n', n, l, n_S) &= \int dr r^2 \left[\left(2 \frac{r}{n_S} \right)^l e^{-r/n_S} L_{n'-l-1}^{2l+1} \left(2 \frac{r}{n_S} \right) \right] r^p \\ &\quad \times \left[\left(2 \frac{r}{n_S} \right)^l e^{-r/n_S} L_{n-l-1}^{2l+1} \left(2 \frac{r}{n_S} \right) \right], \end{aligned} \quad (\text{F.5})$$

where

$$C(n, l, n_S) = \frac{2}{n_S} \sqrt{\frac{(n-l-1)!}{n_S n (n+l)!}}. \quad (\text{F.6})$$

From eq.(F.3), we can derive the following recursion relation for $I_p(n', n, l, n_S)$

$$\begin{aligned} \frac{2}{n_S} I_p(n', n, l, n_S) &= -(n-l) I_{p-1}(n', n+1, l, n_S) + 2n I_{p-1}(n', n, l, n_S) \\ &\quad - (n+l) I_{p-1}(n', n-1, l, n_S). \end{aligned} \quad (\text{F.7})$$

In addition, we can easily calculate the integral for $p = -1$,

$$I_{-1}(n', n, l, n_S) = \frac{1}{C(n, l, n_S)^2} \frac{1}{nn_S} \delta_{n, n'}. \quad (\text{F.8})$$

Thus, matrix elements of the operator r^p for $(p \geq -1)$ can be deduced from the recursion relation eq. (F.7). Using these integrals, the Hamiltonian and the dipole matrix

elements can be obtained. Note that, for the 3-D dipole operator, we need an integral $\langle \tilde{\phi}_{n',l',m'}^S | r | \tilde{\phi}_{n,l,m}^S \rangle$ with $|l - l'| = 1$. Using another recursion relation of Laguerre polynomials,

$$x^2 L_i^j(x) = -(j-1)(i+2)L_{i+2}^{j-2}(x) - (i+j)(x-j+1)L_{i+1}^{j-2}(x), \quad (\text{F.9})$$

this integral becomes,

$$\begin{aligned} \langle \tilde{\phi}_{n',l+1,m}^S | r | \tilde{\phi}_{n,l,m}^S \rangle &= \frac{n_S}{2} C(n', l+1, n_S) C(n, l, n_S) \\ &\times [-2(l+1)(n' - l) I_0(n' + 1, n, l, n_S) \\ &- \frac{2}{n_S} (n' + l + 1) I_1(n', n, l, n_S) \\ &+ 2(l+1)(n' + l + 1) I_0(n', n, l, n_S)] . \end{aligned}$$

Once these matrices are evaluated in the Sturmian basis, they can be transformed to their representation in the orthonormal Sturmian basis (eq. (3.3))

$$H_{jk} = \sum_{j',k'} (\hat{S}^{-1/2})_{jj'} \langle j' | H_{at} | k' \rangle (\hat{S}^{-1/2})_{k'k} \quad (\text{F.10})$$

$$z(r)_{jk} = \sum_{j',k'} (\hat{S}^{-1/2})_{jj'} \langle j' | z(r) | k' \rangle (\hat{S}^{-1/2})_{k'k} \quad (\text{F.11})$$

where $|j\rangle$ corresponds to $|\tilde{\phi}_{n_j,l_j,m_j}^S\rangle$ for the 3-D system and $|\tilde{\phi}_{n_j}^S\rangle$ for the 1-D system, and $\hat{S}$ is the overlap matrix defined by $S_{jk} = \langle j | k \rangle$. These matrices can be diagonalized numerically,

$$\hat{A} = {}^t \hat{O}_A \hat{D}_A \hat{O}_A \quad (\text{F.12})$$

where $\hat{A}$ is arbitrary real matrix in an orthonormal basis ($\hat{H}$, $\hat{z}$, or $\hat{r}$), and $\hat{D}_A$ is a diagonal matrix whose elements are eigenvalues of $\hat{A}$, i.e., $D_{jk} = \lambda_j \delta_{jk}$, whose corresponding eigenvectors are the column vectors of $\hat{O}$, i.e., O_{jl} . Using these results, the unitary free

evolution and boost operators can be expressed as

$$\hat{U}_A = {}^t\hat{O}_A \exp \left[-i\hat{D}_A \Delta t (\text{or } \Delta p) \right] \hat{O}_A. \quad (\text{F.13})$$

F.2 Matrix elements for a non-unitary calculation

In the RPM, matrix elements are evaluated using Sturmian wave functions with two different basis sizes N and M ($N < M$). As an example, the evaluation of the free evolution operator is explained in this section. The free evolution operator with the RPM consists of two different matrices; a unitary free evolution operator in the $P + Q'$ subspace,

$$U_M^{free} = |P + Q'\rangle e^{-i\langle P+Q'|H|P+Q'\rangle \Delta t} \langle P + Q'|, \quad (\text{F.14})$$

and a projection operator,

$$\mathcal{M} = |P\rangle \langle P|, \quad (\text{F.15})$$

(eq. (3.24)). U_M^{free} can be evaluated as described in the previous section. This procedure involves the diagonalization of the matrix, therefore, it has to be evaluated in the orthonormal Sturmian basis. On the other hand, the projection is implemented in the non-orthogonal Sturmian basis. The projection operator transforms from orthogonal to non-orthogonal Sturmian bases in the $P + Q'$ space, projects onto the P space, and transforms back to the orthogonal Sturmian basis in the P space. It is expressed mathematically by,

$$\mathcal{M} = \hat{S}_P^{-1/2} \hat{D}_1 \hat{S}_{P+Q'}^{1/2} \quad (\text{F.16})$$

or

$$\mathcal{M} = \hat{S}_P^{-1/2} \hat{D}_1 \hat{S}_{P+Q'} \hat{S}_{P+Q'}^{-1/2}. \quad (\text{F.17})$$

where $\hat{D}_1$ is a $N \times M$ matrix whose elements are $D_1, jk = \delta_{jk}$. Note that the matrix elements of $\hat{S}$ are invariant in any subspace but those of $\hat{S}^{-1/2}$ are not. Thus the non-unitary free evolution operator can be evaluated using the non-unitary boost operator for a small momentum transfer can be evaluated with the same strategy.

Appendix G

Non-unitary representation of the boost operator

In general, we can define the 1-D Sturmian basis with an angular momentum, i.e.,

$$\langle q|\tilde{\phi}_{n,l}^{1/\lambda}\rangle = C(n, l, 1/\lambda)(2q\lambda)^l e^{-q\lambda} r L_{n-l-1}^{2l+1}(2a\lambda). \quad (\text{G.1})$$

where $\lambda = 1/n_S$. In this non-orthogonal Sturmian basis, the matrix elements of the boost operator are given by

$$\begin{aligned} \langle \tilde{\phi}_{n',l}^{1/\lambda} | e^{iq\Delta p} | \tilde{\phi}_{n,l}^{1/\lambda} \rangle &= \frac{\lambda}{\sqrt{nn'}} \sqrt{\frac{(n'+1)!(n+l)!}{(n-l-1)!(n'-l-1)!}} \frac{(-i\Delta p)^{n+n'-2l-2}}{(2\lambda - i\Delta p)^{n+n'}} \\ &\times \frac{(2\lambda)^{2l+1}}{(2l+1)!} \left\{ 2n {}_2F_1 \left[-(n-l-1), -(n'-l-1), 2l+2, -\frac{4\lambda^2}{\Delta p^2} \right] \right. \\ &- (n+l+1) \frac{-i\Delta p}{2\lambda - i\Delta p} {}_2F_1 \left[-(n-l), -(n'-l-1), 2l+2, -\frac{4\lambda^2}{\Delta p^2} \right] \\ &\left. - (n-l-1) \frac{2\lambda - i\Delta p}{-i\Delta p} {}_2F_1 \left[-(n-l-2), -(n'-l-1), 2l+2, -\frac{4\lambda^2}{\Delta p^2} \right] \right\} \end{aligned}$$

where ${}_2F_1$ denotes a hypergeometric function.

Since ${}_2F_1$ is evaluated numerically and the result becomes unstable for high quantum

numbers, we need to use an asymptotic form of the hypergeometric function [40] in such a case. To prevent the ${}_2F_1$ function from adopting a huge value, we evaluate

$$\mathcal{F} = \frac{(-i\Delta p)^{-a-b}}{(2\lambda - i\Delta p)^{-a-b+c}} {}_2F_1[a, b, c, z] \quad (\text{G.2})$$

instead of ${}_2F_1[a, b, c, z]$. The asymptotic form of $\mathcal{F}$ can be expressed using an Airy function $Ai(x)$ [40].

Vita

Shuhei Yoshida was born on June 10, 1970, 6:10 am in Osaka, Japan, as the second child of Kazuo and Yoshiko Yoshida and a brother of Mitsunobu Yoshida. At the age of 10, he found interests in music and started playing the guitar. In 1983, he entered Omiya junior high school and joined the wind ensemble orchestra of the school where he played the trumpet. After entering Otemae high school in 1986, he deeply committed himself into the brass ensemble in this high school as a music director, and, at the same time, he became a student of Akira Takehara, who is a principal trumpet player of the Osaka city wind ensemble. After graduation from high school, he experienced one year of "ronin¹" life and, in 1990, he became a freshman at the department of applied mathematics and physics, faculty of engineering, Kyoto University which is one of the most prestigious universities in Japan and has produced several novel prize winners in many fields including physics. His music-oriented mind led him again to the Kyoto university symphony orchestra which is one of the oldest symphony orchestras in Japan. During his college days, in order to make a living, he had several jobs; a clerk in a Japanese-style hotel and in an optical shop, an assistant cook in an Italian restaurant, a personal tutor, and several daily jobs. In 1993, physics finally started attracting him and he joined the statistical mechanics group of Professor Toyonori Munakata. In his undergraduate project, he studied chaos in a very simple dynamical map called the logistic map. One year later, he obtained the Bachelor of Engineering in the spring of 1994. He remained in the same group as a graduate student and started working on the statistical properties of liquids under the influence of intra- and inter-molecular interactions. After obtaining the Master of Engineering in the spring of 1996, he became a student of Professor Joachim Burgdörfer at the department of physics, University of Tennessee. He is working on the theory of quantum chaos with Dr. Carlos Reinhold

¹A "ronin" is originally a "samurai" (warrior) who doesn't belong to any "shogun" (king) but nowadays it is used to express a person who doesn't belong to any school or company.

and expects to receive his Ph.D. in August 1999.

List of publications

1. "Floquet analysis of the dynamical stabilization of the kicked hydrogen atom,"
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3. "Reflection-free propagation of wavepackets,"
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4. "Realization of the kicked atom,"
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