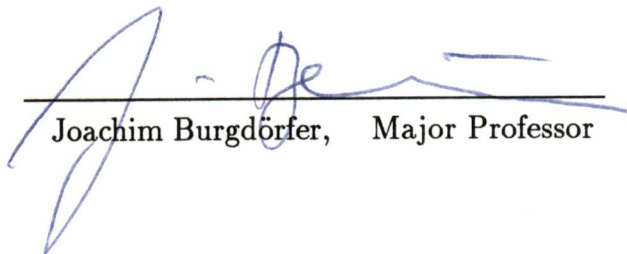
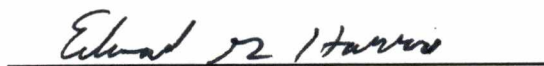


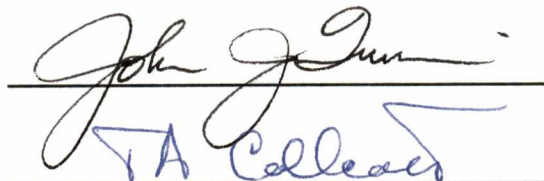
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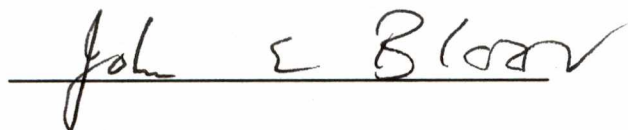
I am submitting herewith a dissertation written by Xiazhou Yang entitled "Parametric Deformation of Quantum Spectra of Classically Chaotic Systems". I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Physics.


Joachim Burgdörfer, Major Professor

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TA Collector


John E. Bloom

Accepted for the Council:


Lew Munkel
Associate Vice Chancellor
and Dean of The Graduate School

Parametric Deformation of
Quantum Spectra of
Classically Chaotic Systems

A Dissertation
Presented for the
Doctor of Philosophy
Degree
University of Tennessee, Knoxville

Xiazhou Yang
August, 1993

DEDICATION

**This dissertation is dedicated to my parents
Prof. Ying Ding and Ms. Ying Yang
for their love and understanding.**

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ABSTRACT

We present theoretical studies of the dynamical origin for the existence of universality classes in quantum spectral fluctuations. The evolution of the quantum spectrum as a function of a control parameter governing the strength of a nonintegrable perturbation can be mapped onto the molecular dynamics of a many-body system. The perturbation causes chaotic motion in the classical dynamics. We show that the classical transition from predominantly regular motion to global chaos is accompanied by a transition from a nonequilibrium to an equilibrium state in the parametric motion of quantum energy levels. The discussion of the source of ergodicity in the parametric motion leads to an equilibrium distribution function which provides an explanation for the existence of the universal fluctuations in the quantum spectra of classically chaotic systems. The microscopic mechanism for the transition from a nonequilibrium to an equilibrium state is the existence of avoided crossings. The width distribution of avoided crossings in quantum systems whose classical counterparts possess a mixed phase space of regular and chaotic dynamics is shown to consist of two components: a near Gaussian distribution suggested by random matrix theory for the chaotic component and an approximately δ -shaped component originating from tori in the regular portion of phase space. The relative weight of these two components is closely related to the structure of classical phase space. The study of relaxation processes in the parametric motion of energy levels reveals that the parametric correlation functions are sensitively dependent on the underlying classical dynamics, and the transition from classically regular to chaotic motion manifests itself in the disappearance of parametric diffusion in quantum spectrum. The parametric motion of resonances is discussed. The two-body approximation indicates that the existence of the repulsion between resonances is independent of the underlying classical dynamics. We suggest that the transition to the thermal equilibrium state in the parametric motion of resonances is the signature of classical chaos.

This thesis is based in part on the following publications:

- J. Burgdörfer, X. Yang and E. Eschenazi, "Quantum Chaology and the Deformation of Spectra of Simple Quantum Systems", Comments in At. and Mol. Phys. 25, 83(1990). Reprinted in "Irregular Atomic Systems and Classical Chaos", Edit. Jean-Claude Gay (Gordon and Breach, 1992) p.91.

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- X. Yang and J. Burgdörfer, "Parametric Correlations and Diffusion in Quantum Spectra", *Phys. Rev. A* 46, 2295(1992).
- X. Yang and J. Burgdörfer, "Statistics of Avoided Crossings for Generic Quantum Systems", *Phys. Rev. A*, July, (1993).
- X. Yang and J. Burgdörfer, "Parametric Motion of Quantum Resonances", in progress. See *Bulletin of the APS* 37, 1645(1992).

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List of frequently used abbreviations

ABC	<u>A</u> quilar- <u>B</u> alslev- <u>C</u> ombes theorem. Page 109
AC	<u>A</u> voided <u>c</u> rossing. Page 55
EBK	<u>E</u> instein- <u>B</u> rillouin- <u>K</u> eller quantization. Page 36
GOE	<u>G</u> aussian <u>o</u> rthogonal <u>e</u> nsembles. Page 26
HFE	<u>H</u> ellman- <u>F</u> eynman <u>e</u> quations. Page 49
KAM	<u>K</u> olmogorov- <u>A</u> rnol'd- <u>M</u> oser theorem. Page 15
MD	<u>M</u> olecular <u>d</u> ynamics. Page 49
NNS	Distribution of <u>n</u> earest- <u>n</u> eighbor <u>s</u> pacings. Page 25
PNV	<u>P</u> arametric <u>n</u> umber <u>v</u> ariance. Page 85
RMT	<u>R</u> andom <u>m</u> atrix <u>t</u> heory. Page 26
VAF	<u>V</u> elocity <u>a</u> utocorrelation <u>f</u> unction. Page 88

Chapter 1

Introduction

1.1 Definition of quantum chaos

Physical systems of classical mechanics can be divided into two categories: deterministic systems and indeterministic systems. The time evolution of the indeterministic system is governed by random forces, thus the future behavior can be predicted only by statistics [1]. The most famous example of this class is the Brownian motion of pollens in liquids. For the deterministic systems, there exist a set of differential or difference equations describing the effect of well-defined non-random forces which determine the evolution of initial conditions. Therefore, successive states evolve in a uniquely defined sequence from each other. One interesting example of deterministic systems is the Kepler problem, for it is realized in nature on both macroscopic and microscopic scales: the classical solar system and the quantum atomic system. By coincidence, both cases are governed by the same central attractive force law in $1/r^2$. Using appropriate units, the Hamiltonian function of two-body Kepler problem can be written as [2]

$$H = \frac{p^2}{2} - \frac{1}{r}. \quad (1.1)$$

Fig. 1.1 displays the motion of the earth around the sun governed by Hamiltonian (1.1). This motion is precisely periodic and accurately predictable for thousands of periods. The intrinsic character which ensures reliable predictions is the stability of this system against both small external perturbations and uncertainties in the initial conditions.

One could assume, at first glance, that all deterministic motions are rather

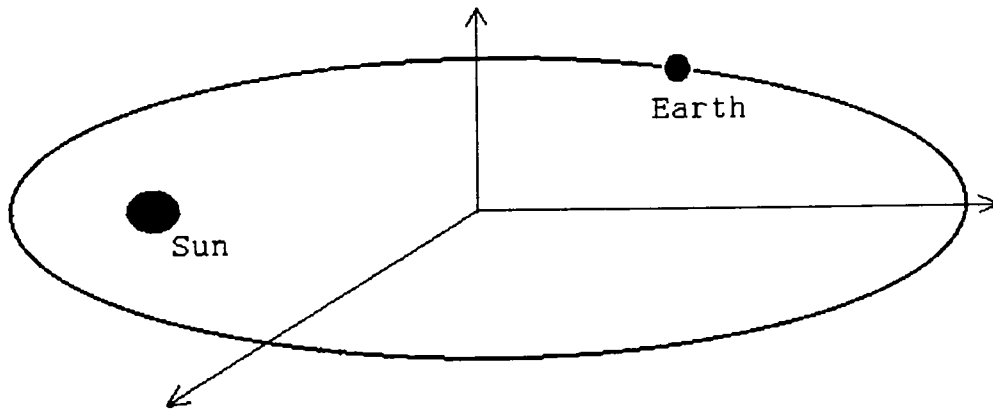


Figure 1.1: The motion of the earth around the sun.

stable under the perturbation as shown by the planetary motion and thus the predictions for the future behavior are guaranteed. It was shown by H. Poincaré [3] at the end of the last century, however, that the three-body Kepler system could display extremely unstable motions, in which a small uncertainty or perturbation upon the trajectory is exponentially enlarged in the course of time. Therefore, the long time behavior of such systems becomes essentially unpredictable because in practice the initial conditions can be prepared only with finite accuracy and errors increase exponentially fast. This complicated behavior is called “deterministic chaos” or “chaos”. Poincaré’s discovery was largely ignored until 1963, when E. N. Lorenz [4] found the chaotic behavior for a simple set of three coupled, first order, nonlinear differential equations describing the hydrodynamics of weather patterns (“Lorenz model”). It was since realized [5] mostly due to the availability of high speed computers that the chaotic motion is by no means exceptional but a typical (or generic) property of deterministic systems. One paradigm of chaotic systems on a microscopic scale is hydrogen atom in a uniform magnetic field [6]. The Hamiltonian of this system is given by replacing momentum p in Eq. (1.1) by $p - \frac{e}{c}A$ where $A = \nabla \times B$ and B is the strength of magnetic field. This procedure simply adds another term,

$$V = \frac{\gamma^2}{8}\rho^2 + \frac{\gamma}{2}L_z \quad (1.2)$$

where $\gamma = B/B_0$ ($B_0 = 2.35 \times 10^5 \text{ Tesla}$) and L_z is a constant (conserved azimuthal component of the angular momentum), to the Hamiltonian of two-body Kepler system (Eq. (1.1)). Under the influence of (1.2), the system

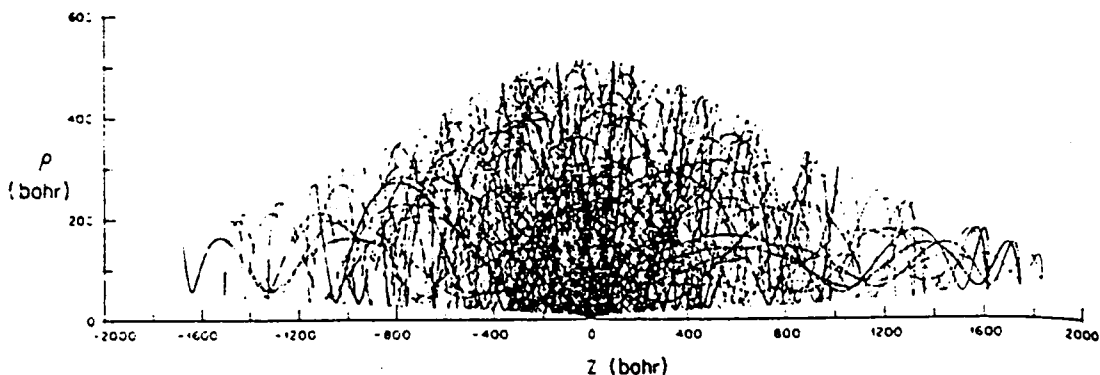


Figure 1.2: An unstable trajectory of hydrogen atom in a magnetic field. This is characteristic of the type of trajectory prevalent near the ionization threshold. Reprinted from M. L. Du and J. B. Delos, *Phys. Rev. A* **38**, 1896(1988).

becomes unstable. Fig. 1.2 displays a characteristic trajectory near the ionization threshold of this system. In contrast to the trajectory of the earth around the sun, this trajectory shows a chaotic, random pattern.

The existence of chaos in classical systems leads to a fundamental problem of whether this irregularity manifests itself in the properties of corresponding quantum systems. This problem is usually referred to as “quantum chaos” or “quantum chaos” [7]. The task is quite general since almost all Hamiltonian systems exhibit classical chaotic dynamics. Among these systems are highly excited states of atoms (in external fields) and of polyatomic molecules.

For a Hamiltonian system with N degrees of freedom, the coordinate q and corresponding canonical momentum p form a $2N$ -dimensional phase space. According to Heisenberg’s uncertainty principle

$$\Delta q \Delta p > \hbar/2, \quad (1.3)$$

if the position q is measured with precision Δq , the momentum p will be inevitably disturbed by $\Delta p \sim \hbar/(2\Delta q)$ or vice versa. Therefore, the notion of a trajectory loses its meaning and so does the notion of any quantities measuring the separation between trajectories. The phase space is “coarse grained”,

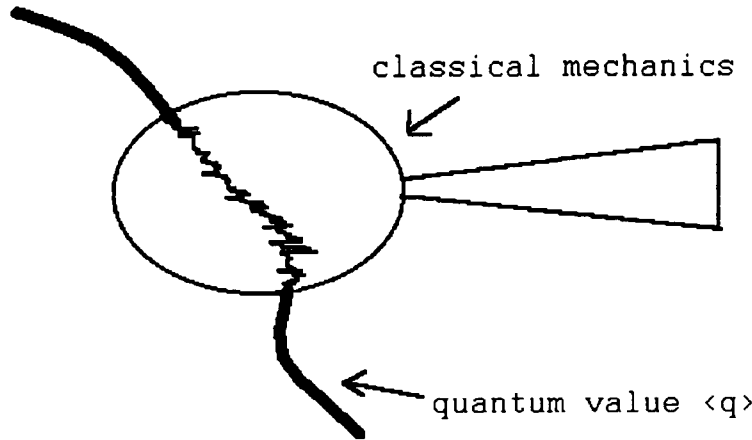


Figure 1.3: Smoothing the phase space structures by quantum mechanics.

i.e. quantum mechanics cannot distinguish the points in $2N$ -dimensional phase space within a volume $\hbar^N$. This means that the classically chaotic motion within a region in phase space with volume smaller than $\hbar^N$ is not “seen” in quantum mechanics (see Fig.1.3). Thus one expects the corresponding quantum systems are not chaotic in the way that classical systems are. This is called the quantum “suppression” of classical chaos. This suppression is easily demonstrated by totally bounded autonomous Hamiltonian systems. In this case the time-dependent Schrödinger equation,

$$H|\Psi\rangle = -\frac{\hbar}{i} \frac{\partial}{\partial t} |\Psi\rangle \quad (1.4)$$

can be solved by Fourier expansion

$$|\Psi\rangle = \sum_n e^{-\frac{i}{\hbar} E_n t} \langle n | \Psi_0 \rangle |n\rangle \quad (1.5)$$

where E_n and $|n\rangle$ are the eigenvalues and eigenvectors of operator H respectively, i.e.

$$H|n\rangle = E_n |n\rangle, \quad (1.6)$$

and $|\Psi_0\rangle$ is the initial wavefunction of the system. (We do not distinguish classical Hamiltonian function and quantum Hamiltonian operator unless

confusion will arise.) Solutions of Eq. (1.5) are strictly quasiperiodic [8] which exclude any exponential separation on time scales on which level spacings are resolvable. Consequently, there is no chaos in quantum mechanics. In the following, the terms “regular” and “chaotic” are always used in the sense of classical dynamics.

Nevertheless, the fundamental question remains: what are the differences between the properties of a quantum system with a regular classical counterpart and a quantum system whose classical analogue displays chaos? The understanding of this problem has been greatly developed during the last decade and several intrinsically quantum mechanical distinction criteria have been established [9]. One well-known criterion is the distribution of the nearest-neighbor spacings of energy levels

$$s_n = (E_{n+1} - E_n) / \langle \Delta E \rangle \quad (1.7)$$

where $\langle \Delta E \rangle$ is the average spacing. Both numerical and experimental evidence shows that depending on the underlying classical dynamics, the distribution of the nearest-neighbor spacings displays universal fluctuations. For classically regular systems, the distribution is Poissonian

$$P_{Poisson}(s) = e^{-s} \quad (1.8)$$

whereas the distribution for classically totally chaotic systems with time reversal symmetry is of the Wigner type

$$P_{Wigner}(s) = \frac{\pi}{2} s e^{-\pi s^2/4}. \quad (1.9)$$

Fig. 1.4 depicts these two distributions. They are easily distinguished: at the origin, the Wigner distribution becomes 0 (“level repulsion”) while the Poisson distribution reaches its maximum value of 1 (“level clustering”). Therefore one can learn about the dynamics of a classical system by studying level fluctuations of the quantum analog or vice versa.

Finding the dynamical origin of the universal classes (Poisson distribution and Wigner distribution) in the fluctuations of quantum spectra is one of the main tasks of quantum chaos. The investigations of this problem have proceeded along two different but complementary lines. One is the traditional theory of semiclassical method and the other is the newly developed parametric dynamics of quantum levels. We present theoretical studies of these approaches in this thesis.

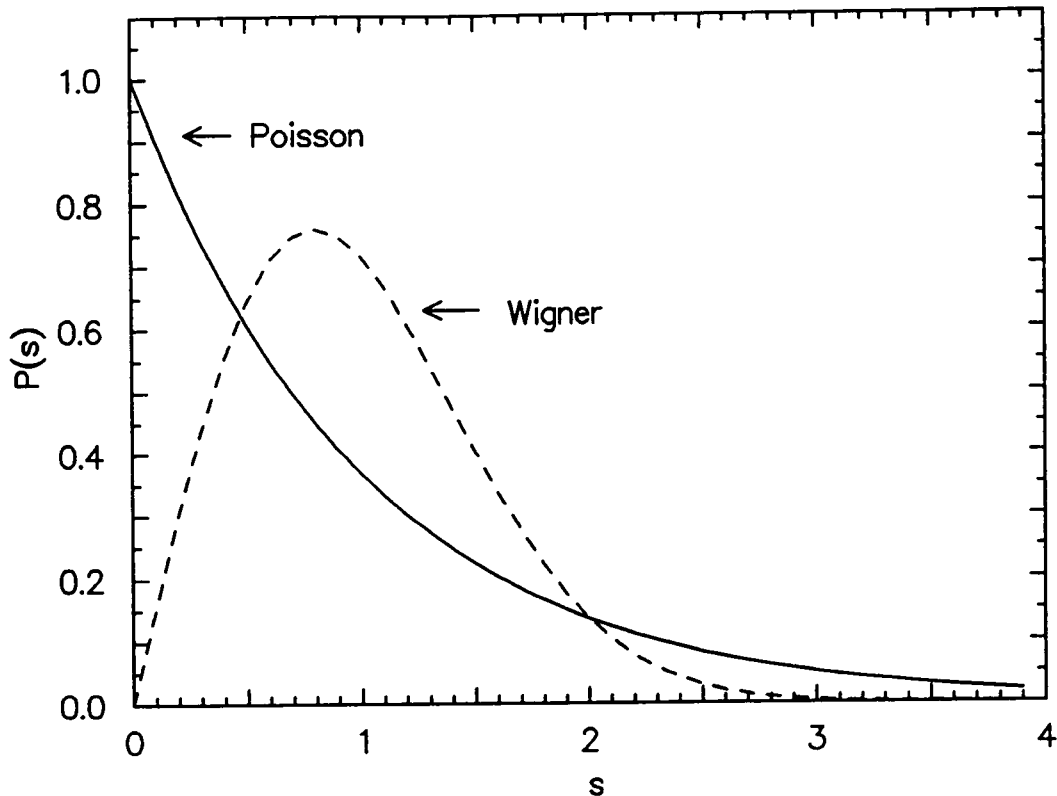


Figure 1.4: Two universality classes in the nearest-neighbor spacing distributions.

1.2 Plan of the thesis

In Chapter 2, we briefly review the classical mechanics and introduce two measures of classical chaos, the mean rate of exponential separations of nearby trajectories and the fraction of the volume of the accessible phase space in which the motion is chaotic. We prove that for continuously deformed periodic orbits, the dependence of the mean rate of separation on a perturbation obeys a square-root law. In Chapter 3, the level statistics are briefly discussed. By the examination of several level sequences, we show that the distributions of nearest-neighbor spacings of quantum levels are sensitively dependent on the underlying classical dynamics. For classically regular systems, the distribution is Poissonian whereas the distribution for chaotic systems are Wigner-type. We discuss the semiclassical quantization theory

in Chapter 4. From this theory, one is able to prove that the nearest-neighbor spacing distribution for a classically regular system is indeed Poissonian. But this theory fails to provide the information about individual levels in the chaotic case, and therefore faces the difficulty to give the dynamical origin of the Wigner distribution of nearest-neighbor spacings for classically chaotic systems. The application of this theory to the system of hydrogen atom in a magnetic field demonstrates that deeper insights on quantum spectrum can be obtained from the corresponding classical dynamics. We show that the reason for the existence of Rydberg series in the classically totally chaotic regime of this system is the existence of the families of classical orbits which spend most of their time in the near separable region. The parametric level dynamics is discussed in Chapter 5. This approach considers the spectrum of a one-parameter family of Hamiltonians $H(\lambda)$. The λ -evolution of the energy levels can be described by a set of ordinary first-order differential equations which closely resemble Newton's equations of motion and hence is formally equivalent to the molecular dynamics of a many-body system with each particle representing an energy level. The basic microscopic mechanism of the parametric evolution is the occurrence of avoided crossings ("collisions") between energy levels. The width distribution of avoided crossings in quantum systems whose classical counterparts possess a mixed phase space of regular and chaotic dynamics is shown to consist of two components: a near Gaussian distribution suggested by random matrix theory for the chaotic component and an approximately δ -shaped component originating from tori in the regular portion of phase space. The behavior of wavefunctions around avoided crossings is investigated. A statistical measure for overlapping avoided crossings based on parametric correlations of energy levels is introduced and shown to be sensitive to the fraction of classically chaotic phase space. Chapter 6 shows that, as λ elapses, the classical transition from predominantly regular motion to global chaos is accompanied by a transition from a nonequilibrium state to an equilibrium state in the parametric motion of quantum energy levels. The discussion of the source of ergodicity in the parametric motion leads to an equilibrium distribution function which provides an explanation for the Wigner-type distribution of nearest-neighbor spacings for classically chaotic systems. In Chapter 7, we will study the relaxation processes in the parametric motion of energy levels. The parametric energy-level dynamics is described in terms of the velocity autocorrelation function and the friction kernel of a many-body system. We show that the parametric motion is sensitively dependent upon the underlying classical dynamics, and there-

fore provide new measures of quantum chaos. The transition from classically regular to chaotic motion manifests itself in the disappearance of parametric diffusion. Semiclassical arguments give analytic approximations for the spectrum of the velocity autocorrelation function, and we compare these autocorrelation functions with those found in gases, liquids, and glasses. The effects of the continuum on the parametric level dynamics is discussed in Chapter 8. The set of ordinary first-order differential equations describing the parametric motion of the energy levels can be extended to include resonances (i.e., positions and widths). The two-body approximation indicates that the repulsion between the resonances is independent of the underlying classical dynamics and the distribution of nearest-neighbor spacings may not be sensitive to the underlying dynamics any longer. Therefore, parametric correlations rather than the distribution of nearest-neighbor spacings may play a crucial role in the identification of classical chaos. We suggest that the transition to the thermal equilibrium state in the parametric motion of resonances is the signature of classical chaos. We investigate the numerical solutions of this set of differential equations. The major advantage of this approach lies in the fact that a single solution provides "en route" the resonances for all parameters in the integration interval. Therefore, each resonance can be easily identified in contrast to other methods when the density of resonances is high and resonances begin to overlap. Using this method we determine parametric "trajectories" of resonances for a hydrogen atom in a strong electric field. The behavior of the width is quite different when real energies cross the top of the potential barrier. The distribution of the velocity of resonances for this regular system is far from a Maxwell-Boltzmann distribution. Chapter 9 is devoted to conclusions.

Chapter 2

The measures of classical chaos

Two quantities of classical chaos, the mean rate of exponential separation of nearby trajectories and the fraction of the volume of the accessible phase space in which the motion is chaotic, are introduced in this chapter. They measure the degrees of chaoticity of an individual classical orbit and the entire accessible phase space respectively and are needed in the study of quantum chaos. We shall prove the universal square-root law for the mean rate of separation of continuously deformed periodic orbits on a perturbation strength.

2.1 Character of classical regular and chaotic motion

An autonomous nondissipative system [2] with N degrees of freedom is described by a time-independent Hamiltonian function $H(q, p)$ where $q = (q_1, \dots, q_N)$ are the system's coordinates and $p = (p_1, \dots, p_N)$ are the canonical momenta conjugate to q . The canonical variables $x = (q, p)$ form a phase space of dimension $2N$. The trajectory in phase space $x(t) = (q(t), p(t))$ is determined by Hamilton's equations

$$\begin{aligned}\frac{d}{dt}q &= \nabla_p H \\ \frac{d}{dt}p &= -\nabla_q H\end{aligned}\tag{2.1}$$

with given initial conditions $x(0)$. One important result of the Hamiltonian equations (2.1) is that the Hamiltonian function is a constant of the motion,

i.e.

$$\frac{d}{dt}H(q, p) = \nabla_q H \cdot \frac{d}{dt}q + \nabla_p H \cdot \frac{d}{dt}p = 0 \quad (2.2)$$

where Eq. (2.1) has been used. The immediate consequence of Eq. (2.2) is that each trajectory is confined to an “energy surface” defined by

$$H(q, p) = E \quad (2.3)$$

which is a $(2N-1)$ -dimensional manifold embedded in the $2N$ -dimensional phase space.

Another important result of Eq. (2.1) is the Liouville’s theorem

$$\nabla_x \cdot \frac{dx}{dt} = \nabla_q \cdot \nabla_p H - \nabla_p \cdot \nabla_q H = 0 \quad (2.4)$$

which states the conservation of volume elements in phase space.

Eq. (2.1) can be written in a more compact way

$$\frac{d}{dt}x = J \frac{\partial H}{\partial x} \quad (2.5)$$

where $(\partial H / \partial x_i)$ is a vector of dimension $2N$ and J is a $2N \times 2N$ matrix

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (2.6)$$

The stability of a trajectory against perturbations and uncertainties can be measured by the rate of separation of nearby trajectories [10]. Consider two adjacent orbits $x(t)$ and $x'(t)$ in $2N$ -dimensional phase space with initial conditions x_0 and $x'_0 = x_0 + \Delta x_0$, respectively, as shown in Fig. 2.1. These trajectories evolve with time as described by Hamilton’s equations (2.5) yielding the separation $\Delta x(x_0, t) = x'(t) - x(t)$ with its Euclidean norm

$$d(x_0, t) = |\Delta x(x_0, t)|. \quad (2.7)$$

The mean rate of exponential separation

$$d(x_0, t) \approx d(x_0, 0)e^{\sigma t}, \quad (2.8)$$

is given by

$$\sigma(x_0) = \lim_{t \rightarrow \infty} \lim_{d(x_0, 0) \rightarrow 0} \frac{1}{t} \ln \frac{d(x_0, t)}{d(x_0, 0)}. \quad (2.9)$$

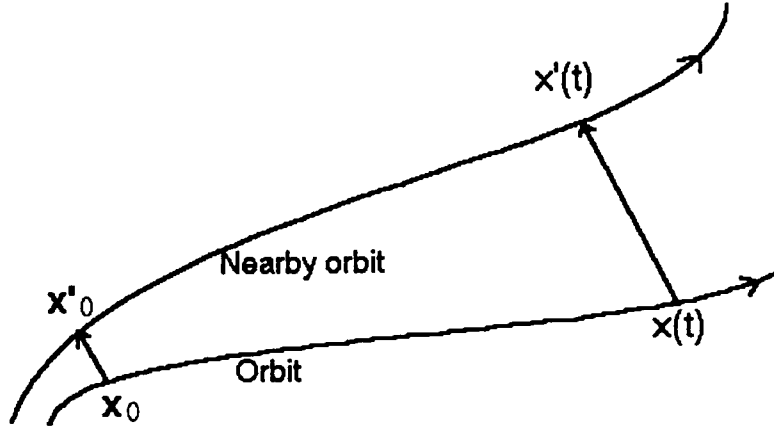


Figure 2.1: The separation of nearby trajectories.

Note that the two limits do not commute, hence $\sigma(x_0)$ is well-defined in the case of finite volume of the accessible phase space. $\sigma(x_0)$ will, in general, depend on the phase space direction of the initial separation Δx_0 . Since the phase space has $2N$ dimensions it is expected to find $2N$ σ 's (possibly nondistinct) for a given trajectory. These are named Lyapunov indices. A practical way of calculating the Lyapunov indices proceeds via the stability matrix $M(t)$ defined by [11]

$$\Delta x(x_0, t) = M(t)\Delta x_0 \quad (2.10)$$

where $\Delta x_0 \rightarrow 0$ and $M(t)$ is a $2N \times 2N$ matrix

$$M_{ij}(t) = \frac{\partial x_i(x_0, t)}{\partial (x_0)_j}. \quad (2.11)$$

Using an orthogonal transformation to diagonalize $M(t)$ in Eq. (2.10) and comparing the result with Eq. (2.8), the Lyapunov indices are determined by the eigenvalues of $M(t)$, ζ_i , through

$$\sigma_i = \lim_{t \rightarrow \infty} \frac{1}{t} \ln |\zeta_i|. \quad (2.12)$$

Because the stability matrix $M(t)$ is symplectic, i.e.

$$MJM^T = J, \quad (2.13)$$

where T denotes the transpose, its eigenvalues occur in pairs with the product of 1, i.e. for each ζ_i , there must be another ζ_j such that

$$\zeta_j = 1/\zeta_i. \quad (2.14)$$

For two-dimensional systems ($N = 2$), they are either complex conjugate pairs on the unit circle or reciprocal real numbers. Thus the corresponding Lyapunov indices are symmetric, i.e. for each σ_i there is another $\sigma_j = -\sigma_i$. Therefore, if a trajectory exponentially separates from the given orbit, there must be another trajectory exponentially approaching with the same rate. This is the consequence of Liouville's theorem (Eq. (2.4)) which states the incompressibility of the Hamiltonian flow in phase space.

The maximal Lyapunov index, σ_{max} , which is called the Lyapunov exponent, is of particular interest since it is a quantitative measure for the degree of chaoticity of a classical orbit. The trajectories with a vanishing Lyapunov exponent are stable under perturbations while those with a positive one are unstable. Unstable trajectories are the source of chaos. Q_{cl} , the fraction of the energy surface which is filled with unstable trajectories provides a measure of the irregularity for the system. Accordingly, autonomous Hamiltonian systems can be further divided into three groups. At one extreme, one has regular systems with all trajectories stable ($Q_{cl} = 0$), showing simple, predictable motion. At the other extreme are the totally chaotic systems with all trajectories unstable ($Q_{cl} = 1$). Then the separation between nearby trajectories is exponentially fast, the motion appears to be random and has strong statistical nature. The third and largest class is that of typical (or generic) systems with both stable and unstable trajectories ($0 < Q_{cl} < 1$), hence their phase space have mixed structures of regular and chaotic dynamics. Q_{cl} can be estimated by dividing the energy surface into cells and by counting the number of cells which are filled with unstable trajectories. One can also calculate the Lyapunov exponents for a large number of trajectories with uniformly distributed initial conditions, and Q_{cl} is given as the fraction of trajectories with non-zero Lyapunov exponent.

In one degree of freedom, the fact that energy E is conserved allows to express the momentum p as a function of the coordinate q alone, independent of the time, by inverting Eq. (2.3)

$$p = p(q, E). \quad (2.15)$$

The first of Hamilton's equations (2.1) yields

$$dt = \frac{dq}{\partial H / \partial p}. \quad (2.16)$$

Since the momentum p is replaced by Eq. (2.15) and $\partial H / \partial p$ is a function of the coordinate q only, the equation of motion has been reduced to quadratures

$$t - t_0 = \int_{q_0}^q \frac{dq}{\partial H / \partial p}. \quad (2.17)$$

This result excludes any exponential separation between bounded trajectories and therefore one-dimensional systems are regular. The integral in Eq. (2.17), however, can often only be evaluated numerically.

The key property which makes one-dimensional systems regular is the existence of one constant of motion. In general [11], for a regular N-dimensional system (possibly nonseparable) there exist N independent analytic single-valued functions $F_i(q, p)$ which are constants of motion, i.e.

$$\frac{d}{dt} F_i(q, p) = \{F_i, H\} = 0 \quad (2.18)$$

and are "in involution"

$$\{F_i, F_j\} = 0 \quad (2.19)$$

where $\{A, B\}$ is the Poisson bracket

$$\{A, B\} \equiv \nabla_p A \cdot \nabla_q B - \nabla_p B \cdot \nabla_q A. \quad (2.20)$$

These functions $F_i(q, p)$ are called "first integrals". A regular system is also said to be "integrable". As shown by Eq. (2.3), $H(q, p)$ is an integral of the system.

The existence of N constants of motion implies that trajectories of the system are confined in an N -dimensional manifold $\mathcal{M}$ defined by $F_i(q, p) = \text{constant}$ in the $2N$ -dimensional phase space. Except for one-dimensional case, the dimension of this manifold is smaller than the dimension of energy surface $H(q, p) = E$, which is $2N - 1$. It can be shown [12] that for bound motion in which the region of accessible phase space is finite, the manifold $\mathcal{M}$ is an N -dimensional torus. The topological character of a torus ("donut") is that there are N independent irreducible circuits c_i that cannot be shrunk to zero, as shown in Fig.(2.2).

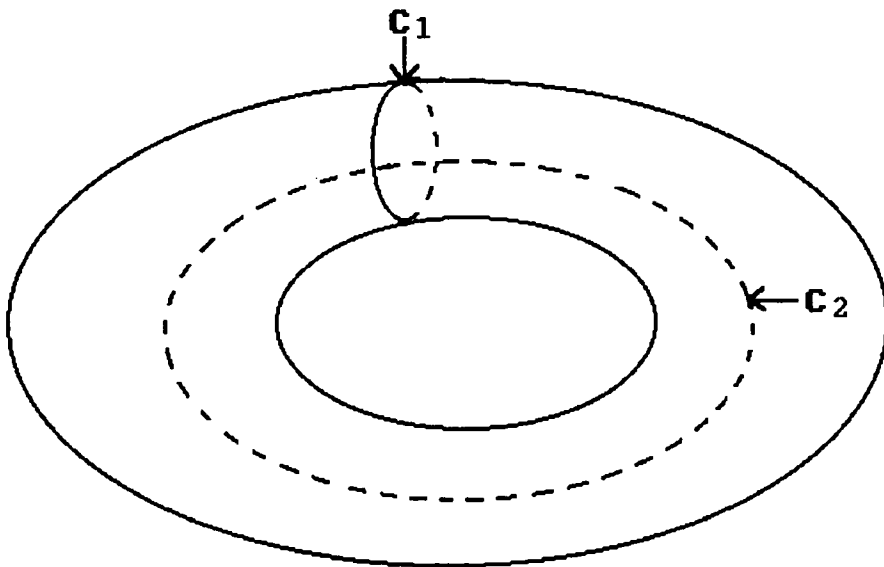


Figure 2.2: Illustration of two-dimensional torus where c_1 and c_2 are two irreducible circuits.

These tori are called invariant because an orbit starting out on one torus remains on this torus forever. One can define action-angle canonical variables which are topologically natural, i.e. the actions I_i measure the areas enclosed by circuits c_i , and the angles θ_i give the locations on the circuits. The actions can be defined by

$$I_i \equiv \frac{1}{2\pi} \oint_{c_i} p \cdot dq. \quad (2.21)$$

Eq. (2.21) gives the actions in terms of the first integrals (F_i) and vice versa. Since H is a first integral, it can be expressed as a function of the actions

$$H = H(I). \quad (2.22)$$

This result plays the central role in the semiclassical quantization of a regular system (see Chapter 4). The angles are canonically conjugate to the actions, i.e.

$$\theta \equiv \nabla_I S(q, I) \quad (2.23)$$

where the generating function $S(q, I)$ is the solution of the Hamilton-Jacobi equation

$$H(q, \nabla_q S) = H(I). \quad (2.24)$$

For a typical system ($Q_{cl} > 0$), the Hamiltonian contains perturbations which are “nonintegrable”, i.e. because of the perturbations, the number of the first integrals F_i is smaller than N , the number of degrees of freedom. Consider an autonomous system described by the Hamiltonian

$$H(\lambda) = H_0 + \lambda V, \quad (2.25)$$

where H_0 is a integrable Hamiltonian and V is, in general, a nonintegrable perturbation. When the control parameter λ is sufficiently small, most tori persist under the perturbation, although in distorted form. Some are destroyed, however, and they occupy a finite volume in phase space. Inside this volume, the motion is chaotic. These assertions were proved by Kolmogorov [13], Arnol’d [14] and Moser [15] and therefore are called “KAM theorem”. When λ increases, regular regions are invaded by chaotic parts and the system undergoes a transition from regular to chaotic motion. When the system reaches the state of being “metrically transitive”, i.e. is totally chaotic, all tori are destroyed and the only invariant manifolds left consist of one-dimensional isolated periodic trajectories and the energy hypersurface itself. We will later discuss their relevance for the semiclassical quantization of chaotic systems. The process of the destruction of tori will be demonstrated by a model system in the next section.

2.2 Coupled Morse oscillators

For our numerical studies in this thesis, we use the model system of two coupled Morse oscillators which provides a simple model for the stretching vibronic motion of linear triatomic molecules as shown in Fig. 2.3. This system has been extensively studied as a model for the quantum mechanics of a classically chaotic system with two degrees of freedom [16]. The Hamiltonian of this system is of the form of Eq. (2.25) and is given by [17]

$$\begin{aligned} H_0 &= \sum_{i=1}^2 H_0^i \\ H_0^i &= P_i^2/2M_i + V_i(r_i) \\ V &= -P_1 P_2/m, \end{aligned} \quad (2.26)$$

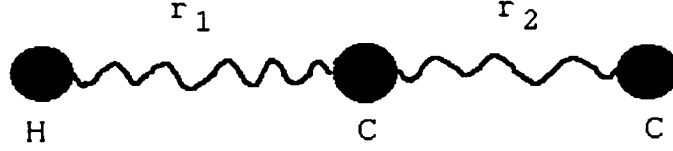


Figure 2.3: Illustration of the collinear vibronic motion of the triatomic molecule H-C-C represented by coupled Morse oscillators.

where M_i are the reduced masses for the two diatomic pairs in the molecule, m is the mass of the central atom and $V_i(r_i)$ are the corresponding Morse potentials [18],

$$V_i(r_i) = D_i \{1 - \exp[-a_i(r_i - r_{i0})]\}^2, \quad (2.27)$$

with r_{i0} the equilibrium distance, D_i the dissociation energy and a_i the scale parameter for the i^{th} diatomic pair. We use the molecular parameters for H-C-C.

The nonintegrable perturbation of the system is provided by the kinetic coupling between the two non-linear oscillators. The diagonalization of the kinetic energy part by an orthogonal transformation of coordinates r_i to q_i yields

$$\begin{aligned} q_1 &= \frac{1}{\sqrt{2}} [a_1(r_1 - r_{10}) + A a_2(r_2 - r_{20})] \\ q_2 &= \frac{1}{\sqrt{2}} [A a_1(r_1 - r_{10}) - a_2(r_2 - r_{20})] \end{aligned} \quad (2.28)$$

where $A = 2\lambda/(\sqrt{B^2 + 4\lambda^2} + B)$, and $B = (a_2^2/M_2 - a_1^2/M_1)m/(a_1 a_2)$. The trajectory with q_1 (or q_2) $\approx$ constant represents antisymmetric (or symmetric) vibration. We denote the corresponding canonical momentum by p_i .

For a system with two degrees of freedom, the phase space structure is easily seen with the help of a Poincaré surface of section which is defined as follows: Referring to Fig. 2.4, we consider a two-dimensional surface Σ_R in the phase space. The consecutive intersections generated each time the trajectory crosses the surface in a particular way (say, with $p_2 > 0$) are studied. The inversion of the energy conservation law $H(q_1, q_2, p_1, p_2) = E$

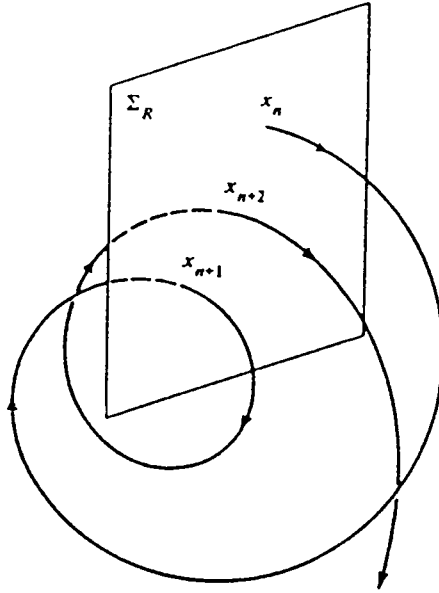


Figure 2.4: Definition of the Poincaré surface of section. Reprinted from A. J. Lichtenberg and M. A. Lieberman, *Regular and Chaotic Dynamics* (Springer-Verlag, New York, 1992).

gives p_2 , for example, in terms of the other three variables:

$$p_2 = p_2(p_1, q_1, q_2). \quad (2.29)$$

One needs, therefore, only to consider the projection of the orbit onto a three-dimensional volume (p_1, q_1, q_2) . The plane $q_2 = \text{constant}$ within this volume consists of a single coordinate q_1 and its canonical momentum p_1 . This plane is repeatedly pierced by the orbit if the motion is bounded and the consecutive crossings are obtained from one another by a canonical (thus area-preserving) transformation generated from original Hamilton's equations [10]. Therefore, the structure of the intersections is topologically invariant of the choice of the value of q_2 and the plane is a convenient choice for the surface of section. The consecutive intersections of the motion with the surface of section will in general occur anywhere within the classically allowed area on the plane. If in addition to E there exists another constant of the motion along the trajectory

$$F(q_1, q_2, p_1, p_2) = \text{constant}, \quad (2.30)$$

then Eqs. (2.29) and (2.30) lead to

$$p_1 = p_1(q_1, q_2). \quad (2.31)$$

Thus the consecutive intersections of the trajectory with the surface of section must lie on a curve, i.e. a one-dimensional manifold given by Eq. (2.31) with $q_2 = \text{constant}$. Hence the existence of constants of the motion can be determined by examination of the intersection of an orbit with a surface of section. Note that the $F(q_1, q_2, p_1, p_2)$ does not need to be global constant of motion. The only requirement here is that $F(q_1, q_2, p_1, p_2)$ remains constant for the particular trajectory under investigation.

Fig. 2.5 shows the Poincaré surfaces of section ($q_2 = 0$) for the coupled Morse oscillators at several selected values of the perturbation. The energy is fixed at $E = 0.75$ in the units of dissociation energy. In the integral limit (a: $\lambda = 0$), all intersections of trajectories fall on smooth curves. For the case of small perturbation (b: $\lambda = 0.2$), the motion is still mostly regular and we see two types of orbits: the simple invariant curve as in the integral limit and a multi-loop trajectory represented by the chain of small “islands”, in which the intersections jumps from one loop to another. The second type of motion is caused by the distorted tori. For large perturbation (c: $\lambda = 0.6$), the structure is dominated by chaotic orbits, in which the random dots are consecutive intersections of the surface of section. The invariant curves are limited to three isolated “islands” surrounded by a chaotic “sea”, the one island with $p_1 \approx 0$ represents antisymmetric vibration and the other two with $p_1 \neq 0$ represents symmetric vibration. In the strong perturbation region (d: $\lambda = 1$), the regular islands for symmetric motion are destroyed and the motion is mostly chaotic. The most striking feature is that the antisymmetric vibration is exceedingly stable and the system possesses a mixed classical phase space with coexisting regular and chaotic motion. We will show that this parametric change of the classical phase space structure as a function of λ manifests itself in the properties of quantum eigenenergies.

2.3 The universal behavior of the Lyapunov exponent

Since the Lyapunov exponent is the central quantity of classical chaos, it is interesting to analyze the λ -dependence of σ_{max} or, at least, to have a partial insight into its analytic properties. Note that σ_{max} can be, in general,

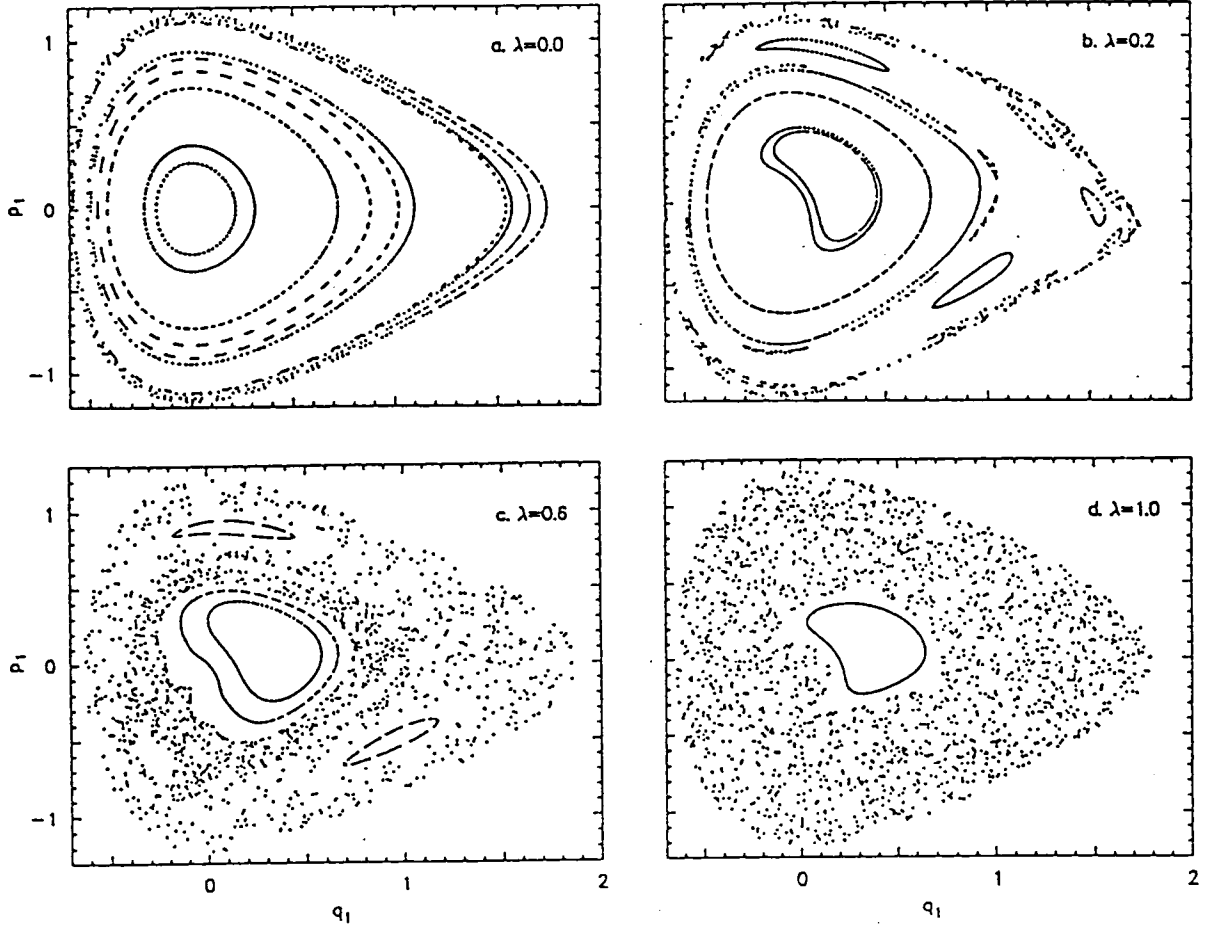


Figure 2.5: Poincaré surfaces of section ($q_2 = 0$) for coupled Morse oscillators at energy $E = 0.75$ in the units of dissociation energy.

calculated only numerically. For a periodic trajectory with period T we have [19]

$$M(nT) = M(T)^n. \quad (2.32)$$

Eq. (2.12) becomes

$$\sigma_i = \frac{1}{T} \ln |\zeta_i|, \quad (2.33)$$

where ζ_i is the eigenvalue of the stability matrix $M(T)$. The periodic motion allows one to avoid the execution of the long time limit ($t \rightarrow \infty$). Near the

integrable limit (i.e. λ is small), for those periodic orbits which are smoothly deformed by the perturbation, the stability matrix $M(T)$ is obtained in Appendix A to the leading order of λ . The eigenvalues of the matrix $M(T)$ are, in turn, approximately given by

$$\zeta_{3,\dots,2N} \approx 1, \quad (2.34)$$

and

$$\zeta_{1,2} \approx 1 \pm T\sqrt{C\lambda} \quad (2.35)$$

with

$$C = \sum_{i,j=1}^N \frac{\partial^2 H_0}{\partial I_i \partial I_j} < -\frac{\partial^2 V}{\partial \theta_j \partial \theta_i} >, \quad (2.36)$$

where $< >$ denotes time average over one period. If $C < 0$, by the requirement of Eq. (2.14), the solutions of Eq. (2.35) should be

$$\begin{aligned} \zeta_{1,2} &\approx 1 \pm iT\sqrt{|C|\lambda} \\ &\approx \exp(\pm iT\sqrt{|C|\lambda}). \end{aligned} \quad (2.37)$$

Hence the trajectory is stable, $\sigma_{max} = 0$ (Eq. (2.33)), and the winding number ν_w is given by

$$\nu_w \approx T\sqrt{|C|\lambda}/(2\pi). \quad (2.38)$$

The winding number ν_w describes the frequency ratio with which neighboring trajectories wind around the periodic orbit in phase space. If $C > 0$, then

$$\begin{aligned} \zeta_1 &\approx 1 + T\sqrt{C\lambda} \\ \zeta_2 &\approx \frac{1}{1 + T\sqrt{C\lambda}} \approx 1 - T\sqrt{C\lambda}. \end{aligned} \quad (2.39)$$

This corresponds to the unstable case and the Lyapunov exponent is given by (Eq. (2.33))

$$\sigma_{max} = \ln(\zeta_1)/T \approx \sqrt{C\lambda}. \quad (2.40)$$

We have therefore proved Benettin's conjecture [20] of the square-root law for the dependence of the Lyapunov exponent on the perturbation and found the winding numbers obey the same law (Eq. (2.38)). Because our proof is constructive, we also get the proportionality constant ($\sqrt{C}$) and a criterion which determines whether such a trajectory is chaotic or not. An example

of the square-root law is the near circular periodic trajectory of a hydrogen atom in a magnetic field [19].

The square-root law is violated when $C = 0$. This is the case of harmonic oscillator, since the unperturbed Hamiltonian of such system is $H_0 = \omega \cdot I$ (see Eq. (2.36)). As we will see repeatedly in this thesis, the linear dependence of the Hamiltonian on the action makes the harmonic oscillator very peculiar.

Chapter 3

Level statistics

In quantum chaos investigations, the most surprising and important discovery concerning spectral properties is that, depending on the underlying classical dynamics, the fluctuation of the spectra belongs to different universality classes (e.g. the Poisson distribution and the Wigner distribution for the nearest-neighbor spacings). These classes are well-reproduced by random matrix theory, the theory of level statistics. This theory is a rather old subject [21] in nuclear physics, developed nearly at the same time as the nuclear shell theory. The statistical theory, whose nature is essentially different from the study of individual levels, reveals new features of the system. Even for regular systems where the individual levels are known from semiclassical quantization, statistical methods are still essential for a more complete understanding. The situation is analogous to that in statistical mechanics where, instead of the positions and momenta of individual particles, the quantities such as temperature and entropy are very often more useful for many-body systems. In this chapter, the elementary measures of level statistics are discussed.

3.1 Different level sequences

Consider an interval of energy δE centered at E where E is measured from the energy of ground state. This interval is much smaller than E , whereas it contains many levels; that is

$$E \gg \delta E \gg \langle \Delta E \rangle, \quad (3.1)$$

where $\langle \Delta E \rangle$ is the mean distance between neighboring levels. The energy levels distributed in the interval form a sequence of $(E_1, E_2, \dots)$. In order to compare the level sequences from different systems, we first need to express the level spacings in common units. This can be done by rescaling the levels by its average spacing

$$\varepsilon_n = E_n / \langle \Delta E \rangle. \quad (3.2)$$

The procedure is known as “unfolding of the spectrum” which has been used in Eq. (1.7). After unfolding, the system-dependent mean level spacing has been eliminated and the new sequence $\{\varepsilon_n\}$ has a universal mean spacing of unity

$$\langle \varepsilon_{n+1} - \varepsilon_n \rangle = 1 \quad (3.3)$$

where $\langle \rangle$ denotes the average over the interval δE . The density of the sequence $\{\varepsilon_n\}$ is constructed by

$$\tilde{n}(\varepsilon) = \sum_n \delta(\varepsilon - \varepsilon_n). \quad (3.4)$$

As a consequence of Eq. (3.3), we have

$$\tilde{n}_{av} = 1. \quad (3.5)$$

The integrated density of the unfolded spectrum $\{\varepsilon_i\}$ is given by

$$N(\varepsilon) = \int_{-\infty}^{\varepsilon} d\varepsilon' \tilde{n}(\varepsilon'). \quad (3.6)$$

Fig. 3.1 displays a few examples of level series. The Poisson sequence (a) is generated randomly by a uniform distribution with no correlations. There are many near-degenerate pairs or sometimes even near-degenerate triples of levels as well as large gaps in this sequences. The sequence of prime numbers (b) is quite similar as the Poisson sequence, i.e. it is characterized by both quasi-degeneracies and large gaps. The excited levels of ^{167}Er within a subspace of given angular momentum and parity (c) is obtained from experiments. Small spacings in this sequence have a small probability of occurrence, and the case is similar for large spacings. But it is still far from being equally spaced. Sinai's billiard is defined as a particle moving freely inside the area specified by the inequalities, $y \geq 0, x \geq y, x \leq 1/2$, and $x^2 + y^2 \geq R$ where R is a parameter; i.e. the area bounded by 1/8 of a unit square and a circular arc whose center is the midpoint of the square. The

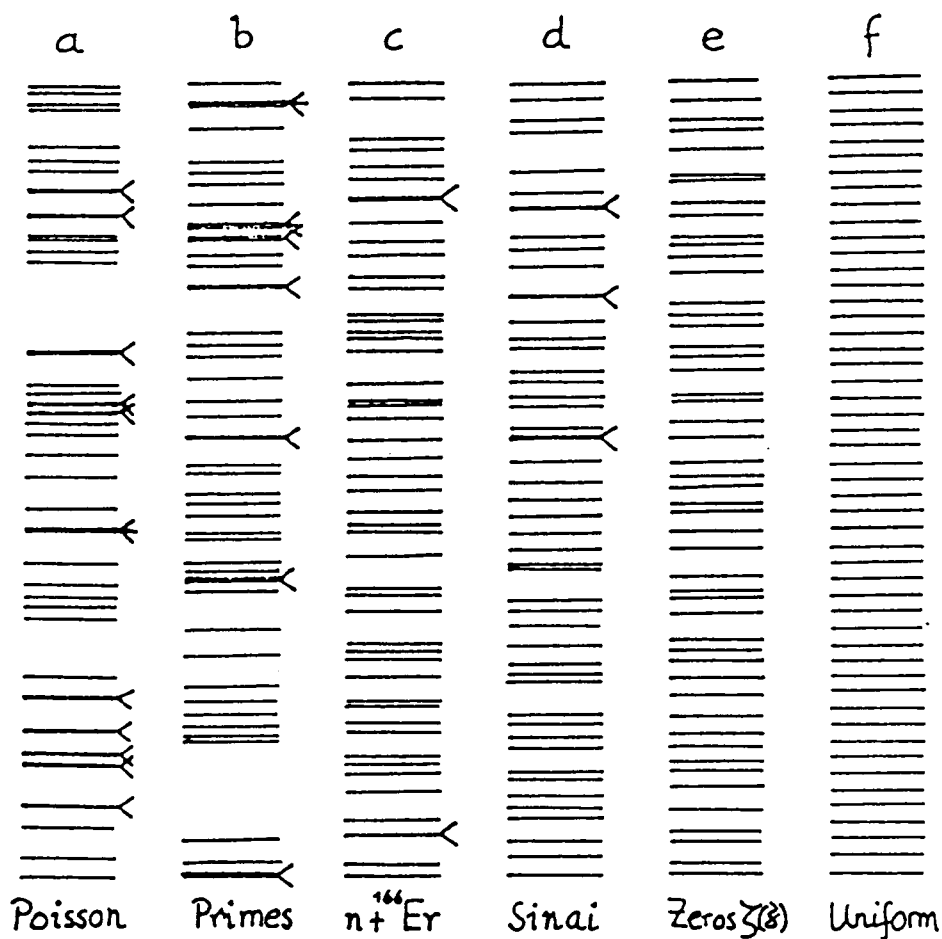


Figure 3.1: Some typical level sequences. (a) Poisson series. (b) Sequence of prime numbers. (c) Slow neutron resonance levels of the Erbium 166 nucleus. (d) Energy levels of Sinai's billiard. (e) The zeros of the Riemann zeta function on the line $\text{Re } z=1/2$. (f) A sequence of equally spaced levels (harmonic oscillators). Reprinted from O. Bohigas, R. U. Haq and A. Pandey, in *Nuclear Data for Science and Technology*, edited by K. H. Böckhoff, (Kluwer Academic Publ., Brussels, 1983), p.809.

system is classically chaotic. Its spectrum (d) appears similar as the spectrum of ^{167}Er . This observation is surprising considering the Hamiltonian of Sinai's billiard is much simpler than the Hamiltonian of the heavy nucleus ^{167}Er . The Riemann zeta function is defined by $\zeta(z) = \sum_{n=1}^{\infty} n^{-z}$ for $\text{Re } z > 1$ and its analytical continuation for other values of z . The spectrum of the zeros of this function in the line $\text{Re } z = 1/2$ (e) is more uniform than previous examples. The spectrum of one-dimensional harmonic oscillator (f) is equally spaced.

It is evident that there are both differences and similarities among the level sequences in Fig. 3.1. The level statistics provides a quantitative description of these properties. The simplest statistical measure is the distribution of the nearest-neighbor-spacings.

3.2 The distribution of the nearest-neighbor spacing

Let $(E_1, E_2, \dots, E_{\tilde{N}})$ be the positions of the successive levels in the interval δE and let $(\varepsilon_1, \varepsilon_2, \dots, \varepsilon_{\tilde{N}})$ be the corresponding unfolded spectrum. We define the relative spacing $s_n = \varepsilon_{n+1} - \varepsilon_n$. The nearest-neighbor-spacing (NNS) distribution $P(s)$ is defined by the condition that $P(s)ds$ is the probability for any s_n to have a value between s and $s+ds$, i.e.

$$P(s) = \lim_{\tilde{N} \rightarrow \infty} \frac{1}{\tilde{N}} \sum_{n=1}^{\tilde{N}} \delta(s - s_n). \quad (3.7)$$

Let $g(\Delta)d\Delta$ denote the pair correlation function, i.e. the conditional probability for finding a level in the interval $[\varepsilon + \Delta, \varepsilon + \Delta + d\Delta]$ when there is one at ε , i.e.

$$g(\Delta) = \text{average over } \varepsilon_n \text{ of } \sum_{m>n} \delta(\Delta - (\varepsilon_m - \varepsilon_n)). \quad (3.8)$$

Then $P(s)$ can be expressed as $g(s) \times$ (the probability for not having another level within spacing s). Therefore

$$P(s) = g(s) \int_s^{\infty} P(s') ds'. \quad (3.9)$$

This equation establishes an one-to-one relation between $P(s)$ and $g(\Delta)$. Solving it for the level spacing distribution, one finds

$$P(s) = g(s) \exp\left(-\int_0^s g(\Delta) d\Delta\right). \quad (3.10)$$

For the case of Poisson sequence in which the positions of the energy levels are generated randomly by a uniform distribution with no correlations, the probability for any ϵ_n to fall between ϵ and $\epsilon + d\epsilon$ is independent of ϵ and is simply given by $d\epsilon$. Consequently,

$$g(\Delta) = 1. \quad (3.11)$$

Substitution of (3.11) into (3.10) immediately leads to

$$P(s) = e^{-s} \quad (3.12)$$

which is the Poisson distribution of Eq. (1.8).

For a complex system with many degrees of freedom like a heavy nucleus, detailed properties of the spectrum are not readily accessible to calculation. Random matrix theory (RMT) makes the hypothesis that the local statistical properties of the energy levels of such systems behave as if they were obtained from the eigenvalues of a matrix with randomly distributed elements. Based on the assumptions that the matrix elements are independently distributed and that the distributions are invariant under orthogonal transformations, the distribution of the Hamiltonian matrix for the systems with the symmetry of time reversal is given by the Gaussian orthogonal ensembles (GOE) [22], i.e. the distributions of diagonal elements H_{ii} and off-diagonal elements H_{ij} are given by

$$\begin{aligned} P(H_{ii}) &= (1/2)^{1/2} e^{-\pi H_{ii}^2/2} \\ P(H_{ij}) &= e^{-\pi H_{ij}^2}. \end{aligned} \quad (3.13)$$

Notice that

$$2 \langle H_{ij}^2 \rangle = \langle H_{ii}^2 \rangle = \frac{1}{2\pi}. \quad (3.14)$$

We have chosen the value of $\langle H_{ii}^2 \rangle$ such that the average spacing is equal to one. For a small spacing where the two-level approximation is valid, the eigenenergies are determined by

$$\det \begin{pmatrix} H_{11} - \epsilon & H_{12} \\ H_{12} & H_{22} - \epsilon \end{pmatrix} = 0. \quad (3.15)$$

After a straightforward calculation, one finds

$$\Delta\epsilon = \epsilon_+ - \epsilon_- = \sqrt{(H_{11} - H_{22})^2 + 4H_{12}^2}. \quad (3.16)$$

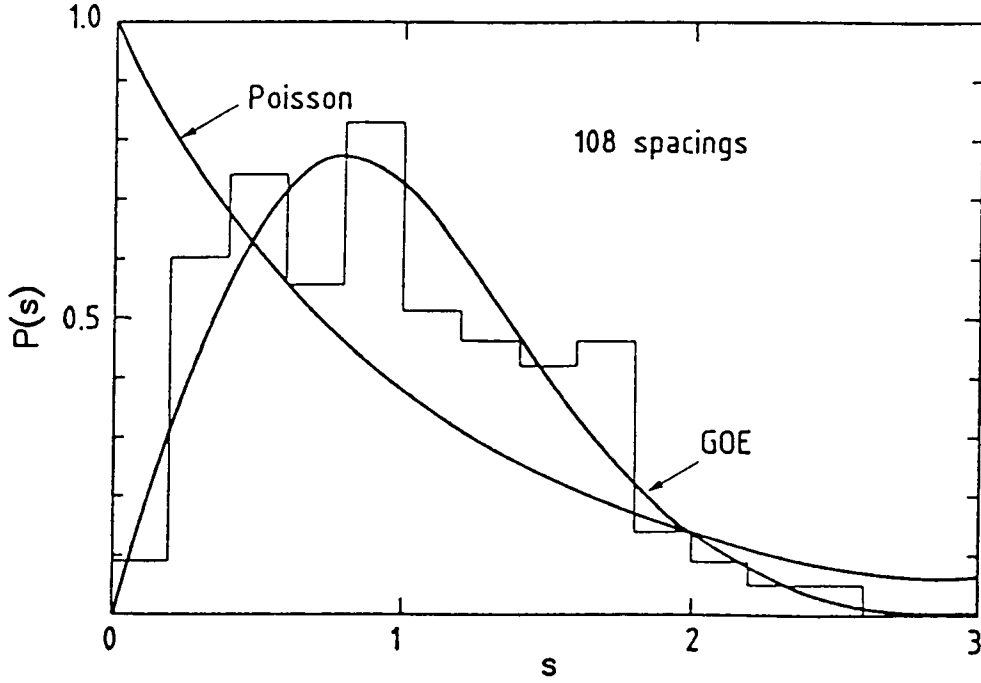


Figure 3.2: NNS distribution for $^{167}\text{Erbium}$. The histogram shows the first 108 levels observed. The solid curves correspond to Poissonian and Wigner distributions. Reprinted from H. I. Liou et al., Phys. Rev. C 5, 974(1972).

Hence the NNS distribution becomes [9]

$$\begin{aligned}
 P(s) &\approx \int \delta(s - \sqrt{(H_{11} - H_{22})^2 + 4H_{12}^2}) P(H_{11})P(H_{22})P(H_{12}) dH_{11}dH_{22}dH_{12} \\
 &= \frac{\pi}{2} s e^{-\pi s^2/4}.
 \end{aligned} \tag{3.17}$$

This is the Wigner distribution of Eq.(1.9). From (3.17) one finds (Eq. (3.10))

$$g(\Delta) \approx \frac{\pi}{2} \Delta. \tag{3.18}$$

Fig.3.2 compares the NNS distribution of the first 108 levels of $^{167}\text{Erbium}$ with Wigner distribution. The overall agreement is obvious.

The remarkable discovery of quantum chaos investigations [23] is that, although the Hamiltonian of a classically chaotic system with a few degrees

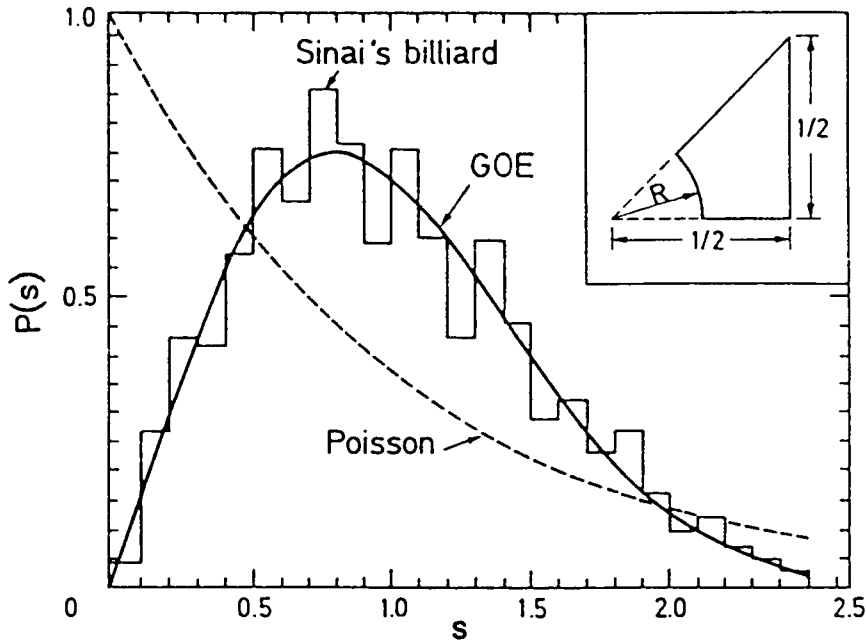


Figure 3.3: NNS distribution for Sinai's billiard. The histogram shows the distribution of calculated energy levels. Reprinted from O. Bohigas, M. J. Giannoni and C. Schmit, *Phys. Rev. Lett.* **52**, 1(1984).

of freedom is simple and the elements of the Hamiltonian matrix are well-defined, the fluctuations of energy levels for such a system still follow the predictions of the random matrix theory. Fig. 3.3 shows the NNS distribution of Sinai's billiard compared with the GOE distribution.

The results of the spectral fluctuations for classically regular systems are also surprising [24]. Apart from untypical exceptions, i.e. one-dimensional systems and harmonic oscillators, the classically integrable systems have scaled levels that are locally uncorrelated and well described by the Poissonian sequences.

Therefore, dependent on the underlying classical dynamics, the NNS distributions of quantum spectra belong to different universality classes. The main feature is that the spectra of classically regular systems are dominated by level clustering,

$$P_{\text{Poisson}}(s)_{s \rightarrow 0} \approx 1, \quad (3.19)$$

while the spectra of classically totally chaotic systems with time reversal

symmetry are characterized by linear repulsion , i.e.

$$P_{Wigner}(s)_{s \rightarrow 0} \propto s. \quad (3.20)$$

The level repulsion is caused by avoided crossings between adjacent levels when a nonintegrable perturbation is turned on. Avoided crossings provide the microscopic mechanism for the transition of the spectra from Poissonian distribution to a GOE distribution. The properties of avoided crossings will be discussed in Chapter 5.

The situation concerning fluctuations in mixed systems, which is the generic case, is more complicated and less clear [25]. In order to understand the level statistics in the transition regime, Brody [26] suggested an empirical formula which describes the NNS distribution for generic systems of Eq. (2.25) quite well

$$g(\Delta) = A\Delta^\kappa. \quad (3.21)$$

From Eq. (3.10) we get

$$P(s) = As^\kappa \exp(-Bs^{1+\kappa}) \quad (3.22)$$

where $A = (1 + \kappa)B$, $B = \Gamma^{1+\kappa}((2 + \kappa)/(1 + \kappa))$, and κ is found by fitting the “experimental” NNS distribution (usually obtained from large-scale matrix diagonalization) with a distribution of the form Eq. (3.22). The Brody distribution (Eq. (3.22)) interpolates between the Poissonian distribution ($\kappa = 0$) and the Wigner distribution ($\kappa = 1$). As λ in Eq. (2.25) increases, κ should (not always monotonically) increase from 0 to 1. A microscopic analysis of the behavior of the Brody parameter $\kappa(\lambda)$ will be given in Chapter 6.

Fig. 3.4 illustrates the NNS distribution for the coupled Morse oscillators (histogram) with a superimposed Brody distribution where the Brody parameter κ is determined by the best fit of Eq. (3.22) to the histogram. The energy levels contributing to the statistics are within the interval of 0.75 ± 0.1 in the units of the dissociation energy. In the integrable region, $\kappa \approx 0$ and therefore the distribution is Poissonian while in the mostly chaotic region, $\kappa \approx 0.8$, indicating a Wigner-type distribution.

Fig. 3.5 displays the corresponding pair correlation functions for the coupled Morse oscillators (histogram) with Eq. (3.21) where the Brody parameter κ is taken from the NNS distribution. In the integrable region, the data are described by a Poisson distribution quite well corresponding to an approximate constant (≈ 1) pair correlation function. In the mostly chaotic region, a “hole” appears near the origin and $g(\Delta)$ saturates (≈ 1) for large

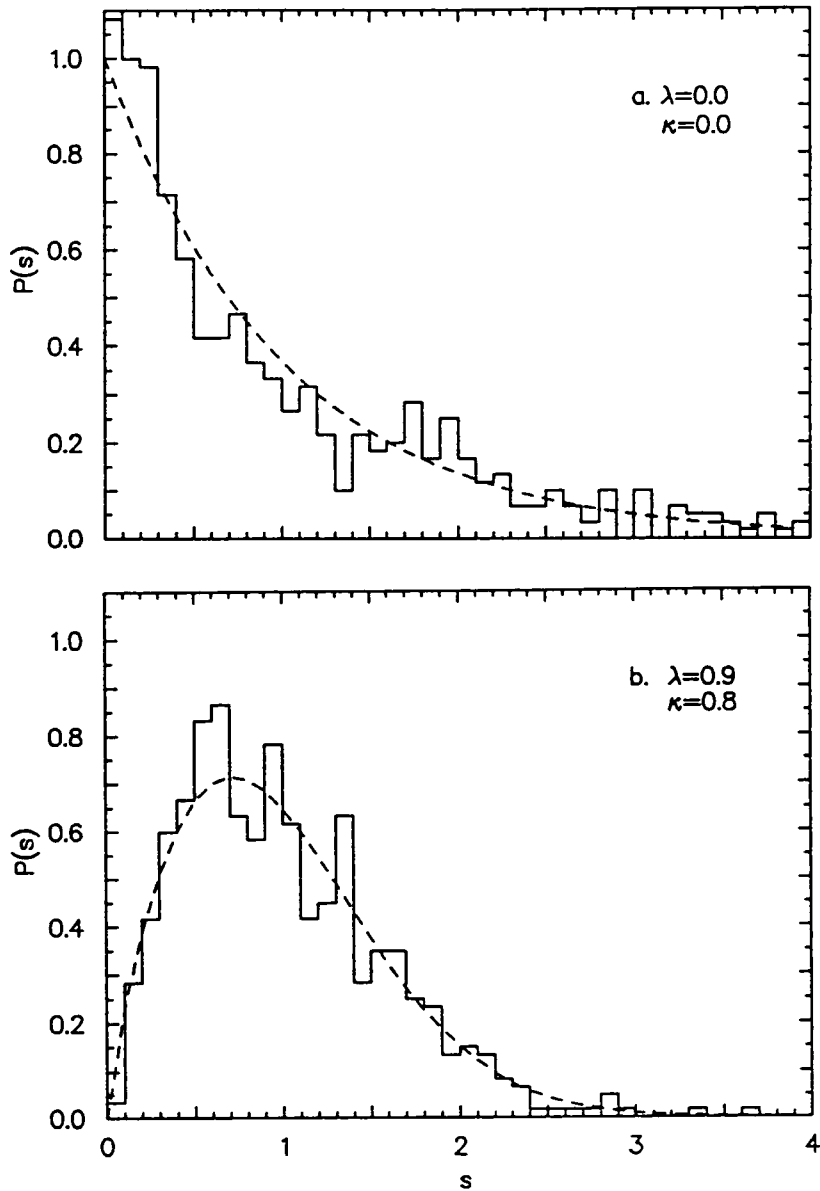


Figure 3.4: NNS distribution for coupled Morse oscillators $P(s)$ (histograms) for: (a) in the integrable regime ($\lambda = 0$) where the dashed line is the Brody distribution with $\kappa = 0$. (b) in the mostly chaotic regime ($\lambda = 0.9$) where the dashed line is the Brody distribution with $\kappa = 0.8$.

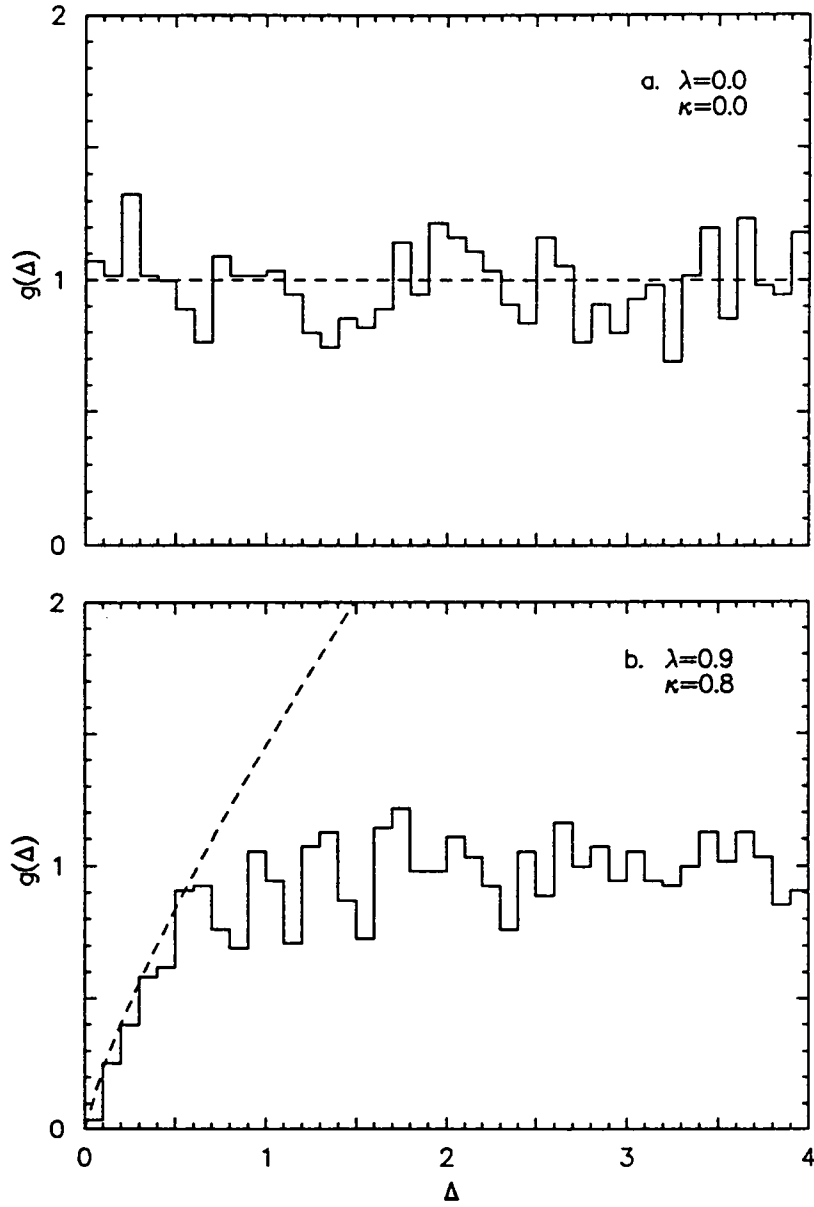


Figure 3.5: Pair correlation function $g(\Delta)$ for coupled Morse oscillators (histogram): (a) in the integrable regime ($\lambda = 0$) where the dashed line is Eq. (3.21) with $\kappa = 0$. (b) in the mostly chaotic regime ($\lambda = 0.9$) where the dashed line is Eq. (3.21) with $\kappa = 0.8$.

Δ , representing the existence of short range ($\Delta \leq 1$) correlations and large range randomness. We note here an interesting correspondence: the pair correlation function in the regular domain resembles that of a gas while $g(\Delta)$ for the mostly chaotic domain resembles that of a liquid. This gas-liquid transition will be discussed in Chapter 7. Note that in the classically mostly chaotic regime, Eq.(3.21) fits the data only in the range of $\Delta \leq 1$. For larger Δ , it increases continuously rather than saturating around a constant. The interesting observation is that although $g(\Delta)$ (Eq. (3.21)) does not behave correctly for large Δ (Fig.3.5b), the corresponding $P(s)$ (Eq.(3.22)) still gives overall a good description of the distribution (Fig.3.4b) indicating that $P(s)$ is insensitive to the behavior of $g(\Delta)$ in the region of large Δ . The reason is that for large s , $P(s)$ is exponentially small, hence the contributions as well as deviations become unimportant. Consequently, if one knows $P(s)_{s \rightarrow 0} \propto s^\kappa$, one can approximately obtain $P(s)$ for all s by Eq.(3.22) without introducing a significant error. This is the standard procedure for deriving the Wigner distribution [22], and we will use it in Chapter 6.

Chapter 4

Semiclassical quantization theory

Although the random matrix theory describes the universality classes of the fluctuations of quantum spectra very well, it is an empirical theory. We need to justify the application of such a theory. Ensembles involving a large number of energy levels for a given Hamiltonian represent properties of the quantum system in a state of high excitation far away from the ground state and can therefore be described by semiclassical mechanics. The success and failure of semiclassical mechanics to provide insights into the origin of the universality classes in level statistics will be discussed in this chapter. We shall apply the semiclassical quantization to the system of a hydrogen atom in a magnetic field and show that the analysis of isolated unstable periodic orbits can lead to a deeper understanding of the structure of complex spectra.

4.1 Semiclassical trace formula for the density of quantum states

We start with the eigenfunction expansion of the propagator $K(q', q, t)$

$$K(q', q, t) = \sum_n e^{-iE_n t/\hbar} \langle n|q' \rangle \langle q|n \rangle \quad (4.1)$$

where $\langle q|n \rangle$ is the coordinate representation of the eigenvector $|n \rangle$. Its Laplace transform leads to the Green's function

$$G(q', q, E) = \frac{1}{\pi \hbar} \int_0^\infty e^{iEt/\hbar} K(q', q, t) dt. \quad (4.2)$$

This gives an expression for the density of physical energy levels

$$n(E) = \sum_n \delta(E - E_n) \quad (4.3)$$

in terms of the Green's function:

$$n(E) = 2 \text{Re} \int d^N q G(q, q, E). \quad (4.4)$$

Feynman's path integral [27] provides a general connection between classical paths and the quantal propagator $K(q', q, t)$:

$$K(q', q, t) = \int D[q] e^{iS(q', q, t)/\hbar}, \quad (4.5)$$

where

$$S(q', q, t) = \int_0^t d\tau (p(\tau) \dot{q}(\tau) - H(p(\tau), q(\tau))) \quad (4.6)$$

is the action along a path $q(\tau)$, $p(\tau)$ (possibly classically forbidden) with the boundary condition $q(0) = q$, $q(t) = q'$ and $D[q]$ denotes the functional integration over all paths with the above boundary conditions. The path integral is therefore a natural starting point for semiclassical mechanics [28]. In the semiclassical limit ($S/\hbar \rightarrow \infty$), the contributions of $e^{iS/\hbar}$ to the functional integral have a sharp maximum around the saddle point of the action S , i.e. for the classically allowed path, and the contributions from other points cancel each other since $e^{iS/\hbar}$ fluctuates rapidly around these points. Then one can expand the action S to second order in the departure δq from the saddle point and evaluate the resulting Gaussian integrals. This method is called the stationary phase evaluation. After stationary phase evaluation of Eq. (4.5) one gets the semiclassical approximation of the propagator ("van Vleck propagator") [29]

$$K_{sc}(q', q, t) = \frac{1}{(2\pi i \hbar)^{N/2}} \sum_\nu |D_\nu|^{1/2} \exp i \left(\frac{S_\nu}{\hbar} - \frac{\alpha_\nu \pi}{2} \right) \quad (4.7)$$

where ν denotes different classically allowed orbits, S_ν the action round the ν^{th} trajectory, α_ν the number of caustics encountered along orbit ν , and

$$D_\nu(q', q, t) = \det\left(-\frac{\partial^2 S_\nu}{\partial q' \partial q}\right). \quad (4.8)$$

Caustics are the envelopes of the families of classical orbits which are given by $\det(\partial q_i(t)/\partial p_j(0))_{q(0)} = 0$ [28]. After substitution K_{sc} into Eq. (4.2), the integration over time can be easily performed by stationary phase evaluation and one has the semiclassical approximation of the Green's function

$$G_{sc}(q', q, E) = \frac{1}{i\hbar(2\pi i\hbar)^{(N-1)/2}} \sum_\nu |\Delta_\nu|^{1/2} \exp i\left(\frac{S_\nu}{\hbar} - \frac{\alpha_\nu \pi}{2}\right) \quad (4.9)$$

with

$$\Delta_\nu = -\left(\frac{\partial^2 S_\nu}{\partial E^2}\right)^{1-N} \det\left(\frac{\partial^2 S_\nu}{\partial E^2} \frac{\partial^2 S_\nu}{\partial q' \partial q} - \frac{\partial^2 S_\nu}{\partial q' \partial E} \frac{\partial^2 S_\nu}{\partial q \partial E}\right). \quad (4.10)$$

However, the evaluation of the trace $\int d^N q$ in Eq. (4.4) for a generic system is not obvious. If the underlying Hamiltonian is integrable, the trajectories form continuous families of tori and it is possible to transform to action-angle variables. Then the operation of taking the trace corresponds to a trivial multiplication [30]. On the other hand, if all closed trajectories are isolated, the trace can be evaluated by the method of stationary phases [31]. This is the case for totally chaotic systems and one-dimensional (hence integrable) systems. Therefore, these two extremes, the case of the existence of tori and the case of the isolated periodic orbits, are equivalent only for one-dimensional systems and do not, in general, contain each other. Nevertheless, they lead to the similar expressions for the spectral density

$$n(E) = n_{av} + \sum_\nu \frac{A_\nu}{\hbar^{1+\mu}} \exp\left(i\frac{S_\nu(E)}{\hbar} - \frac{\pi}{2}\alpha_\nu\right). \quad (4.11)$$

In this formula, ν labels either all isolated periodic trajectories for totally chaotic systems or all rational tori which are formed by families of periodic trajectories for integrable systems, including multiple traversals (negative – i.e. retracings – as well as positive) so that the sum is real. The information about the stability of trajectory ν is contained in the real amplitude A_ν . For a regular system with N freedoms the exponent μ is given by $\frac{1}{2}(N-1)$ (periodic trajectories form $(N-1)$ parameter families filling tori), while for a

totally chaotic system it is zero (isolated unstable periodic trajectories form zero parameter families). n_{av} is given by the Thomas-Fermi approximation [32]

$$n_{av} = \frac{1}{(2\pi\hbar)^N} \int d^N p d^N q \delta(E - H(p, q)). \quad (4.12)$$

This result is the old quantum mechanics rule that there is one quantum state per Planck cell in phase space. Consequently, the mean level spacing is in the order of

$$\langle \Delta E \rangle = 1/n_{av} \propto \hbar^N. \quad (4.13)$$

We can see from Eq. (4.11) that the spectrum of eigenvalues is determined by a background contribution from the whole energy surface, n_{av} , and oscillatory modulations from the periodic orbits, n_{fl} :

$$n(E) = n_{av} + n_{fl}. \quad (4.14)$$

For an integrable system [33], Eq. (4.11) is convergent resulting in the familiar Einstein-Brillouin-Keller (EBK) quantization rule

$$E_n = H(I_n), \quad I_n = (n + \frac{\alpha}{4})\hbar \quad (4.15)$$

which provides the essential information about individual levels. Using the EBK quantization, Berry and Tabor [24] proved rigorously that the distribution of nearest-neighbor spacings $P(s)$ for an integrable system is indeed a Poissonian distribution. The two exceptions are harmonic oscillators and one-dimensional systems. Berry and Tabor showed that there is no general NNS distribution for multi-dimensional harmonic oscillators. Based on the EBK quantization, we show in Appendix B that the unfolded spectra of one-dimensional systems form a universality class of equally spaced sequence and the NNS distribution for such systems is $\delta(s - 1)$. Therefore, semiclassical theory provides the dynamical origin for the existence of universality classes in the spectrum fluctuations of integrable systems.

For a chaotic system, on the other hand, the trace formula Eq. (4.11) is divergent [34]. The reason is that the number of orbits with period T proliferates exponentially with T [35], or more precisely,

$$\begin{aligned} \rho(T) &= \frac{\text{number of orbits with periods between } T \text{ and } T + dT}{dT} \\ &= \exp(h_K S T)/T \quad T \rightarrow \infty \end{aligned} \quad (4.16)$$

where h_{KS} is the Kolmogorov-Sinai entropy defined by the sum of the Lyapunov indices larger than 0, i.e.

$$h_{KS} = \sum_{\sigma_i > 0} \sigma_i. \quad (4.17)$$

The explicit expression of the trace formula for chaotic systems [31] is given by

$$n(E) = n_{av} + Im \sum_{\nu} \frac{iT_{\nu}}{\pi \hbar} \frac{t_{\nu}}{1 - t_{\nu}} \quad (4.18)$$

with

$$t_{\nu} = \exp(iS_{\nu}(E)/\hbar - i\alpha_{\nu}\pi/2 - h_{KS}T_{\nu}/2), \quad (4.19)$$

where the sum runs over all primitive periodic orbits ν and we have used the long period limit for the expression of the stability matrix. In this limit, we can replace the sum in (4.18) by $\int dT \rho(T)$ resulting

$$n_{fl} \propto \int dT \exp(h_{KS}T/2) \quad (4.20)$$

which is divergent. From the uncertainty principle for energy and time

$$\Delta E \Delta T \sim \hbar, \quad (4.21)$$

one expects that the orbits that contribute to resolve the structures on the scale smaller than the mean level spacing (Eq. (4.13)) have periods

$$T > \hbar n_{av} \propto \hbar^{-(N-1)} \rightarrow \infty \quad \text{when } \hbar \rightarrow 0. \quad (4.22)$$

Because of divergence, the trace formula Eq. (4.18) is, in general, unable to provide the detailed information on a large number of individual highly excited levels for chaotic systems [36] and fails to give the dynamical origin for the existence of the Wigner-type NNS distribution. This result suggests the need of other approaches.

4.2 Application of semiclassical quantization to hydrogen atom in a magnetic field

Although the trace formula (Eq. (4.18)) is divergent and not suited to give the information on individual levels, it is still useful to understand the cluster structures in quantum spectra qualitatively or some times even quantitatively, because those structures are related to either one particular trajectory

[37] or a set of trajectories as we will show in this section for the system of hydrogen atom in a magnetic field. In order to improve the convergence of the trace formula for a given set of trajectories, we consider the integrated density of states, i.e. the number of states with energy $\leq E$

$$\mathcal{N}(E) = \int_{-\infty}^E dE' n(E') = \mathcal{N}_{av} + \mathcal{N}_{fl}. \quad (4.23)$$

Because of the classical identity

$$\frac{dE}{dS} = \frac{1}{T}, \quad (4.24)$$

the convergence of the integrated density $\mathcal{N}(E)$ is improved by the factor $1/T$ for a given set of classical trajectories compared with the density of states $n(E)$ and hence $\mathcal{N}$ is easier for a numerical calculation. Substituting Eq. (4.18) into Eq. (4.23) and using Eq. (4.24) to change the variable of integration from energy to action, we have

$$\mathcal{N}_{av}(E) = \frac{1}{(2\pi\hbar)^N} \int d^N p d^N q \Theta(E - H(p, q)). \quad (4.25)$$

and

$$\mathcal{N}_{fl} = -\frac{\theta}{\pi} \quad (4.26)$$

where θ is the argument of the complex number $\prod_{\nu}(1 - t_{\nu})$.

The Hamiltonian of a hydrogen atom in a uniform magnetic field [6] is given by (in atomic units $m_e = e = \hbar = 1$)

$$H = \frac{P^2}{2} - \frac{1}{r} + \frac{\gamma}{2} L_z + \frac{\gamma^2}{8} \rho^2, \quad (4.27)$$

where the direction of the field is taken as the z -direction and $\gamma = B/B_0$ ($B_0 = 2.35 \times 10^5 Tesla$). The derivation of (4.27) is briefly discussed in Chapter 1 (see Eq. (1.2)). The azimuthal component of angular momentum L_z is conserved because of rotational symmetry and it can be therefore replaced by a number. The z -parity π defined with respect to reflection at the xy -plane which is perpendicular to the direction of the magnetic field is also conserved. In each L_z^{π} subspace of the Hilbert space, the Schrödinger equation defined by the Hamiltonian (4.27) remains nonseparable in the two coordinates z , parallel, and ρ , the cylindrical coordinate perpendicular, to the field. Leaving

out the contribution of the normal Zeeman term $\frac{\gamma}{2}L_z$ because it contributes a L_z -dependent but trivial additive constant to the energy, the Hamiltonian (4.27) is of form of Eq. (2.25) with $\lambda \propto \gamma^2$. This system is an experimentally accessible physical system that has been studied in the laboratory [38] and provides a prototype for the study of quantum chaos. We apply now the trace formula Eq. (4.26) to this system and show that the analysis of the classical dynamics, and in particular of the important role of isolated unstable periodic orbits embedded in the chaotic part of the phase space, can lead to a deeper understanding of the structure of complex spectra. We restrict ourselves to the case of $L_z = 0$.

In the limit of large magnetic field $\gamma \rightarrow \infty$, the motion in ρ -direction is strongly bounded by the diamagnetic term $\frac{\gamma^2}{8}\rho^2$, therefore $\langle \rho \rangle \ll \langle z \rangle$. The problem approaches that of a one-dimensional hydrogen atom parallel to the field [39] with the potential

$$-\frac{1}{r} \approx -\frac{1}{|z|} \left(1 + O\left(\frac{\langle \rho \rangle^2}{\langle z \rangle^2}\right)\right) \quad (4.28)$$

and the spectrum is given by

$$E_{N,n} = (N + 1/2)\gamma - \frac{1}{2(n - \mu)^2} \quad (4.29)$$

which form a sequence of Rydberg series converging to the respective ionization threshold $(N + 1/2)\gamma$, where N ($= 0, 1, 2, \dots$, the Landau quantum number) and n (the principle quantum number) are the quantum numbers in ρ and z directions respectively, and μ is the quantum defect (in fact, quantum excess since $\mu < 0$) caused by residual coupling between z and ρ directions. As the field strength is reduced to values around $\gamma = 1$, the Rydberg series associated with the different Landau channels begin to overlap and couple. At the laboratory field strength ($\gamma \sim 10^{-5}$), a huge number ($\sim 10^5$) of Rydberg series are overlapping and the interchannel coupling makes the spectrum extremely complicated.

However, in the region of ionization threshold, the structures on the scale of the average spacing was revealed by the high resolution ($\sim 10^{-8}$) experiments at fields around 6T ($\gamma \sim 10^{-5}$) by Iu et al. [40] and confirmed by a numerical diagonalization of $90,000 \times 90,000$ complex matrices by Delande et al. [41]. Fig. 4.1 is the result of experiment. The ionization threshold is around 2.8cm^{-1} ($1\text{cm}^{-1} = 0.4556 \times 10^{-5}$ atomic units). The most striking feature of the observed spectra is the existence of Rydberg series which are

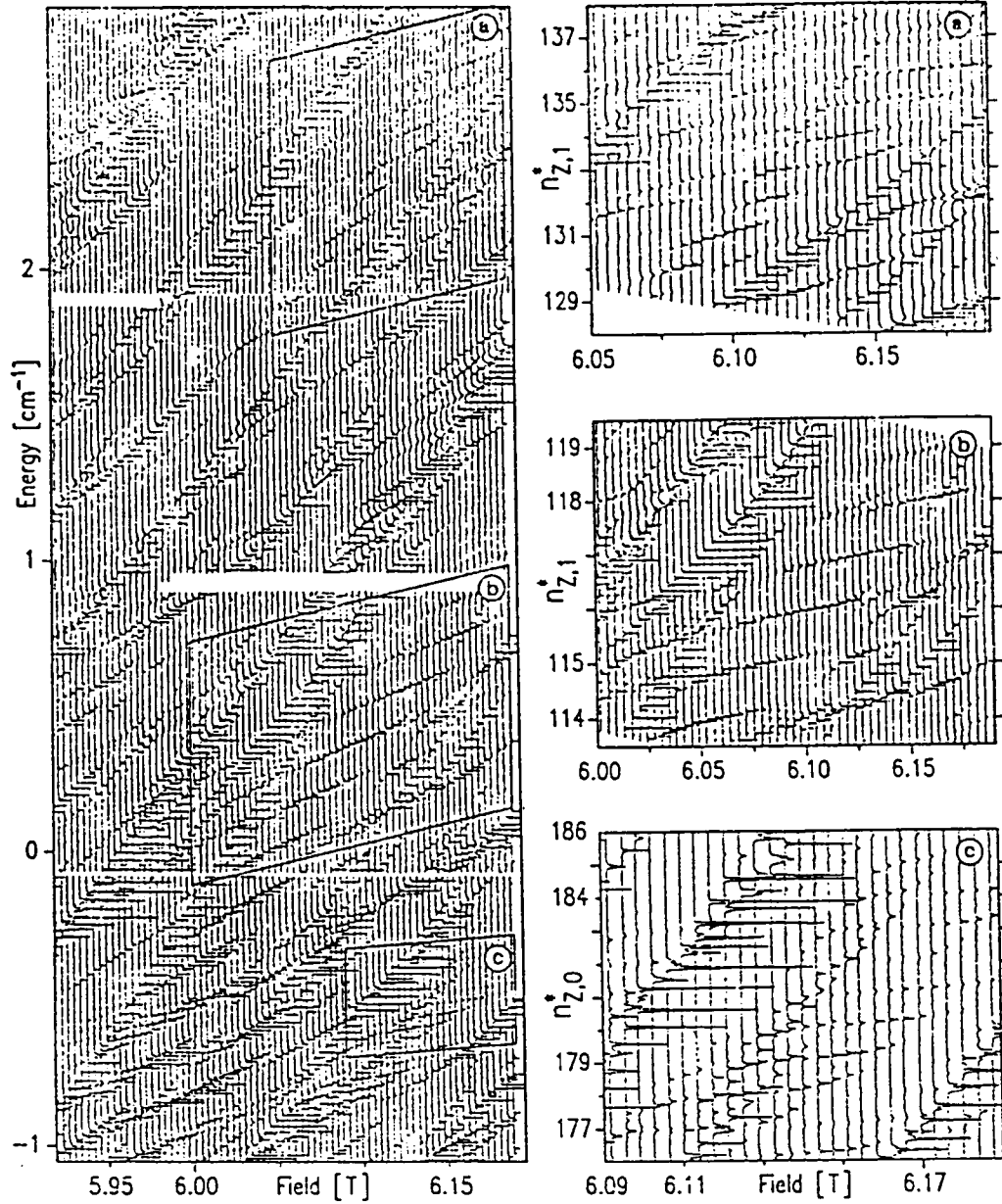


Figure 4.1: Energy-level map of odd-parity $L_z = 0$ states of lithium in an applied magnetic field (in Tesla units). Horizontal peaks are field ionization signals. The plots for the outlined regions are shown at the right by $n_{z,N}^* = n - \mu$ which is derived from Eq.(4.29). (a), (b) $N = 1$; (c) $N = 0$. A progression of Rydberg states appears as a series of lines with unit separation. The ionization threshold lies at approximately $+2.8\text{cm}^{-1}$. Reprinted from C. Iu et al., Phys. Rev. Lett. 63, 1133(1989).

disturbed by a number of widely spaced strong lines with large slopes with the magnetic field. Avoided crossings and other phenomena associated with level couplings are apparent, but they do not completely destroy the orderly structures.

The detailed investigation of the structure is based on Eq.(4.29). A Rydberg series has two features. The slope of the family is determined by its Landau quantum number

$$\frac{dE_{N,n}}{d\gamma} \approx (N + 1/2), \quad (4.30)$$

and the spacing between the family members is given by the principle quantum number

$$E_{N,n+1} - E_{N,n} \approx 1/(n - \mu)^3 \quad (4.31)$$

After using Eq. (4.30) to get N , one can express $n^* \equiv n - \mu$ as a function of E (Eq. (4.29)) and therefore an implicit function of the magnetic field. The right part of Fig. 4.1 plots the dependence of n^* on the magnetic field. A progression of Rydberg states appears as a series of lines with unit separation. The other striking feature revealed by this plot is that the Rydberg series very near the ionization threshold is not convergent to the nearest threshold ($N = 0$, i.e. the ionization threshold itself) but to the next one ($N = 1$), while those Rydberg series relatively far away from the ionization threshold are indeed convergent to the nearest threshold ($N = 0$). The third striking feature is that the members of the Rydberg series, in general, have fine structures. Therefore they are not individual levels but modulations of the spectra.

The existence of the Rydberg series at the laboratory field strengths range ($\gamma \sim 10^{-5}$) is a priori not expected because the classical dynamics is fully chaotic and the coupling between two directions (z and ρ) should, at first glance, destroy the Rydberg progressions. This leads naturally to the question whether the correspondence between quantum and classical mechanics is broken in the region of ionization threshold. We use the trace formula Eq. (4.26) to answer this question. The cross section of a photoabsorption measurement is proportional to

$$< D\psi_i | G(q, q, E) | D\psi_i > \quad (4.32)$$

where ψ_i is the initial state, $G(q', q, E)$ is the Green's function (4.2) and D is the component of the dipole operator in the direction of polarization of the

exciting electromagnetic field. Substitution of semiclassical approximation of Green's function (Eq. (4.9)) into (4.32) leads to a simple physical picture explaining how the absorption spectrum is correlated with closed classical orbits [37]. Initially, the electron is located near the nucleus. When the atom absorbs a photon, the electron propagates away from the nucleus to large distances as an outgoing wave. Through the semiclassical approximation (Eq. (4.9)), the outgoing wave fronts are guided by outgoing classical orbits. A pencil of trajectories are turned back by the magnetic field; some of them return to the nucleus, and the associated waves become incoming. The interference between outgoing and incoming waves produce the observed spectrum. Hence one expects those orbits which pass by the nucleus to be important. Since the amplitude A_ν in the trace formula decays exponentially with the increase of the Lyapunov exponents, we also expect that the main contribution to the spectrum is from those orbits with the smallest Lyapunov exponents. The family of trajectories which satisfies these conditions are shown in Fig. 4.2. We have calculated the first 140 members of this family at the laboratory field strength $B = 6.1T$ and extrapolated their actions, periods and Lyapunov exponents as functions of k , the number of intersections of the orbit with z -axis. When $k \rightarrow \infty$, the trajectories spend most of their time in the nearly separable region ($z \gg \rho$) and the actions and the periods reach their asymptotic forms[42]

$$T_k = k2\pi/\gamma, \quad (4.33)$$

$$S_k = 2\pi \frac{k}{\gamma} [E + 1.5(\frac{\gamma}{k})^{2/3}]. \quad (4.34)$$

The most important input are the Lyapunov exponents. We find that for large k (or equivalently large T_k), the stability constant defined by the product of Lyapunov exponent and period increases logarithmically with k or T_k , as shown in Fig. 4.3. Therefore, the amplitudes A_k (see Eq. (4.11)) of these orbits decrease with k algebraically rather than exponentially. Substituting these classical quantities into Eq. (4.26) we get the fluctuations of the integrated density as a function of energy as shown in Fig. 4.4. First we notice the discontinuity around threshold. This is due to the algebraic decay of the amplitudes A_k as a function of T_k , therefore the effect of long orbits accumulates and resolves the structure near the threshold. This is consistent with the full quantum calculation [41]. Experiments with finite resolution average over these fine structures and therefore observe a continuous spectrum around the threshold. Note that some irregular patterns near the threshold

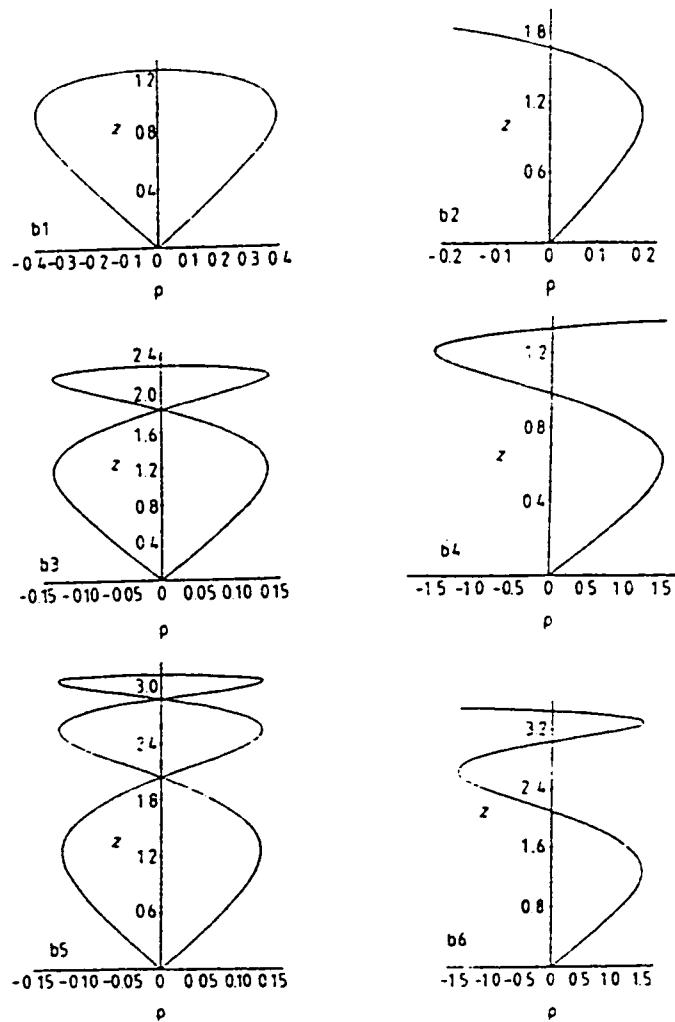


Figure 4.2: A family of classical orbits (b_k) of hydrogen atom in a magnetic field. The shapes of the orbits can be decomposed into “balloons” and “snakes”. Reprinted from M. A. Al-Laithy and C. M. Farmer, J. Phys. B20, L747(1987).

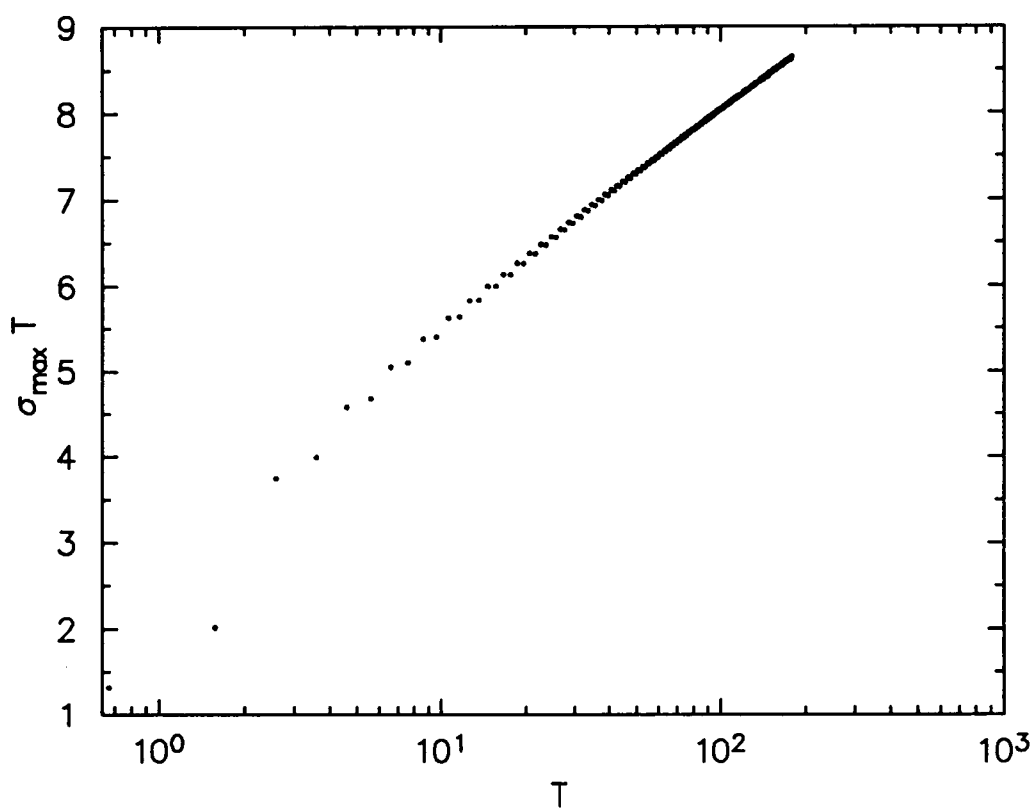


Figure 4.3: The stability indices $T \times \sigma_{\max}$ for a family of classical orbits of hydrogen atom in a magnetic field at $E = 0$.

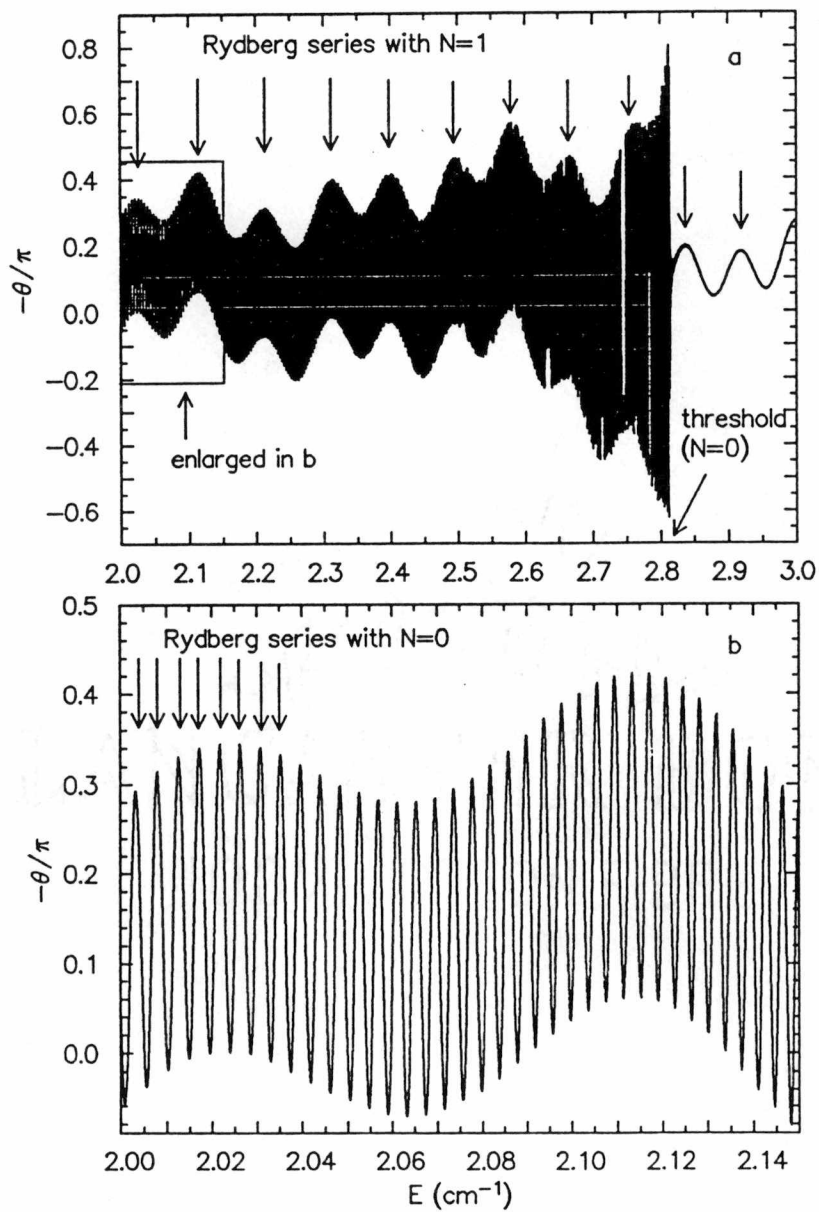


Figure 4.4: a. Semiclassical approximation of the fluctuations of the integrated density for hydrogen atom in a magnetic field as a function of energy where the ionization threshold is at 2.8cm^{-1} . The plot for the outlined region is shown in b.

are due to the numerical noise since a huge number (around 150,000) of orbits are included. There are two main modulations around the threshold. The one on larger scale forms Rydberg series convergent to the next threshold. The positions of the modulations are given by Eq. (4.29) with $N = 1$ and $n \sim 130$, hence $\Delta E \sim 0.1 \text{ cm}^{-1}$ (Eq. (4.31)). The other on a finer scale is the Rydberg series convergent to the nearest threshold. Its positions are given by Eq. (4.29) with $N = 0$ and $n \geq 360$ so that $\Delta E \leq 0.005 \text{ cm}^{-1}$ by Eq. (4.31). The latter appears as the fine structure of the former. Hence, near the ionization threshold, the experiments with finite resolution observed the dominant Rydberg series of larger scale which has fine structure and convergent to the next threshold. When the energy range is far away enough from the ionization threshold that the resolution can resolve the structure of the Rydberg series with smaller scale, one observes the Rydberg series convergent to the nearest threshold. These are the qualitative features observed in the experiments. We conclude therefore that the existence of the Rydberg series is due to the existence of such families of classical orbits which, though chaotic (i.e. with nonvanishing Lyapunov exponents), spend most of their time in the near separable region ($z \gg \rho$), thus their actions and periods behave as separable ones.

Chapter 5

Molecular-dynamics approach to quantum spectra

The difficulty of the semiclassical theory to describe the dynamical origin of the Wigner-type NNS distribution for classically chaotic systems suggests the need for another method to be applied to the investigation of the validity of random matrix theory. The parametric level dynamics provides an attractive alternative approach. This method uses a set of differential equations to describe the deformation of the quantum spectrum as a function of the control parameter for the strength of a perturbation. As we will show in this chapter, because these differential equations closely resemble Newton's equations of motion, the parametric evolution of the quantum spectrum is formally equivalent to the molecular dynamics of a many-body system with each particle representing an energy level. Equilibrium as well as non-equilibrium properties of this equivalent many-body system are expected to be directly linked to the quantum dynamics of classically chaotic systems. The basic microscopic mechanism of the parametric level dynamics is the collision between particles, i.e. avoided crossing between adjacent levels. The distribution and morphology of avoided crossings is therefore an important local property of quantum chaos. We suggest a simple formula for the distribution of avoided crossings for generic systems and introduce a statistical measure for overlapping avoided crossing which is sensitive to the fraction of classically chaotic phase space.

5.1 Molecular-dynamics calculation of energy levels

As discussed by Pechukas [43], and further developed by Yukawa [44] and Nakamura and Lakshmanan [45], the deformation of the energy levels of quantum system Eq. (2.25) as a function of λ can be described completely by a set of coupled ordinary differential equations

$$\begin{aligned}\frac{d}{d\lambda}x_n &= \langle n|V|n \rangle = V_{nn} = p_n \\ \frac{d}{d\lambda}p_n &= 2 \sum_{i \neq n} \frac{V_{in}^2}{x_n - x_i} = F_n \\ \frac{d}{d\lambda}V_{in} &= \sum_{j \neq i,n} V_{ij}V_{jn} \left(\frac{1}{x_i - x_j} + \frac{1}{x_n - x_j} \right) - \frac{V_{in}(p_i - p_n)}{x_i - x_n}\end{aligned}\tag{5.1}$$

where $x_n(\lambda) = E_n(\lambda)$ are the energy levels. For reasons of simplicity we have assumed in the above equations the coupling matrix V_{in} to be real (i.e. a system with time-reversal symmetry). Furthermore, the spectrum is assumed to be entirely discrete. We will relax these conditions and discuss the effects of the continuum in Chapter 8.

We give first a short outline of the derivation of Eqs. (5.1). Differentiating the Schrödinger equation (1.6) with Hamiltonian (2.25) with respect to λ , we find

$$V|n \rangle + H \frac{d|n \rangle}{d\lambda} = \frac{dx_n}{d\lambda}|n \rangle + x_n \frac{d|n \rangle}{d\lambda}.\tag{5.2}$$

Forming expectation values with $\langle m|$ in (5.2), we get the first equation of (5.1) for $m = n$, provided we choose the phase of eigenvector $|n \rangle$ such that [46]

$$\langle n| \frac{d|n \rangle}{d\lambda} = 0,\tag{5.3}$$

and

$$\langle m| \frac{d|n \rangle}{d\lambda} = \frac{V_{mn}}{x_n - x_m}\tag{5.4}$$

for $m \neq n$. We have used the Hermitian property of the Hamiltonian, i.e. $\langle m|H = \langle m|E_m (= x_m)$. Repeating this process for p_n and V_{in} , we obtain the second and the third equations of (5.1) with the help of Eqs. (5.4)

and (5.3). This set of coupled ordinary differential equations is an obvious generalization of the Hellman-Feynman theorem (the first equation of (5.1)) and will be referred to in the following as Hellman-Feynman equations (HFE) of motion. Extensions to the quasienergies of kicked systems [47], to the systems with multiple nonintegrable-parameters [46] and to quadratic parameter-dependent perturbations [48] have become available. We stress that the linear dependence of a perturbation on λ is essential in arriving at (5.1).

Heretofore, the HFE have been primarily used to analyze the energy level statistics in the semiclassical limit invoking statistical mechanics arguments. “Quasi-equilibrium” is expected to be attained during the λ -evolution. This state of quasi-equilibrium should represent the energy level distribution of an irregular quantum system. This approach goes back to Dyson’s observation [49] that different ensembles of random matrix theory can be mapped onto the equilibrium statistical mechanics of a circular one-dimensional Coulomb gas at different temperatures embedded in a two-dimensional space. These works leave several key hypotheses to be verified by a numerical calculation. We have developed a code to numerically integrate HFE for a large number of energy levels (presently up to 10^4 levels) [50] by a 5th order Runge-Kutta integrator with variable step size. Our approach is directly modeled after molecular dynamics (MD) calculations for classical liquids [51]. We identify Eq. (5.1) as Newton’s equations of motions for $\tilde{N}$ ($=$ number of levels) particles with canonical coordinates (x_n, p_n) , each particle representing one energy level. The particles move in a one-dimensional space and interact pairwise via a singular repulsive potential U_{in} with “time”-(λ -)dependent “charge” V_{in}

$$U_{in} = 2V_{in}^2 \ln |x_n - x_i| \quad (5.5)$$

We chose a linear configuration where the position coordinates form an ordered sequence $(x_1 < x_2 < \dots < x_{\tilde{N}})$ which will be conserved because of the singular repulsive force between levels of given exact symmetry. This singularity is a direct manifestation of level repulsion. The only non-standard feature in HFE are the additional degrees of freedom of fluctuating “charges” $V_{in}(\lambda)$ whose variations are coupled to the parametric motion. The initial conditions $(x_n(0), p_n(0), V_{in}(0))$ are calculated from the eigenvalues and eigenvectors of the integrable Hamiltonian H_0 . Avoided crossings which are generic for nonintegrable systems correspond to collisions between particles within the MD approach.

The analogy to molecular dynamics reaches much further: From MD cal-

culations of classical liquids it is well known that the propagation of ensembles is facilitated by the fact that the number of $\tilde{N}(\tilde{N} - 1)/2$ mutual interactions in the $\tilde{N}$ particle system can be reduced to those within a reaction range of J nearest neighbors provided the forces are sufficiently short-ranged. The number of interaction pairs of particles is thus reduced from $\tilde{N}(\tilde{N} - 1)/2$ to $\tilde{N} \times J/2$ where $J \ll \tilde{N}$. Application of such a reaction window to Eq. (5.1) implies the use of an λ -dependent self-adjusting "banded" Hamiltonian matrix, which is crucial in gaining computational speed. Since the forces in HFE are short-ranged only if $V_{in}(\lambda) \rightarrow 0$ as $|i - n| \gg 1$, the convergence as a function of the reaction range J must be checked. We find the convergence as a function of the reaction range to be rather slow for individual levels (typically, $J \geq 50$); however, it is much faster for ensemble properties. To illustrate the effects of the reaction range, we use a solvable system with long-range couplings between energy levels

$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + x_1^2/2 + x_2^2 + \lambda x_1 x_2. \quad (5.6)$$

Because the parity is conserved we have calculated 1000 levels (including ground state) with positive parity. The error is measured by the absolute values of the differences between the exact levels and calculated levels, i.e.

$$error_n = |E_n^{exact} - E_n^{calculated}| / <\Delta E>. \quad (5.7)$$

where $<\Delta E>$ is the mean spacing. This is a very sensitive measure as it heavily weighs small absolute errors by $<\Delta E>^{-1}$. We use the criterion that if $error_n$ is smaller than the tolerance used in the calculation (here the tolerance = 10^{-8}), the value of level E_n is considered exact. Fig. 5.1 displays the fraction of the "exact" levels as a function of reaction range J . One can see that for this system most levels become exact when $J > 50$.

Another key feature of MD simulations of which we can make use is the choice of appropriate boundary conditions. Instead of periodic boundary conditions used in calculations for classical liquids, we use at the lower end of the stretch of spectrum (ground state x_1) the correct open boundary conditions while at the top ($x_{\tilde{N}}$) we use a boundary layer ($x_{\tilde{N}+1}, \dots, x_{\tilde{N}+J}$) whose thickness J is determined by the effective range of the coupling and whose λ motion is explicitly prescribed. The boundary layer delimits the upward motion of particles, taking into account the level repulsion by truncated levels and thereby reducing truncation errors. If we choose open boundary conditions on the top instead, the method yields results identical to those of

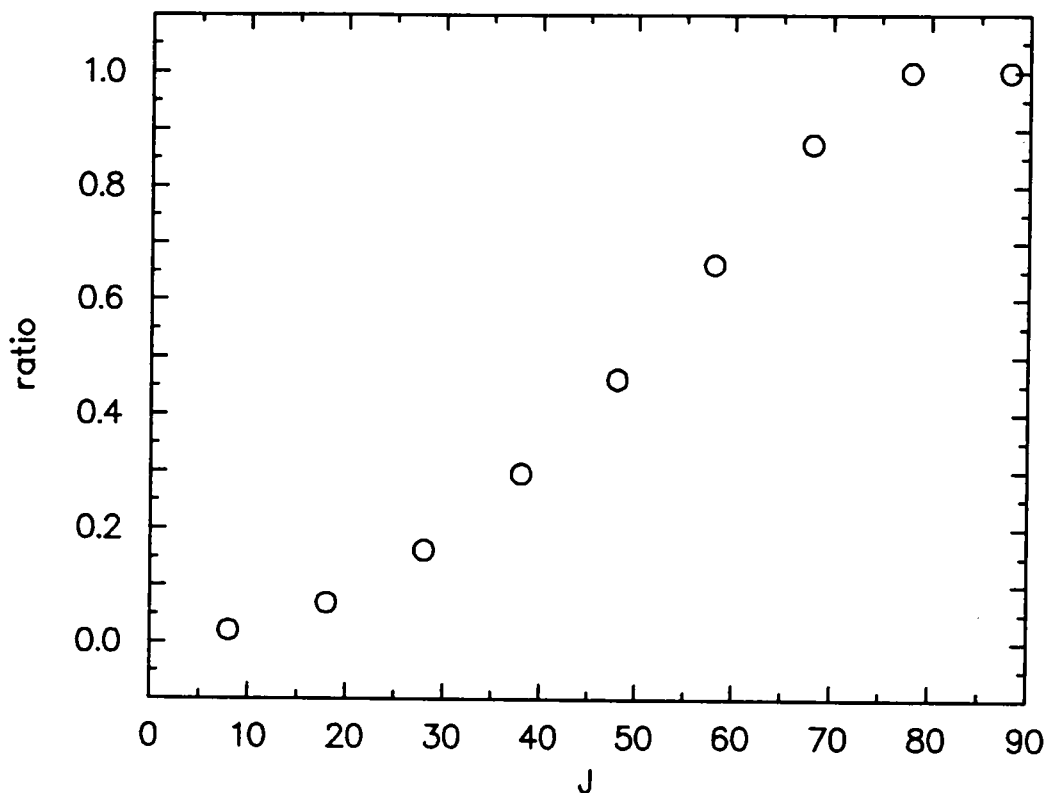


Figure 5.1: Fraction of “exact” energy levels as a function of reaction range for the solvable coupled harmonic oscillators (see text).

matrix diagonalization at fixed λ . The effects of boundary conditions can be beautifully demonstrated by the solvable model of one-dimensional harmonic oscillator in an electric field

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x. \quad (5.8)$$

Fig. 5.2 shows the errors (see Eq. (5.7)) caused by different boundary conditions as a function of the state n (counted from the ground state up) where the number of the levels involved in the calculation is 1000. The “hard-wall” boundary condition is given by fixing the position of the last level, i.e. $p_N(\lambda) = 0$. It is clear that the hard-wall boundary condition takes into account the level repulsion by truncated levels and thereby reduces truncation errors compared with the result of open boundary condition (or equivalently

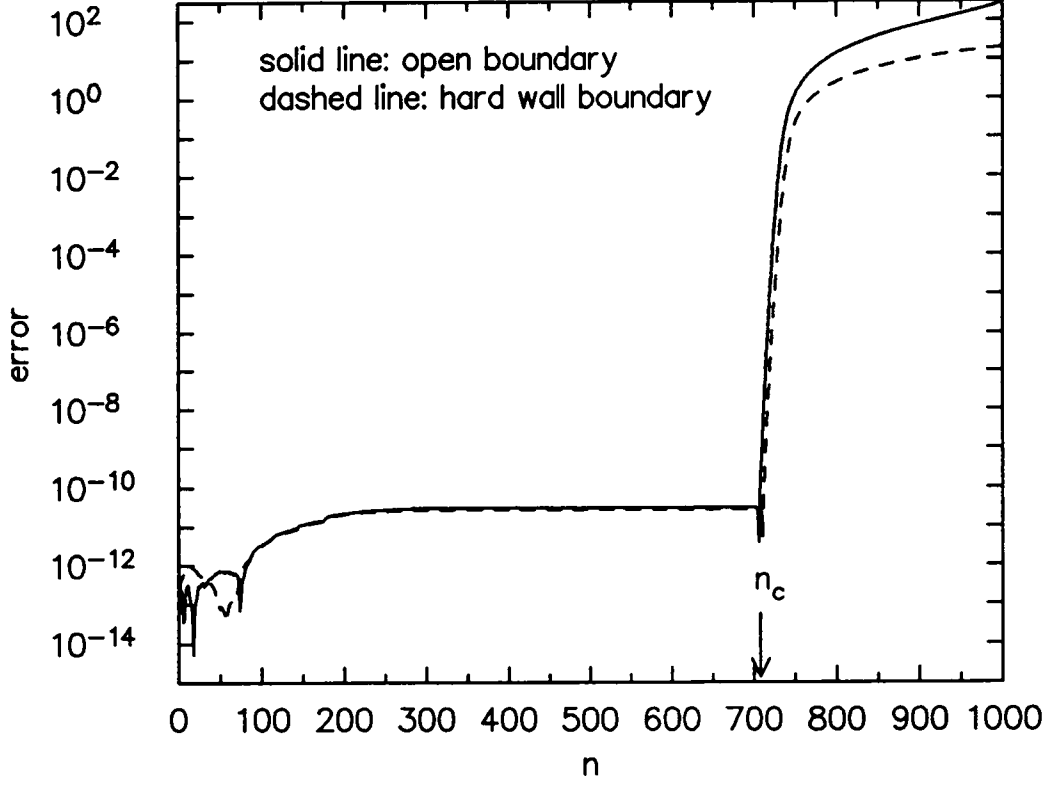


Figure 5.2: Errors caused by boundary conditions of level dynamics for the system of a harmonic oscillator in an electric field (Eq. (5.8)) as a function of the state n (counted from the ground state up), where the field strength $\lambda \approx 6.3$.

the result of diagonalization). Another interesting aspect of Fig. 5.2 is that the influence of boundary conditions decays abruptly and there exists a level n_c independent of the boundary conditions imposed below which ($n < n_c$) all the levels are weakly influenced by boundary conditions. This behavior is system-independent. We define the quantity

$$b_n(\lambda) = - \sum_{k=\tilde{N}+1}^{\infty} | \langle \psi_n(\lambda) | \psi_k(0) \rangle |^2 \ln(| \langle \psi_n(\lambda) | \psi_k(0) \rangle |^2), \quad n \leq \tilde{N} \quad (5.9)$$

where $|\psi_n(\lambda)\rangle$ is the perturbed state under the consideration and $|\psi_k(0)\rangle$ are the unperturbed states. This quantity is the amount of the informa-

tion (“information entropy”) needed from the truncated levels to calculate level x_n . It can be used to describe the influence of boundary conditions to the given level x_n . The information entropy $b_n(\lambda)$ increases with the perturbation λ . When $b_n(\lambda)$ deviates significantly from zero, the level x_n is strongly influenced by the boundary conditions. For systems in which the coupling between levels is short-ranged (as for the system Eq. (5.8)), the major contribution to the information entropy b_n is from the first truncated level, $\langle \psi_n(\lambda) | \psi_{\tilde{N}+1}(0) \rangle$, when b_n is near zero. From the semiclassical approximation for wavefunctions, we know that when the turning point of the wavefunction $|\psi_n(\lambda)\rangle$ coincides with the turning point of $|\psi_{\tilde{N}+1}(0)\rangle$, the product $\langle \psi_n(\lambda) | \psi_{\tilde{N}+1}(0) \rangle$ should be large. Hence, for a given λ the state $|\psi_{n_c}(\lambda)\rangle$ is the state whose turning point coincides with the turning point of the state $|\psi_{\tilde{N}+1}(0)\rangle$. This leads to

$$n_c(\lambda) = \tilde{N} + 1 - \sqrt{2\tilde{N} + 3\lambda + \lambda^2/2}. \quad (5.10)$$

which fits the numerical observation very well.

One difficulty of the MD approach lies in the occurrence of singularities in the integrable limit ($\lambda \rightarrow 0$). The completely integrable Hamiltonian H_0 possesses typically non-accidental degeneracies of energy levels, $x_i(0) - x_j(0) = 0$, which result in singular, ill-defined initial conditions of Eq. (5.1). The numerical convergence problems associated with degeneracies are very likely one reason why systematic numerical investigations of HFE are, up to this point, rare [52]. However, these singularities can be removed by applying lowest-order nonvanishing perturbation theory for $\Delta\lambda \ll 1$, yielding non-degenerate initial conditions $x_i(\Delta\lambda) - x_j(\Delta\lambda) \neq 0$ which are then suitable for propagation to large λ according to Eq. (5.1). A similar complication arises from isolated avoided crossings (or hard collisions) during the λ evolution. As will be discussed in the following sections, these near singularities can be removed by treating them analytically. On the other hand, a major advantage of the MD simulation over matrix diagonalization or the Feit-Fleck Fourier transform method [53] lies in the fact that a single molecular dynamics run provides “en route” the spectra of $H(\lambda)$ for all λ in the integration interval, thereby giving detailed information on the deformation of spectra during the transition from a regular to a chaotic classical phase space structure. In analogy to the dynamics of liquids we will refer to our numerical solutions of HFE as molecular dynamics simulations (or computer “experiments”). Analytic predictions of distributions and dynamical correlation functions for the pseudo-Newtonian many-body system (Eq. (5.1)) will

be tested by comparing with our computer experiments. It is important to realize that despite its classical appearance, Eq. (5.1) is fully equivalent to the original Schrödinger equation (1.4) for the quantum system of Eq. (2.25). It should be noted that the terms “classically regular” or “chaotic motion” will in the following always refer to the dynamics governed by the original Hamiltonian system (Eq. (2.25)) and not to the pseudo-Newtonian $\tilde{N}$ -body system (Eq. (5.1)).

Although the systematic comparison of the relative computational efficiencies of the MD approach and traditional matrix diagonalization is not yet completed, a simple estimate can be given. Virtually all modern eigen-system routines diagonalize non-sparse matrices by a sequence of similarity transformations [54]. The number of operations for each transformation is proportional to $\tilde{N}^3$ [53] where $\tilde{N}$ is the dimension of the matrix. To resolve the spectrum in the interval of λ , the number of diagonalizations is proportional to $\lambda(N_{AC} + 1)$ where N_{AC} is the number of avoided crossings. Consequently, the computation time for matrix diagonalization is proportional to $\lambda(N_{AC} + 1)\tilde{N}^3$. On the other hand, the computer time for the evaluation of parametric dynamical equations is proportional to $\tilde{N}(1 + J + J^2)$ and the number of evaluations is proportional to $\lambda(N_{AC} + 1)$. Hence the computer time required is proportional to $\lambda(N_{AC} + 1)\tilde{N}(1 + J + J^2)$. Therefore, the ratio of the computer time of the MD approach to the matrix diagonalization is

$$r_{cpu} = C \frac{1 + J + J^2}{\tilde{N}^2} \approx C \left(\frac{J}{\tilde{N}} \right)^2. \quad (5.11)$$

where C is system-dependent. Consequently, in general, when $J/\tilde{N} \ll 1$ our MD approach will be more efficient.

5.2 Parametric trajectories of quantum levels

The parametric trajectories of energy levels for the solvable (and therefore integrable) systems are analytic, smooth and structureless. We discuss now the parametric level dynamics of generic systems whose classical counterparts possess a mixed phase space of regular and chaotic motion. The model system we use is the coupled Morse oscillators (Eq. (2.26)) with molecular parameters of H-C-C. The coupling to the continuum is neglected.

Fig. 5.3 depicts the λ -trajectories of a few particles in the (x,p) phase space of the $\tilde{N}$ particle system representing the energy levels of the coupled Morse oscillators. The trajectories of low-lying states are obviously smooth while for high-lying states the trajectories very much resemble those of Brownian particles undergoing a seemingly erratic motion and sharp turns which are due to close collisions (avoided crossings) with adjacent particles. Note that $\hbar \rightarrow 0$ is a short-hand notation for the approach to the semiclassical limit. The complexity increases with decreasing $\hbar$. This indicates that the properties of semiclassical spectrum (i.e. high-lying levels) can be quite different from the properties of the levels near ground state and there may be interesting structures in those high-lying levels.

Fig. 5.4 shows an example of the dependence of energy levels (or the position coordinates of the particles in the language of MD) of excited states on λ for coupled Morse oscillators in mostly chaotic region. This plot shows the absence of any obvious regularity of the spectrum, suggesting that a statistical description would be appropriate. Another feature of Fig. 5.4 is the existence of a large number of avoided crossings between high-lying energy levels. It is well-known [55] that for $H(\lambda)$ with no additional symmetry the quantum levels generally do not cross each other as λ varies. Instead, two levels may approach and recede from each other along two branches of a hyperbola. This behavior is termed avoided crossing (AC). As indicated in the figure, there are "isolated" and "overlapping" avoided crossings and even "triple" avoided crossings which essentially involve three levels. Avoided crossings play an important role in parametric level dynamics. From the viewpoint of molecular dynamics, avoided crossings (collisions between levels) redistribute the "kinetic energies" and "potential energies" of particles and therefore provide the microscopic mechanism for the transition from nonequilibrium state to equilibrium state. During such an avoided crossing, the properties of two levels involved are mixed and hence the original quantum numbers are not "good" any more. According to the EBK quantization (Eq. (4.15)), these processes correspond to the destructions of classical tori, therefore the classical motion changes from regular to chaotic. Avoided crossings are fine structures in quantum spectra and, based on the uncertainty principle for energy and time (Eq. (4.21)), they should be very sensitive to the long-time behavior of the underlying classical dynamics. Thus the distribution and morphology of the avoided crossings is an important property of quantum chaos. Such an interconnection had been proposed in early studies as the fingerprints of classical chaos [56], though at that time only on a qualita-

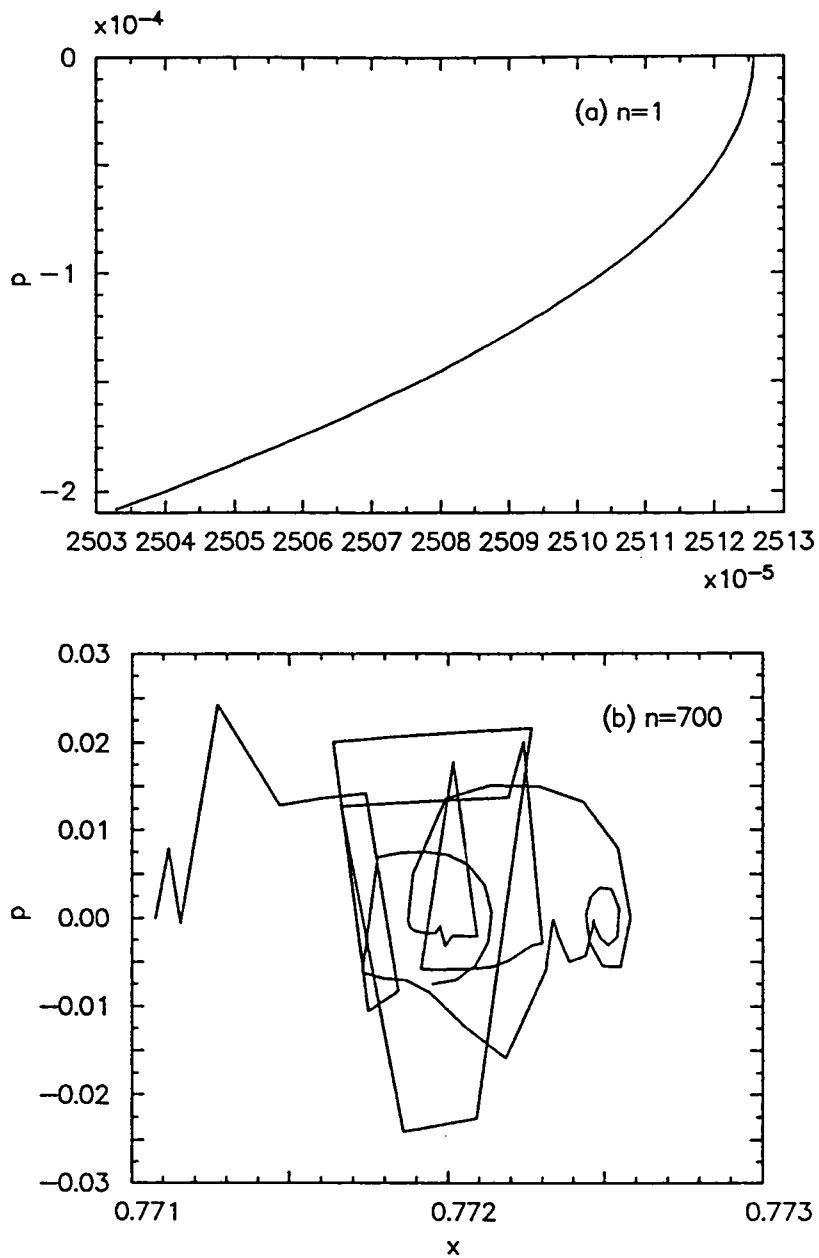


Figure 5.3: “Phase space” trajectories of energy levels of the coupled Morse oscillators for the interval of perturbation strength $0 \leq \lambda \leq 0.7$: (a) ground state $n = 1$ and (b) excited state $n = 700$.

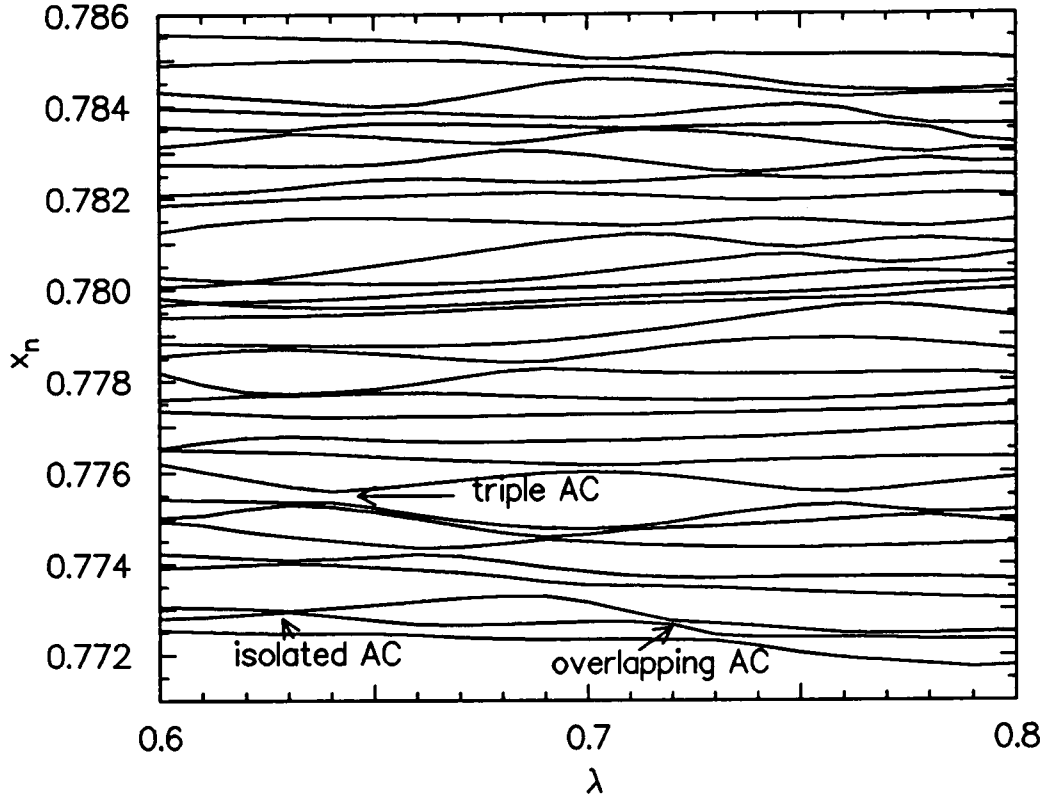


Figure 5.4: “Coordinate space” trajectories of energy levels of the coupled Morse oscillators for excited states ($700 \leq n \leq 730$) in the classically mostly chaotic region. Due to the finite resolution of the plot, some narrow avoided crossings look like crossings.

tive level. The HFE (Eq. (5.1)) are particularly convenient to study avoided crossings quantitatively [57, 58]. Virtually all two-body collisions within a given λ interval can be found by searching for zeros in the relative momentum $\Delta p = p_{n+1}(\lambda) - p_n(\lambda)$ with positive slope $\Delta p' \geq 0$. Extensions to three-body collisions (i.e. triple avoided crossings) or multiple collisions are straightforward. It is important that the interval of λ within which the avoided crossings are counted for statistics must be small compared to the range of λ when the classical phase space of Eq. (2.26) undergoes structural changes.

5.3 Width distribution of avoided crossings

Around the point of the closest approach, λ_c , the distance between two levels involved in an avoided crossing can be approximated by the Wigner-von Neumann formula

$$\Delta E = E_{n+1}(\lambda) - E_n(\lambda) = \sqrt{C^2 + 4\Delta\lambda^2 V_0^2} \quad (5.12)$$

where $C = E_{n+1}(\lambda_c) - E_n(\lambda_c)$ is the minimum distance, $V_0 = V_{n,n+1}(\lambda_c)$ is the coupling among two levels at the point of the closest approach, and $\Delta\lambda = \lambda - \lambda_c$.

Eq.(5.12) corresponds to the “adiabatic” representation (in the terminology of collisions) of an isolated avoided crossing. A more detailed quantitative criterion for an isolated AC will be given below. An alternative diabatic representation follows from the description of the effective 2x2 Hamiltonian for the levels $(n, n+1)$, denoted by (1,2) in the following, by the matrix

$$H_{eff}(\Delta\lambda) = \begin{pmatrix} a\Delta\lambda & \Delta/2 \\ \Delta/2 & -a\Delta\lambda \end{pmatrix} \quad (5.13)$$

where $\Delta/2$ is the coupling matrix element between two diabatic levels and a is the slope with which the levels approach each other and would cross if Δ would be zero. Solving the eigenvalue problem (5.13) and comparing with (5.12) leads to the correspondence

$$\begin{aligned} \Delta &= C \\ a &= V_0. \end{aligned} \quad (5.14)$$

Note the interchange of the role of (off-)diagonal elements in the (a-)diabatic representation

$$\Delta = 2 \langle 1|H_{eff}|2 \rangle_{dia} = (\langle 2|H|2 \rangle - \langle 1|H|1 \rangle)_{adia}. \quad (5.15)$$

Note, furthermore, that Δ and a in (5.13) are assumed to be independent of $\Delta\lambda$, i.e. the diabatic state vectors $|1, 2 \rangle$ to be invariant under variation of $\Delta\lambda$ for small $\Delta\lambda$. The latter plays an important role for the correlated motion of energy levels near avoided crossings.

It is worth noting that the HFE (5.1) describe the parametric evolution of the matrix element V_{in} in the adiabatic representation. In the following,

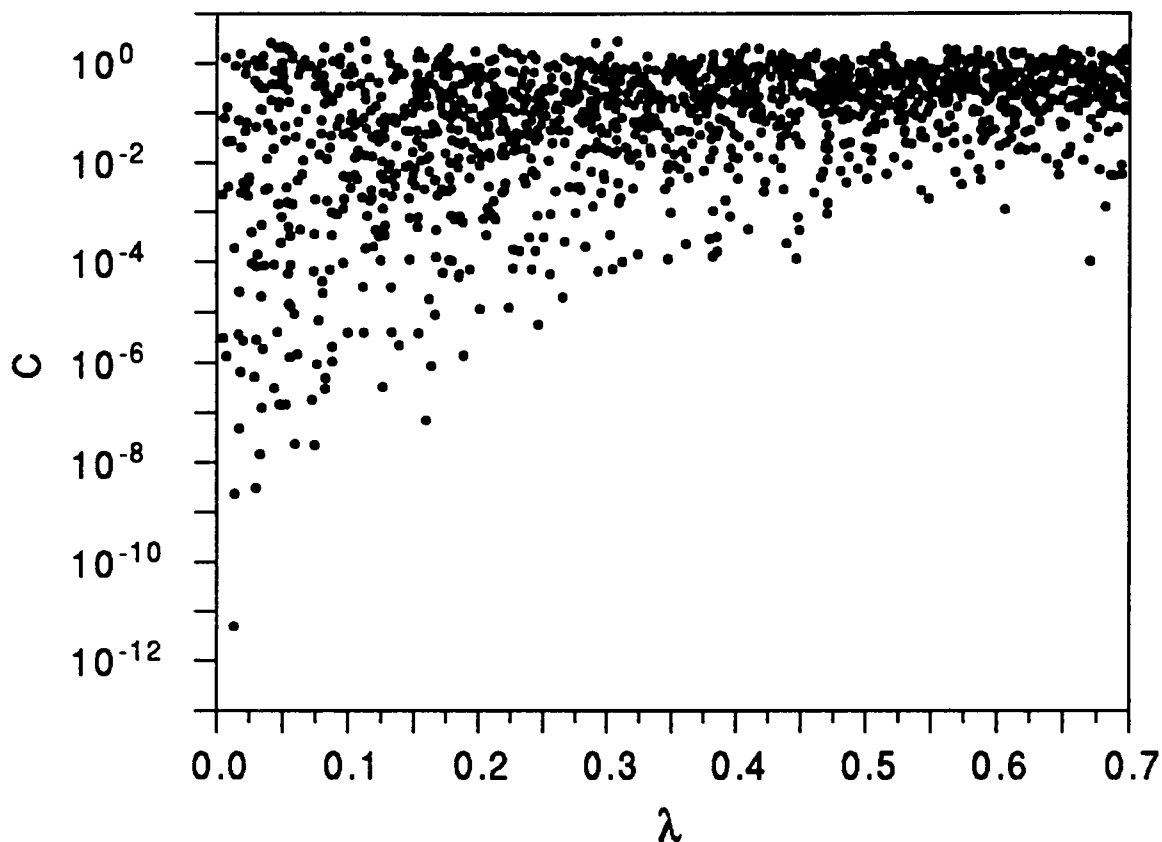


Figure 5.5: Scatterplot of widths, in units of the local mean level spacing, for avoided crossings in the interval $0 \leq \lambda \leq 0.7$.

we use this set of equations for determination of the width distributions and the λ (“temporal”) correlation between avoided crossings.

Fig. (5.5) displays the scatterplot of widths in units of the mean level spacing within the interval $0 \leq \lambda \leq 0.7$. We may speak of mild avoided crossings when C is of the order of the mean level spacing $\langle \Delta E \rangle$ while hard avoided crossings correspond to $C \ll \langle \Delta E \rangle$. The most remarkable feature in Fig. (5.5) is the dramatic increase of the lower bound of C for a given λ as a function of λ by orders of magnitude as the classical dynamics undergoes a transition from regular to chaotic motion. Near the integrable limit there exist extremely small avoided crossings ($\approx 10^{-9}$ mean spacing) while mild collisions become prevalent in the region of chaotic motion. Extremely narrow avoided crossings have been first observed for hydrogen in a

strong magnetic field and could be traced to the existence of an adiabatic invariant [6]. The C distribution spans many orders of magnitude in the regular regime while it becomes much more uniform in the chaotic regime. Since small C corresponds to near-singularities in Eq. (5.1) we arrive at the somewhat paradoxical conclusion that the evolutions of levels and avoided crossings described by the HFE become smoother at the same time the underlying classical dynamics becomes more chaotic.

For quantitative studies of the distribution of avoided crossings, we restrict ourselves to those avoided crossings which are dominated by a two-level interaction such that two-level approximation (Eq. (5.12)) is locally valid near the point of the closest approach λ_c . The validity of the two-level approximation can be easily tested for each avoided crossing within our calculation by requiring that the residual forces exerted by other levels (see the second equation of (5.1)) on the two levels in question, F_N , are negligible compared to the dominant two-level force, F_2 , between the two levels. i.e.

$$F_N = \text{Max}_{s=n,n+1}(|2 \sum_{k \neq n,n+1} \frac{V_{k,s}^2}{x_s - x_k}|) \ll F_2 = \frac{2V_{n,n+1}^2}{x_{n+1} - x_n} \quad (5.16)$$

for $\lambda_1 \leq \lambda \approx \lambda_c \leq \lambda_2$ where $\lambda_{1,2}$ denotes the “time” the two particles enter (leave) the isolated-collision region as shown by Fig. 5.6. We have found numerically that for $F_N/F_2 < 0.1$ the two-level approximation is sufficiently accurate and used therefore this criterion to define $\lambda_{1,2}$. We note that the results are stable against the variation of the cut-off criterion, provided that $F_N \ll F_2$. We also note parenthetically that within this interval (λ_1, λ_2) the trajectories x_n and x_{n+1} can be propagated analytically according to Eq. (5.12), thereby removing the near-singular terms associated with two-body collisions in Eq. (5.1).

For classically completely chaotic, metrically transitive systems, random matrix theory predicts a Gaussian distribution of the width of an avoided crossing. In its simplest form, the underlying argument can be phrased as follows [59]: The two free parameters in H_{eff} in the diabatic representation (Eq. (5.13)), a and Δ , are independent Gaussian random numbers, while the width of the avoided crossing is given by Δ ($=C$, Eq. (5.14)). Consequently, RMT predicts

$$P(C) = \frac{2}{\pi \langle C \rangle} e^{-C^2/(\pi \langle C \rangle^2)} \quad (5.17)$$

with $\langle C \rangle$ the mean value of the width in the ensemble of avoided crossings.

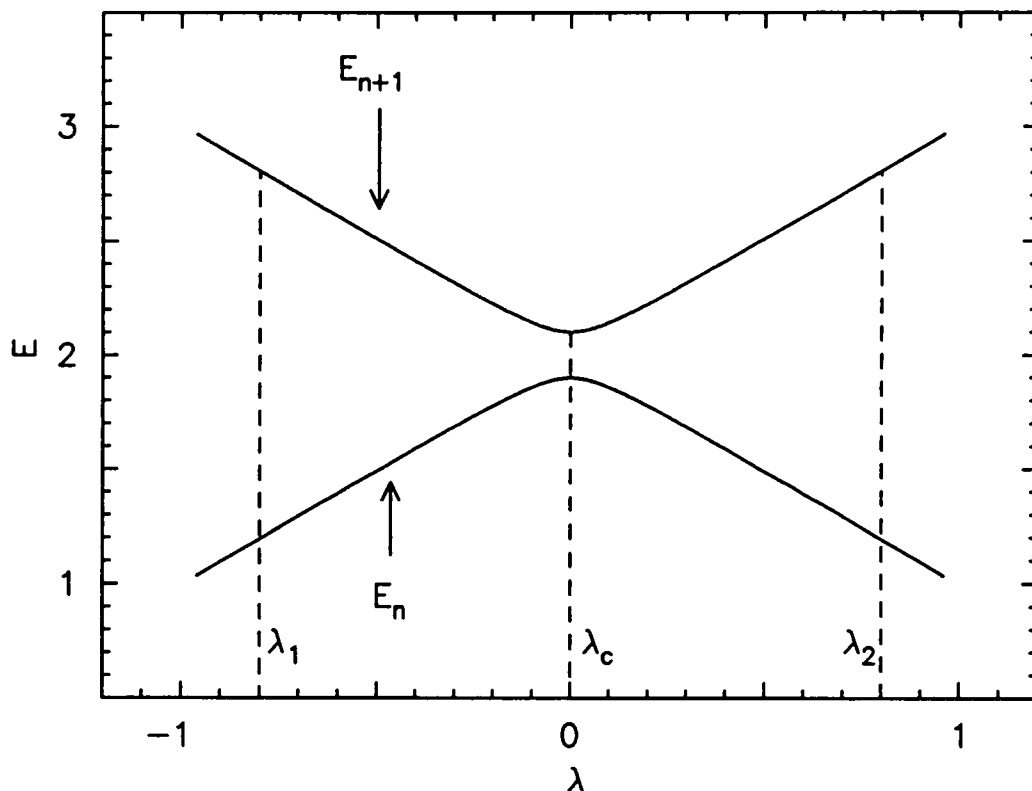


Figure 5.6: Illustration of two-level avoided crossings.

In the quasi-integrable limit, on the other hand, invariant tori fill most of the accessible phase space. The Hamiltonian system can be quantized via torus (EBK) quantization. Energy levels are characterized by complete set of compatible quantum numbers (N actions (I_i , $i = 1, \dots, N$) of the N -torus), i.e.

$$E_n(\lambda) = H(I_i, \lambda)_{I_i = \hbar(n_i + \frac{\alpha_i}{4})}. \quad (5.18)$$

The levels obtained by (5.18) generally do not exhibit any inhibition to cross under the variation of one parameter when the number of degrees of freedom $N \geq 2$. Consider an N -dimensional space with axes $n_1, n_2, \dots, n_N$. In this space, the function $H(I_i \propto n_i, \lambda) = E$ defines a energy surface of dimension $(N - 1)$. As shown in Fig. 5.7, an allowed quantum energy eigenvalue arises from the intersection of the energy surface with a discrete lattice point, say n_i^* , of the primitive cubic space where all components of the vectors are non-

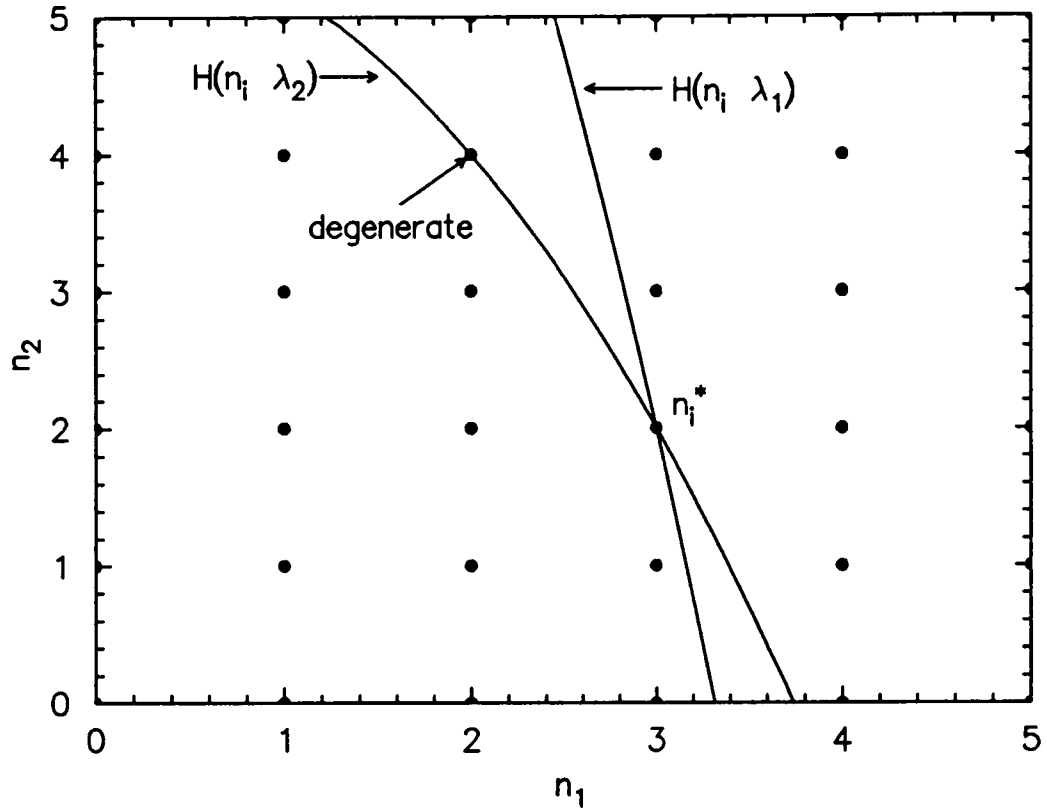


Figure 5.7: Illustration of the level crossing from EBK quantization.

negative. For a fixed value of λ , an energy surface will not, in general, intersect two lattice points simultaneously. The energy surface intersecting n_i^* will, however, smoothly deform upon changing λ . By properly choosing λ , it can, in general, intersect with a second lattice point. The case of harmonic oscillators is exceptional for which the energy surface is a hyperplane. Apart from such exceptional surfaces, one concludes that primitive (i.e. non-uniform) semiclassical quantization (Eq.(5.18)) therefore gives crossings rather than avoided crossings. Uniform quantization [60] lifts these degeneracies and induces small splittings due to dynamical tunneling between tori and narrow phase space zones within which the non-integrable perturbation destroys tori. As other quantities due to the tunneling, the size of avoided crossings in the near integrable limit is of the order $\exp(-S/\hbar)$ where S is the classical action associated with the tunnelling [61]. The size of AC is therefore very small

compared to the average spacing ($\propto \hbar^N$, Eq. (4.13)) in the semiclassical limit ($\hbar \rightarrow 0$). On the scale of the average spacing between energy levels, the distribution for these avoided crossings can be approximately described by a δ function

$$P(C) = \delta(C). \quad (5.19)$$

We note that any other sharply peaked function (on the scale of the mean spacing) is admissible as well, while the advantage of a δ function is that it is without additional free parameters. For generic quantum systems with a mixed classical phase space consisting of regular islands and chaotic seas, we expect $P(C)$ to consist of two components: One with fraction $1 - \gamma$ is formed by avoided crossings involving two adjacent levels from the quantization of the classical tori of regular islands and Eq. (5.19) applies. The other group with fraction γ involves at least one level embedded in the chaotic seas. The Gaussian distribution (Eq. (5.17)) should be applicable to this group. Therefore, the distribution for all AC's reads

$$P(C) = (1 - \gamma)\delta(C) + \gamma\sqrt{\frac{4D}{\pi}}\exp(-DC^2) \quad (5.20)$$

where D is determined by the average width

$$D = \frac{\gamma^2}{\langle C^2 \rangle}. \quad (5.21)$$

This distribution interpolates between a δ distribution Eq. (5.19) ($\gamma = 0$) and a Gaussian distribution Eq. (5.17) ($\gamma = 1$). The parameter γ can be determined by fitting the results of numerical experiments for quantum spectra. At the same time, we expect γ to be closely related to the fraction of the classically chaotic phase space.

Fig. 5.8a displays the AC distribution for coupled Morse oscillators in the perturbative regime ($0 \leq \lambda \leq 0.1$) where C is in units of the average spacing. The circles are the values of Eq. (5.20) averaged over each window of size $\Delta C = 0.05$ and the numerical results are represented by histograms. The dominant feature is clearly the sharp peak near the origin $C = 0$. Note the peak width is not intrinsic but is determined by the window size ΔC . The sharp peak near the origin signifies the approximate separability and the persistence of KAM tori in the classical phase space. A very weak Gaussian component at large C is recognizable. For strong perturbations ($0.5 \leq \lambda \leq 0.8$) chaotic motion becomes prevalent, though some regular islands still exist (see

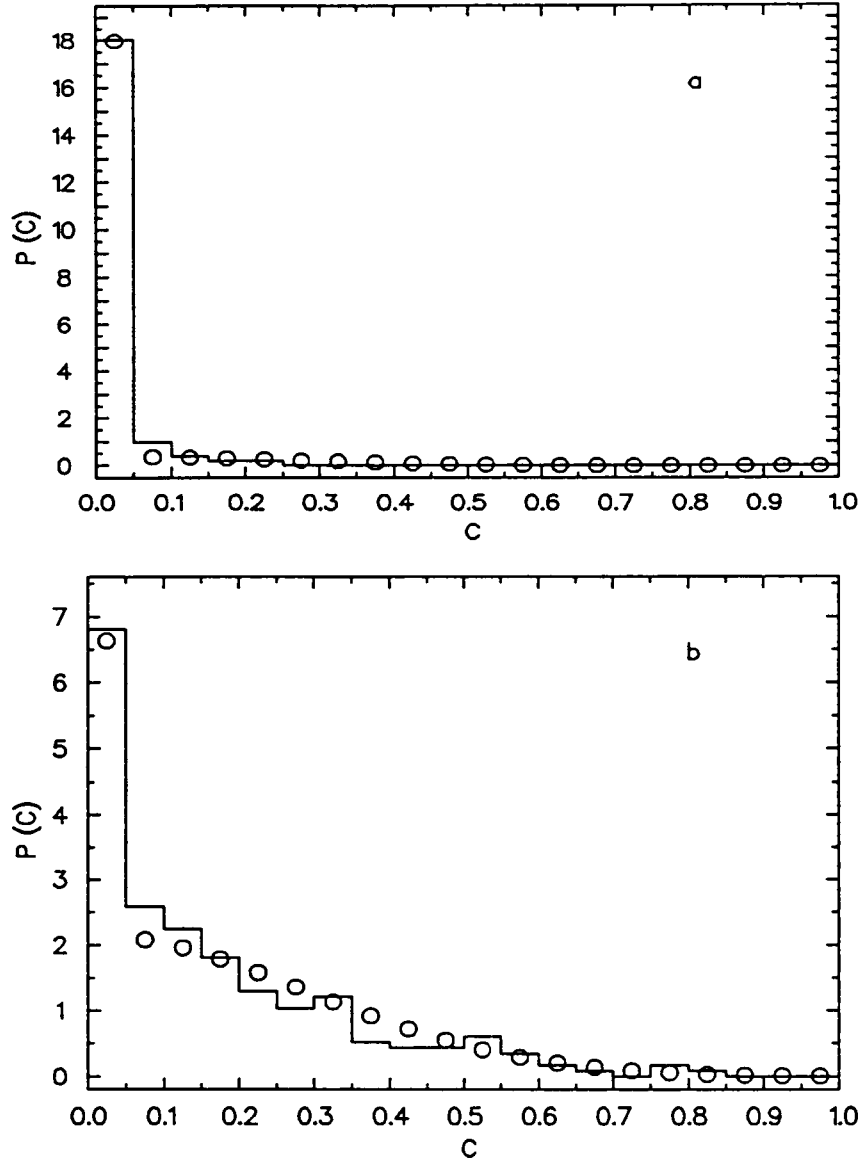


Figure 5.8: The AC distribution (a) in the near-integrable regime ($0 \leq \lambda \leq 0.1$) and (b) in mostly chaotic regime ($0.5 \leq \lambda \leq 0.8$) where C is in units of the average level spacing. The circles are the averages of the distribution function Eq. (5.20) over the window of the histogram (0.05 of mean spacing). The numerical results for coupled Morse oscillators are given by histograms.

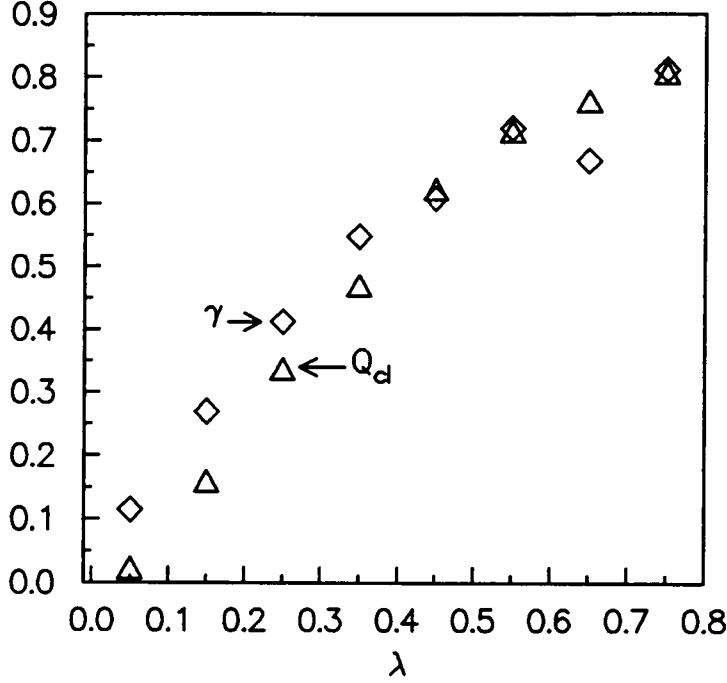


Figure 5.9: Quantum parameter γ (diamond) and the fraction of classically chaotic phase space in the energy shells contributing to the energy level statistics, Q_{cl} , (triangles) as a function of λ for coupled Morse oscillators.

Fig. 5.9). Fig. 5.8b shows that the corresponding AC distribution consists of two components: a dominant Gaussian tail and a small peak near the origin, as predicted by distribution Eq. (5.20). Fig. 5.9 displays the λ -dependence of quantum parameter γ and the fraction of classical chaotic phase space Q_{cl} in the energy hypershells within which the quantum energy levels lie. We averaged the fraction Q_{cl} within each window of $\Delta\lambda = 0.1$. One can see that γ closely follows Q_{cl} . The AC distribution changes from a δ -type to a Gaussian one as the corresponding classical system undergoes a transition from regular to chaotic motion.

As a consequence of (5.20), we find that the validity of the RMT prediction (Eq. (5.17)) for small C cannot be tested for a mixed system since the region near the origin is always “overshadowed” by the δ contribution due to regular islands. Only in the limit of completely chaotic systems, or

systems whose regular islands are too small to accommodate any quantum state, the $C \rightarrow 0$ limit of RMT becomes accessible. For several such systems (strongly “kicked” top, billiards, hydrogen in strong magnetic field) recent investigations [62] found systematic deviations which were detected in the cumulative distribution

$$I(C) = \int_0^C dC' P(C'). \quad (5.22)$$

The width of the avoided crossings for billiards has been recently linked to very long periodic orbits [63]. According to the GOE result (Eq. (5.17), or Eq. (5.20) with $\gamma = 1$), $I(C)$ should be proportional to C in the limit of small C for chaotic systems. Using a sample of $\approx 10,000$ AC's, it was shown in Ref. [59] that $I(C)$ does not grow linearly with C . As found by Goldberg and Schweizer [62], $I(C)$ grows instead quadratically with C for small C , i.e.

$$P(C) = \frac{d}{dC} I(C) \propto C \quad C \rightarrow 0. \quad (5.23)$$

The origin of this deviation is not yet clear. In order to test the proposal that the deviations are due to small ensemble sizes, we generate two samples of 10,000 random numbers and plot the integrated distributions for small C in Fig. 5.10 where C is in units of the average width $\langle C \rangle$. The triangles are generated from the GOE result (Eq. (5.17)) which is proportional to C with the slope $\sqrt{4/\pi}$. The circles are generated from Eq. (5.23) which fits the data of the kicked-top model of Ref. [59] very well. This result shows clearly that the sample size of the numerical data of model systems are large enough to verify the GOE result in the limit of small AC, and the discrepancies are not due to the small sample size. As recently suggested, another possibility would be numerical errors in the determination of the width distribution [64]. The third possibility is strong parametric correlations among matrix elements and effects of overlapping avoided crossings [65]. We will in the following analyze the distribution of non-isolated avoided crossings.

5.4 Overlapping avoided crossings

A multitude of overlapping avoided crossings has been proposed from early on as a signature of classical chaos in quantum spectra [66]. Numerical calculations supported this criterion qualitatively, but a quantitative description

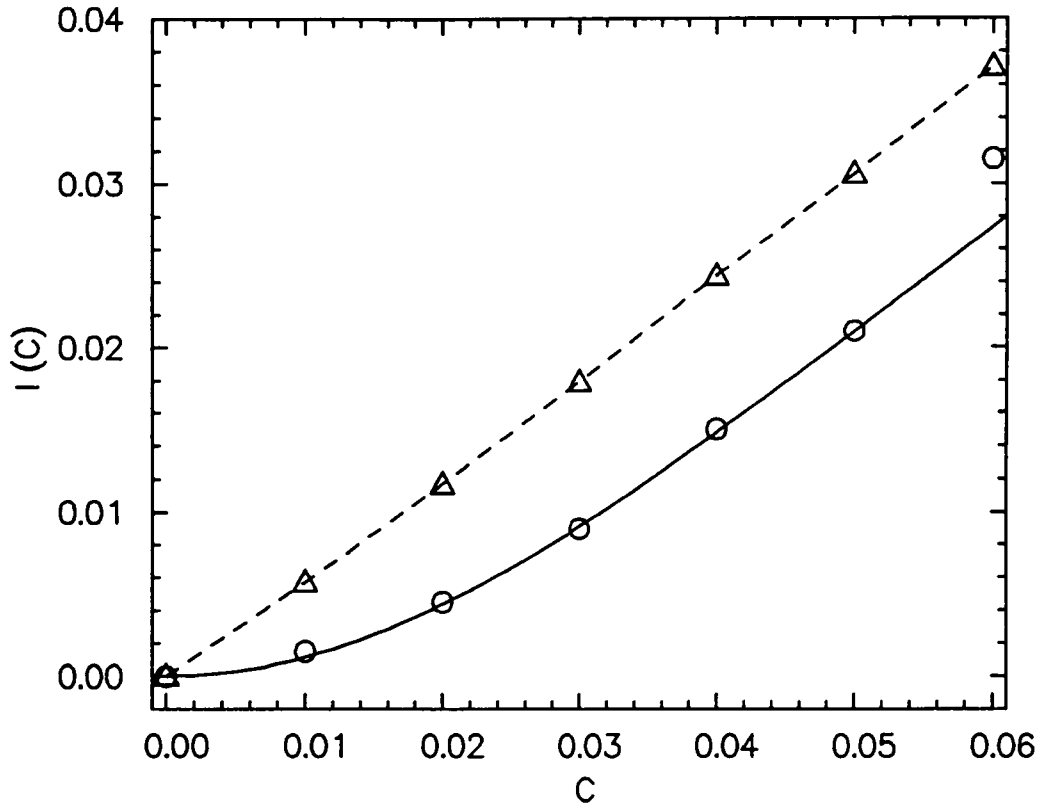


Figure 5.10: The cumulative distributions of 10,000 non-uniform random number distributions. The triangles are generated from Eq. (5.17) (dashed line) and the circles are generated from Eq. (5.23) (solid line) which fits the data of the kicked-top model of Ref. [59]. C is in units of the average width $\langle C \rangle$.

for the amount of overlap has only recently begun to develop by our MD approach. One measure is the mixing angle describing the incomplete exchange of diabatic state vectors across an avoided crossing due to the presence of other nearby levels. The change of the wavefunction during a two-body collisions can be parameterized as [67]

$$\begin{aligned}
 |n(\lambda_2) \rangle &= \cos(\psi/2)|n(\lambda_1) \rangle + \sin(\psi/2)|n+1(\lambda_1) \rangle \\
 |n+1(\lambda_2) \rangle &= \cos(\psi/2)|n+1(\lambda_1) \rangle - \sin(\psi/2)|n(\lambda_1) \rangle
 \end{aligned} \tag{5.24}$$

in term of mixing angle ψ . Note that when $\psi = 2\pi$, $|n, n+1(\lambda_2) \rangle = -|n, n+1(\lambda_1) \rangle$, where “-” represents the remnant of Berry’s phase [68]. For isolated two-body scattering the mixing angle ψ accumulated between λ_1 and λ_2 is π , leading to an “exchange” of the two state vectors. However,

if the residual force F_N due to the coupling to other nearby levels becomes nonnegligible before the exchange of state vectors is complete, the accumulated mixing angle ψ in the close collision region (λ_1, λ_2) is less than π , and the two state vectors remain mixed. We use this property to quantify the amount of overlap of avoided crossings as a function of λ . Fig. 5.11 displays the frequency distributions of ψ for two-body collisions of coupled Morse oscillators in the intervals $0 \leq \lambda \leq 0.1$ (a) and $0.5 \leq \lambda \leq 0.7$ (b). The former lies in the classically regular region while the latter lies in the predominantly chaotic regime. As expected, the distribution is peaked near π in the regular regime. The distribution of mixing angles shifts dramatically towards smaller values in the chaotic region, indicating the increasing statistical significance of overlapping avoided crossings. A peak near $\psi \approx \pi/2$ leads to a rapid spread of probability amplitudes over many states of the unperturbed basis. The latter is a prerequisite for wavefunctions in the chaotic domain to become pseudo-random number distributions [69] in the semiclassical limit.

The definition of mixing angle used above involves the properties of wavefunctions though their calculations are completely determined by the HFE (Eq. (5.1)). We introduce now an alternative measure that is solely based on the parametric variation of the energy levels without explicit reference to wavefunctions. The parametric equations of motion HFE provide a convenient framework in which to analyze the parametric correlations among matrix elements. Specializing to the two level system involved in an isolated avoided crossing the HFE become

$$\begin{aligned}\Delta \dot{E} &= p \\ \Delta \ddot{E} &= 4 \frac{V_{12}^2}{\Delta E} \\ \dot{V}_{12} &= -V_{12} \frac{p}{\Delta E}.\end{aligned}\tag{5.25}$$

The Wigner-von Neumann formula for $\Delta E(\lambda)$ (Eq. (5.12)) solves the system (5.25). Moreover, we find an explicit expression for the $\Delta\lambda$ dependent adiabatic coupling matrix element

$$V_{12}(\Delta\lambda) = V_0 \frac{C}{\sqrt{C^2 + 4(\Delta\lambda V_0)^2}}.\tag{5.26}$$

From the third equation of (5.25) follows that $\Delta E(\Delta\lambda)V_{12}(\Delta\lambda)$ is a constant of λ motion, in particular

$$\Delta E(\Delta\lambda)V_{12}(\Delta\lambda) = V_0 C\tag{5.27}$$

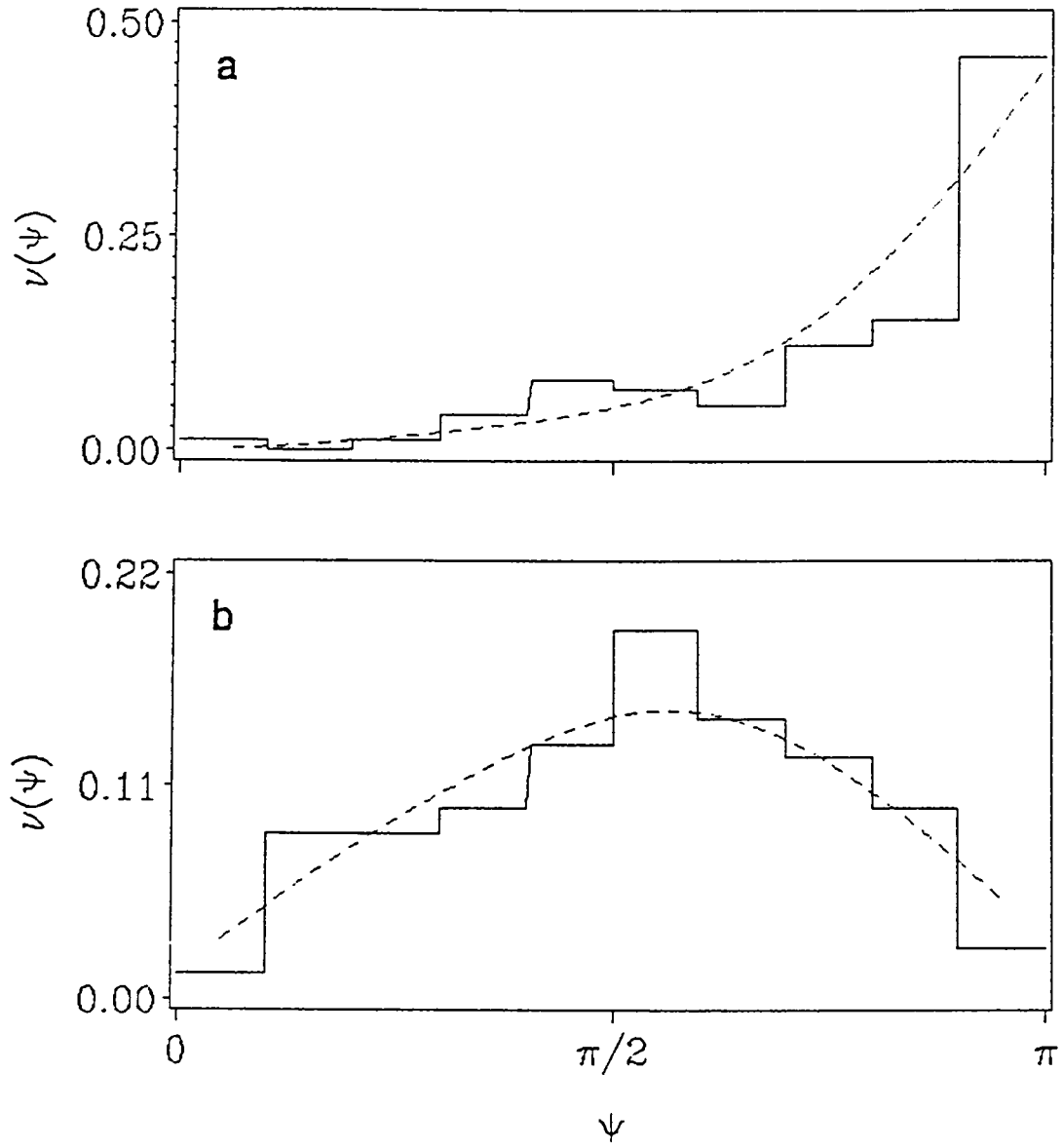


Figure 5.11: Histogram of mixing angles due to two-body collisions (avoided crossings) in (a) the classically mostly regular regime $0 \leq \lambda \leq 0.1$, and (b) in the mostly chaotic regime $0.5 \leq \lambda \leq 0.7$.

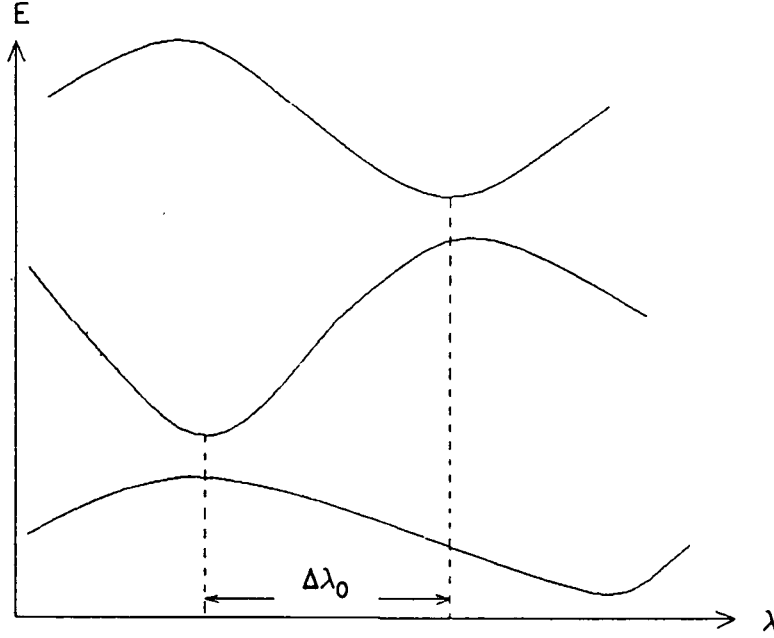


Figure 5.12: Illustration of the multiple avoided crossings.

for all $\Delta\lambda$. In the limit of “large” $\Delta\lambda$ (but still within the range of validity of the two-level approximation), i.e.

$$|\Delta\lambda| \gg \frac{C}{2|V_0|} \quad (5.28)$$

the matrix elements become

$$V_{12}(\Delta\lambda) \simeq \frac{C}{2\Delta\lambda} \text{sign}(V_0\Delta\lambda)$$

$$\Delta E(\Delta\lambda) \simeq 2|\Delta\lambda V_0|. \quad (5.29)$$

Eqs. (5.28) and (5.29) are now used to define a measure for overlapping avoided crossings. As above for wavefunctions, the latter are characterized by a breakdown of the Wigner-von Neumann formula for isolated avoided crossings (Eq. (5.12)). As shown by Fig. 5.12, the two-level approximation

(Eq. (5.25)) underlying Eq. (5.12) becomes invalid due to the presence of levels with which one of the two levels undergoes a subsequent avoided crossing. The avoided crossing can be considered to be isolated if the asymptotic form of the level separation (Eq. (5.29)) is reached prior to the encounter with other levels. Denoting the distance between two adjacent avoided crossings in λ parameter space involving the same level by $\Delta\lambda_0$, the ratio

$$R = \left| \frac{C}{2\Delta\lambda_0 V_0} \right| \quad (5.30)$$

measures the amount of overlap. An isolated avoided crossing corresponds to $R \ll 1$ while $R \simeq 1$ implies strong overlap.

The ensemble average R provides a measure of the overlap of the avoided crossings for the system. Because R varies by orders of magnitude in the classical transition regime, it is convenient to employ for an ensemble of avoided crossings the geometrical mean

$$\langle R \rangle = \sqrt[N]{R_1 R_2 \cdots R_N}. \quad (5.31)$$

Fig. 5.13 depicts $\langle R \rangle$ as a function of λ averaged over all AC's within a given window of $\Delta\lambda = 0.1$. In the perturbative regime ($0 \leq \lambda \leq 0.1$), $\langle R \rangle \approx 10^{-2}$ indicating the avoided crossings are mainly isolated. When $0.7 \leq \lambda \leq 0.8$, $\langle R \rangle$ has risen to $\simeq 0.5$ indicating the prevalence of overlapping avoided crossings. In order to illustrate the correspondence to the classical phase space structure we have overlaid the fraction of classical chaotic phase space Q_{cl} . The relative position and scale between the two axes (left-hand side Q_{cl} and right-hand side $\langle R \rangle$) were determined by a least- χ^2 fit

$$\chi^2 = \text{Min}_{(A,B)} \sum_i [\log_{10} \langle R \rangle (\lambda_i) - (A Q_{cl}(\lambda_i) + B)]^2. \quad (5.32)$$

As expected, the amount of overlap is directly correlated to the fraction of chaotic phase space.

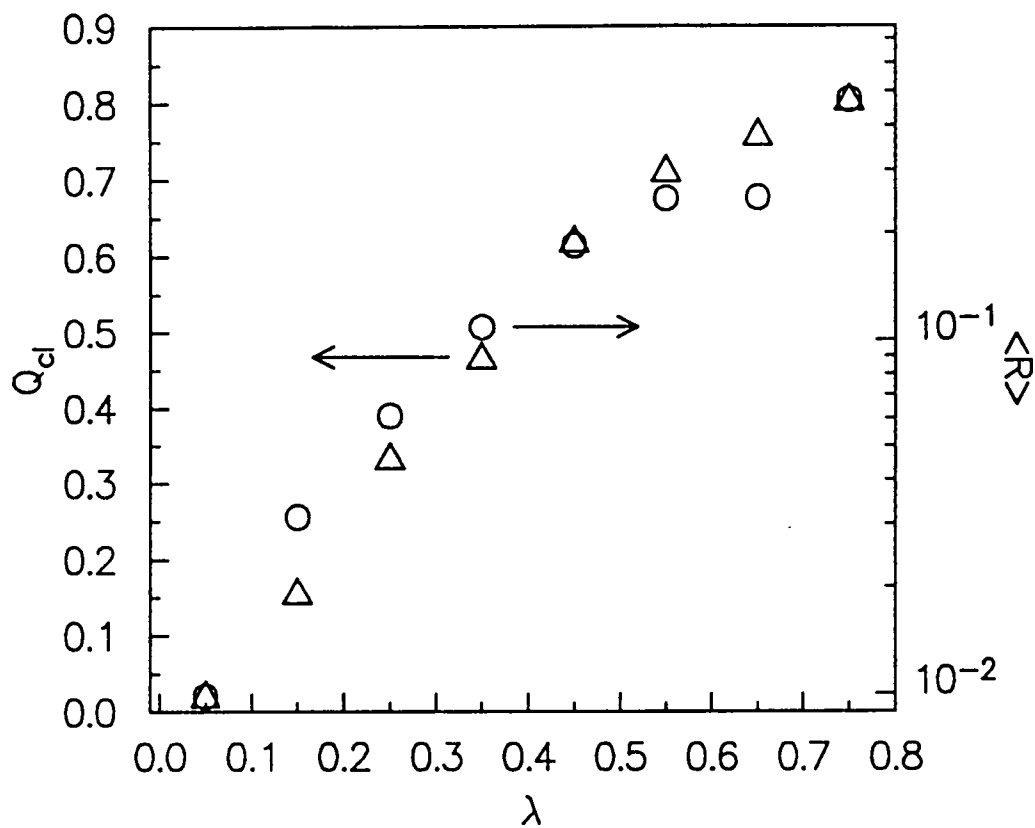


Figure 5.13: Overlap parameter $\langle R \rangle$ (circle) and the fraction of classically chaotic phase space in the energy shells contributing to the energy level statistics, Q_{cl} , (triangles) as a function of λ for coupled Morse oscillators.

Chapter 6

Thermal equilibrium distribution of parametric dynamics

Whether the parametric dynamical system described by Eq. (5.1) can reach thermal equilibrium and what kind of equilibrium is reached are two long-standing problems. It is a major advance that our MD simulations can put these hypotheses to the test of computer “experiments”. Using the model system of coupled Morse oscillators, we show in this chapter that the thermal equilibrium of the parametric dynamical system is indeed reached. The equilibrium distribution allows a direct determination of the Brody parameter in the predominantly chaotic regime and confirms the Wigner-type NNS distribution in this regime.

6.1 Approach to equilibrium

The conceptual beauty of Eq. (5.1) is its generality. The form of Eq. (5.1) is independent of the properties of Hamiltonian (2.25) and the specific features of Hamiltonian only influence the initial conditions $(x_n(0), p_n(0), V_{in}(0))$. From Figs. (5.3) and (5.4), we expect that in the limit of large λ , the many-body system described by Eq. (5.1) may “forget” its initial states due to the huge number of avoided crossings, and reach the state of “thermal equilibrium” which should represent a universal energy level distribution of irregular quantum systems. Equilibration should occur typically within a “mean free path” λ_{MFP} for collisions which should approximately correspond to the

critical value λ_c where the transition from mostly regular to mostly chaotic motion occurs.

It was shown [45] analytically, however, that Eq. (5.1), though complicated and highly nonlinear, constitutes a completely integrable system with internal complex vector space. The integrability is not surprising since Eq. (5.1) is equivalent to the diagonalization of an $\tilde{N} \times \tilde{N}$ matrix. Therefore, the output of the HFE is connected with its initial input by a unitary transformation, hence the HFE can be solved completely algebraically, which excludes any exponential separations among solutions which are initially close. We will construct this unitary transformation explicitly in Chapter 8.

While the integrability of the HFE guarantees the stability of our MD numerical solutions, it challenges the notions of equilibrium statistical mechanics since these notions implicitly invoke ergodicity (or even mixing) which in general requires the system to be nonintegrable. Therefore, a quantitative verification of the thermal equilibrium conjecture which seems conflicting with the integrability of Eq. (5.1) is needed. Since our method amounts, in essence, to the study of non-equilibrium statistical mechanics of the one-dimensional many-body system of the HFE, it is well suited to quantitatively test this conjecture. In order to improve the statistics we have rescaled Planck's constant $\hbar$ to $\hbar/3$ (or equivalently, the dissociation energies D_i to $9D_i$) in this and the next chapters for coupled Morse oscillators with parameters for the triatomic molecule H-C-C, thereby increasing the number of bound states below the dissociation limit to ≈ 1480 in the interval of $0 \leq \lambda \leq 1$.

The ensemble averages discussed contain a stretch of energy levels from the 400th to the 1000th level (counted from the ground state up) with energies of about 0.75 ± 0.1 in units of the dissociation energy.

Based on the correspondence between Newton's equation and the HFE, the thermal equilibrium of system Eq. (5.1) should be signaled by a Maxwell-Boltzmann distribution for the single-particle kinetic energy $p_n^2/2$, i.e.

$$P(p_1, \dots, p_{\tilde{N}}) = \exp\left[-\frac{\beta}{2} \sum_{i=1}^{\tilde{N}} p_i^2\right] \quad (6.1)$$

with

$$\beta^{-1} = \langle p_n^2 \rangle. \quad (6.2)$$

In the present case, the mean momentum vanishes, $\langle p_n \rangle \approx 0$. This test for a Maxwell-Boltzmann distribution has the advantage of being not directly

dependent upon the properties of the fluctuating charges $\langle V_{in}^2 \rangle$ and of the absence of free parameters. Fig. 6.1 displays the distribution function for the kinetic energy at various "times" λ . Note that the peak at zero momentum (all $p_n = 0$) at $\lambda = 0$ is a peculiarity of the system of coupled Morse oscillators. With increasing λ the distribution indeed approaches a Maxwell-Boltzmann distribution represented in Fig. 6.1 by a straight line with "temperature" β^{-1} .

Fig. 6.2(a) displays the temperature, the ensemble averages $\langle V_{in}^2 \rangle$, and the subset of nearest-neighbor couplings $\langle V_{n,n+1}^2 \rangle$ as a function of λ , while Fig. 6.2(b) gives χ^2 for a least square fit with a Maxwell-Boltzmann distribution. Obviously, equilibrium is reached for $\lambda \approx 0.6$ as reflected in both an approximately constant value of β^{-1} and small χ^2 values. The values of the temperature β^{-1} and of the average couplings $\langle V_{in}^2 \rangle$ are system-dependent, but the ratio, $2\beta \langle V_{n,n+1}^2 \rangle$, is independent of the units and is closely related to the Brody parameter in the equilibrium state as shown in the next section.

6.2 The source of ergodicity and equilibrium distribution

There are at least two proposals to explain the apparent contradiction between our numerically verified approach to thermal equilibrium and the complete integrability of the HFE system. Yukawa's [44] proposal that the introduction of boundary conditions reduces the number of constants of parametric motion and thereby restores the ergodicity of the HFE faces the following difficulties: firstly, numerical studies with some classical many-body systems [70] indicate that integrability persists irrespective of imposed boundary conditions; secondly, boundary conditions are a characteristic of the model dependent truncation of the Hilbert space rather than of the Hamiltonian itself. It is therefore unsatisfactory to rely on model dependent approximations in order to approach an "equilibrium" level distribution which is considered to be generic for irregular dynamics.

An alternative proposal was developed within the framework of our molecular dynamics approach [71]. The key observation is that the HFE system lives in an extended phase space with $2\tilde{N} + \tilde{N}(\tilde{N} - 1)/2$ dimensions incorporating the dynamics of the charge fluctuations V_{in} as internal degrees of freedom. The $2\tilde{N}$ dimensional phase space, in which the distribution function

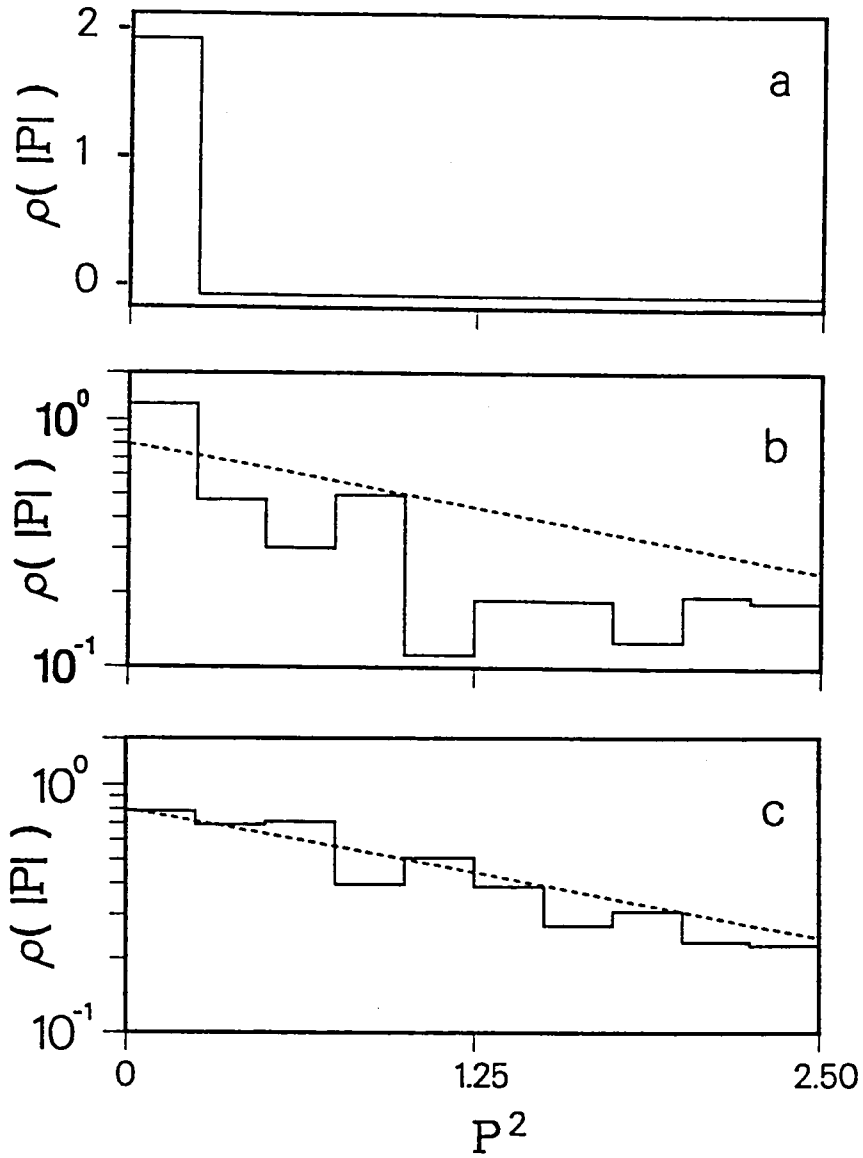


Figure 6.1: Histogram of the single particle kinetic energy distribution at three different “times”: (a) $\lambda = 0$, (b) $\lambda = 0.10$, and (c) $\lambda = 0.65$, where the horizontal axes is in the units of $\langle p^2 \rangle$. The dashed line is the Maxwell-Boltzmann distribution with temperature $\beta^{-1} = \langle p^2 \rangle$.

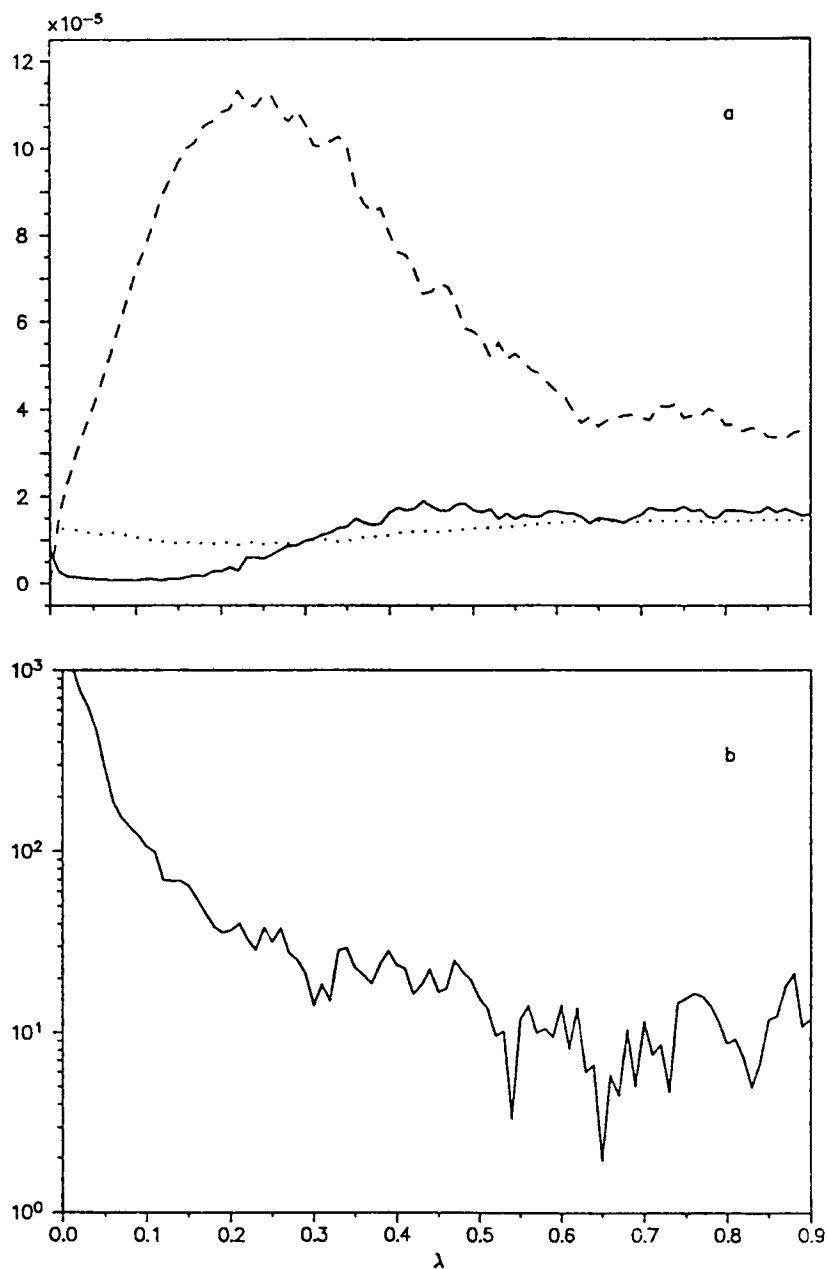


Figure 6.2: (a) Temperature β^{-1} (dashed line), $\langle V_{in}^2 \rangle$ (dotted line), and $\langle V_{n,n+1}^2 \rangle$ (solid line). The perturbation V is in units of the dissociation energy. (b) χ^2 for a Maxwell-Boltzmann distribution as a function of λ .

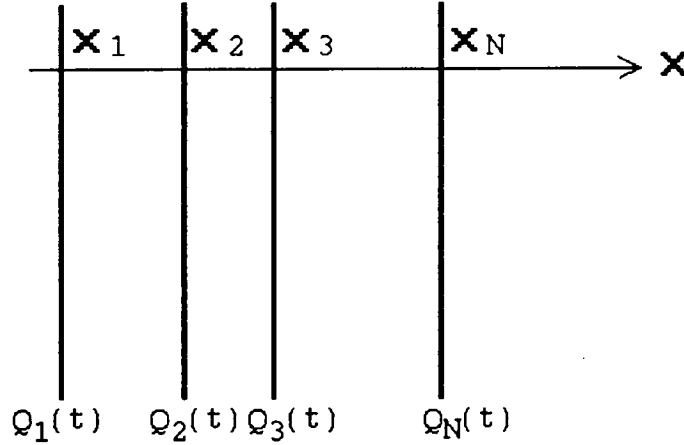


Figure 6.3: The classical system of charged strings. The pairwise coupling potential is given by $Q_i(t)Q_n(t) \ln |x_i - x_n|$ where $Q_i(t)$ is the time-dependent charge density of the string.

of (x_n, p_n) is to be defined, therefore represents a subspace of the extended phase space. In the semiclassical limit, $\tilde{N} \rightarrow \infty$, Eq. (5.1) for the $\tilde{N}$ particles embody the nonequilibrium statistical mechanics of a small system with $2\tilde{N}$ degrees of freedom coupled to a large reservoir (with $\approx \tilde{N}^2/2$ degrees). Almost inevitably, the $\tilde{N}$ particle distribution function will become canonical irrespective of details of the coupling to the reservoir, provided the coupling is sufficiently strong to ensure equilibration within the available “time” interval λ .

We note first that the canonical equations of motion for the $2\tilde{N}$ phase space variables (x_n, p_n) are generated from an effective λ “time”-dependent model Hamiltonian

$$\tilde{H}(\lambda) = \sum_{n=1}^{\tilde{N}} \frac{p_n^2}{2} - 2 \sum_{i < n}^{\tilde{N}} V_{in}^2(\lambda) \ln |x_i - x_n|. \quad (6.3)$$

Eq. (6.3) is similar to the Hamiltonian for a classical system of charged strings with infinite length moving along the x -dimension, as shown in Fig. 6.3. The system of Eq. (6.3) is coupled to a heat bath with $\tilde{N}(\tilde{N} - 1)/2$ degrees of freedom through λ -dependent coupling parameters (“charges”) $V_{in}(\lambda)$. In the semiclassical limit, $\tilde{N} \rightarrow \infty$, the reduced density function of a small system (with $2\tilde{N}$ degrees of freedom) coupled to a reservoir with $\sim \tilde{N}^2/2$

degrees of freedom is expected to be canonical,

$$P(\tilde{H}) = \exp[-\beta\tilde{H}] = \exp[-\frac{\beta}{2} \sum_{i=1}^{\tilde{N}} p_i^2] \exp[2\beta \sum_{i < n} \langle V_{in}^2 \rangle \ln |x_i - x_n|]. \quad (6.4)$$

The essential assumption underlying (6.4) is that the fluctuations in $V_{in}(\lambda)$ are fast on the time scale of the motion in the $2\tilde{N}$ phase space so that we can replace V_{in}^2 by its average $\langle V_{in}^2 \rangle$ [68]. This procedure is similar to deriving the rate equations from the Liouville's equation by averaging over the quantities of the heat bath [72]. The origin of the rapid fluctuations of V_{in}^2 are close collisions (i.e., avoided crossings) between adjacent energy levels.

In order to verify this assumption we study the linear correlation between variables X and Y measured by the covariance

$$\sigma_{XY} = \langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle. \quad (6.5)$$

If $\sigma_{XY} = 0$, X and Y are said to be linearly uncorrelated [73]. The normalized covariance of X and Y is defined as

$$\rho_{XY} = \sigma_{XY} / (\langle X \rangle \langle Y \rangle). \quad (6.6)$$

Let $X = V_{n,n+1}^2$ and $Y = 1/|x_{n+1} - x_n|$, then ρ_{XY} provides a measure of the correlation between the two factors (charge and distance) in the two-body forces

$$F_2 = 2V_{n,n+1}^2 / |x_{n+1} - x_n|. \quad (6.7)$$

Fig. 6.4 displays the correlation between these two factors of F_2 as a function of λ . It fluctuates strongly in the nonequilibrium regime while becoming close to zero when thermal equilibrium is reached. Therefore, $V_{n,n+1}^2$ and $1/|x_{n+1} - x_n|$ are not correlated in the equilibrium state. This result provides a justification of replacing V_{in}^2 by its average $\langle V_{in}^2 \rangle$ in Eq. (6.4). In Fig. 6.2, the ensemble averages $\langle V_{in}^2 \rangle$ show remarkably little variation as a function of λ . This is the key characteristic of a heat bath which has so many degrees of freedom that the effect of the interaction with the small system (here is the $2N$ -dimensional subsystem of (x_n, p_n)) is negligible. The heat bath remains described by several macroscopic constants, irrespective of the amount of energy diffusing into or out of the small system.

Note that tracing out all position coordinates, Eq. (6.4) predicts a Maxwell-Boltzmann distribution for the single-particle kinetic energy Eq. (6.1), as expected. The joint particle-(level-)distribution function follows from Eq. (6.4)

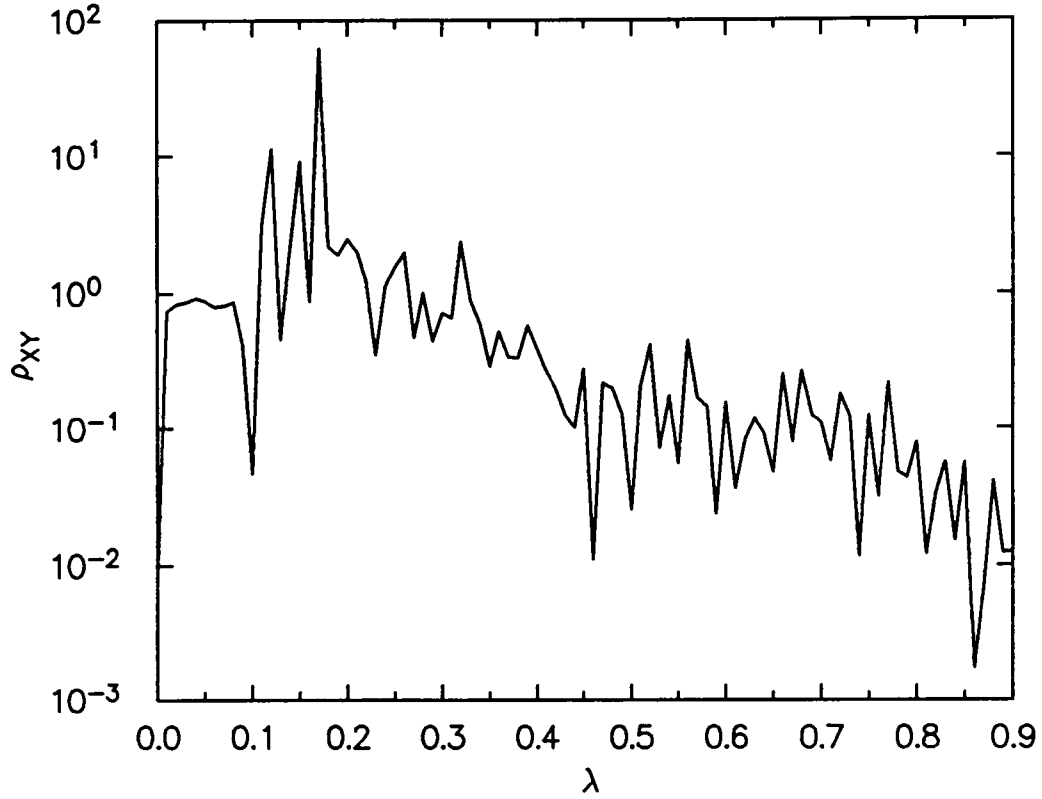


Figure 6.4: Correlation between the couplings and the positions of the nearest neighbors.

upon tracing out all momentum coordinates,

$$P(x_1, \dots, x_{\tilde{N}}) = \prod_{i < n} |x_i - x_n|^{2\beta \langle V_{in}^2 \rangle}. \quad (6.8)$$

Eq. (6.8) implies for the NNS distribution for small s

$$P(s) \propto s^{\gamma_1} \quad s \rightarrow 0 \quad (6.9)$$

where $s \propto x_{n+1} - x_n$ and

$$\gamma_1 = 2\beta \langle V_{n,n+1}^2 \rangle \quad (6.10)$$

Therefore, Eq. (6.8) agrees locally with the GOE prediction $P(s)_{s \rightarrow 0} \propto s$ (Eq. 3.20) if the exponent of it happens to attain the value

$$2\beta \langle V_{in}^2 \rangle = 1. \quad (6.11)$$

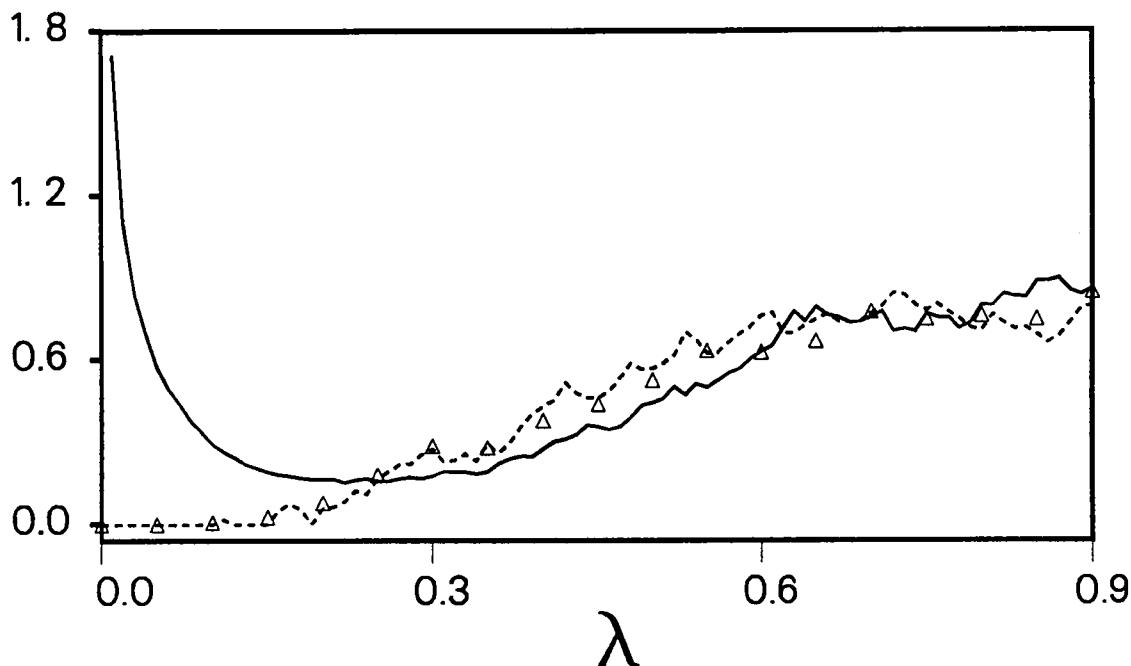


Figure 6.5: Brody parameter κ (dashed line), γ_1 (solid line), and fraction of classically chaotic phase space Q_{cl} (Δ) as a function of λ .

Extending Eq. (6.9) to large s using the standard procedure (see Chapter 3) for deriving the Wigner distribution [22] yields a Brody-like distribution (Eq. (3.22)) with γ_1 playing the role of the Brody parameter κ . The important result is that γ_1 can be directly determined in terms of the equilibrium kinetic and potential energy of the HFE Hamiltonian $\tilde{H}$ (see Eq. (6.10)) provided that equilibrium has indeed been reached. In turn, when

$$\kappa \approx \gamma_1, \quad (6.12)$$

a direct numerical determination of the Brody parameter becomes possible.

Fig. (6.5) displays both the Brody parameter κ determined from fits with NNS distributions and γ_1 determined from Eq. (6.10) together with the fraction Q_{cl} of the classically chaotic area on the energy hypersurface $E = 0.75$ which lies approximately in the center of the stretch from the 400th to the 1000th quantal eigenvalue entering the statistics. We note first that the transition to classical large-scale chaos ($Q_{cl} \geq 0.6$) occurs simultaneously with

the approach of the statistical equilibrium of the energy-level distribution as described by HFE ($\lambda \geq 0.6$). At the same time the exponent γ_1 agrees well with the Brody parameter κ determined from fits to histograms, in agreement with the hypothesis Eq. (6.12). In line with investigations of other systems [16] we find that κ (or γ_1) stays below the GOE predictions, probably because of residual islands of regular motion. In the near regular regime ($\lambda < 0.3$) the ensemble is far from statistical equilibrium and γ_1 deviates strongly from κ . Contrary to Yukawa's assumptions, the Poissonian distribution cannot be derived from equilibrium statistical mechanics for HFE. The latter is a consequence of the fact that in the regular regime avoided crossings become quasi-crossings (i.e. very narrow avoided crossings. See Chapter 5). In this limit the $\tilde{N}$ -body system behaves like an ideal gas which remains its initial distribution of single-particle kinetic energy and does not attain equilibrium. On the other hand, because of the simplicity of such a gas, one can easily derive its properties, such as a Poissonian distribution for the nearest-neighbor spacings [74].

A quasi-crossing implies a weak coupling between the two levels, i.e. $V_{n,n+1} \sim 0$. This is another signal of quasi-integrability since it leads to $[H, V] \sim 0$, i.e. V is an approximately conserved constant in the subspace spanned by the levels E_n and E_{n+1} . Therefore, the ratio of the averaged nearest coupling over the averaged coupling,

$$O = \langle V_{n,n+1}^2 \rangle / \langle V_{n,i}^2 \rangle, \quad (6.13)$$

should be small in the near-integrable region while it becomes of the order of unity in the mostly chaotic region. Fig. (6.6) displays this quantity as a function of λ . In the near-integrable region, O decreases very rapidly from a system-specific value to a generic small one. When chaotic motion becomes significant, O increases to the values around one. Therefore, O provides another measure for the study of quantum chaos.

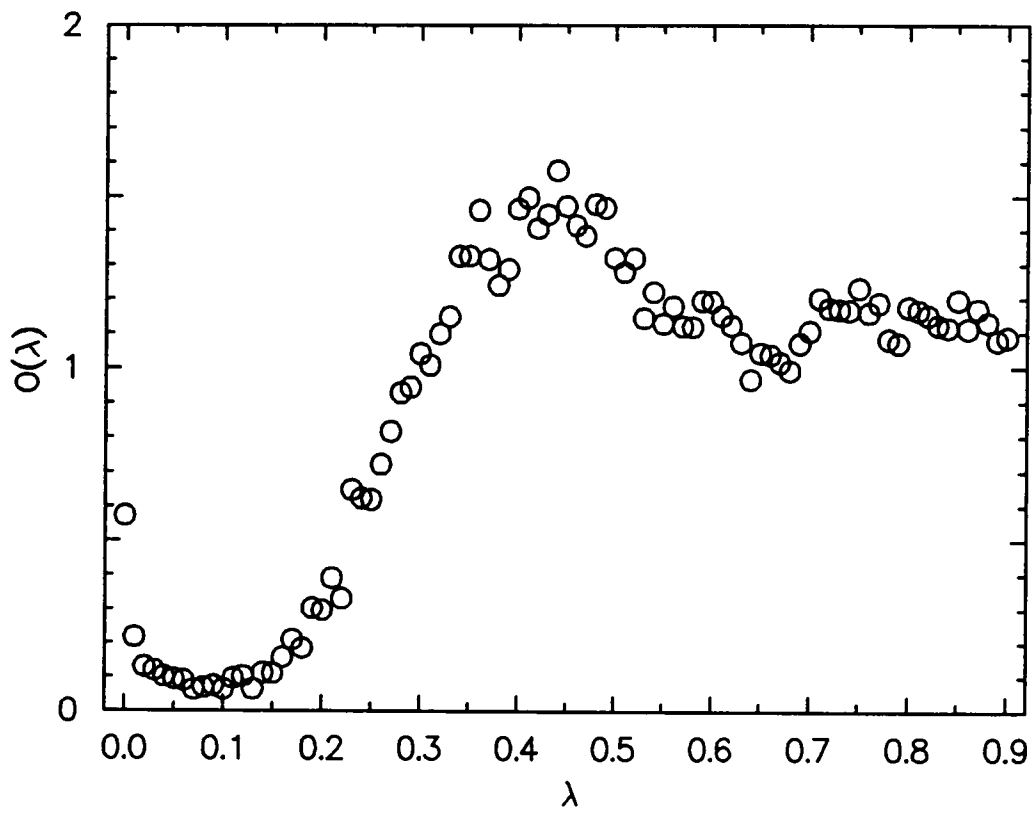


Figure 6.6: The ratio of the couplings as a function of λ .

Chapter 7

Parametric Correlations and Diffusion in Quantum Spectra

Apart from the efforts to confirm random matrix description, the HFE (5.1) have also been used to identify other fingerprints of classical chaos on quantum spectrum [75]. Eq. (5.1) exhibits structures in the parametric motion of energy levels, such as solitons [76] and the universal distribution of the curvatures (i.e. the second derivative of the energy levels with respect to λ) [77]. Parametric motion of energy levels, in particular the sensitivity of the spectra with respect to small changes in λ , was proposed very early as one fingerprint of classical chaos [66]. The study of parametric correlations is important for two reasons. Firstly, they measure the correlations between Hamiltonians at different values of λ , and therefore provide criteria for the statistical independence of spectra such that level statistics can be obtained by treating spectra at different values of λ as effectively independent ensembles. Secondly, they are sensitive to the changes in the underlying classical dynamics and therefore provide new diagnostic tools for quantum chaology. In this chapter, we investigate the relaxation processes in the parametric motion of energy levels. As is well-known from the theory of liquids and, more generally, disordered many-body systems, the dynamics of relaxation can be described in terms of correlation functions [78]. We analyze in the following for the first time the velocity autocorrelation function and the friction kernel of its generalized Langevin equation. One important result [79] is that the frequently invoked picture of the parametric motion of energy levels as that of a “gas” is correct only in the near-integrable regime. The dynamic correlation functions resemble, in the mostly chaotic regime, that of a strongly coupled

liquid. Moreover, we find the transition from classically regular to classically chaotic motion to be associated with a “liquid-glass” type transition in the parametric energy level dynamics characterized by the disappearance of diffusion [80]. A simple analytic approximation for the spectrum of the velocity autocorrelation function whose form is suggested by the periodic orbit (PO) quantization Eq. (4.11) in the semiclassical limit reproduces our results of the molecular dynamics simulation quite well.

7.1 Parametric number variance

The molecular dynamics simulation (Eq. (5.1)) yields the physical energies $(x_1(\lambda), \dots, x_N(\lambda))$. For the implementation of level statistics the spectrum is rescaled by Eq. (3.2) to yield the unfolded spectrum $(\varepsilon_1(\lambda), \dots, \varepsilon_N(\lambda))$. One parametric measure we use in this chapter is the parametric number variance (PNV) proposed by Goldberg et al. [81]

$$V_P(\Lambda) = \langle (N(\varepsilon, \lambda + \Lambda) - N(\varepsilon, \lambda))^2 \rangle \quad (7.1)$$

where N is the λ -dependent integrated density of the unfolded spectrum $\{\varepsilon_n(\lambda)\}$ (Eq. (3.6)), Λ is the increment of the parameter λ and the average is over λ . PNV measures the fluctuations in the number of energy levels lying below the reference point ε and it can be understood pictorially as follows: The “coordinate space” trajectories of the unfolded levels are roughly horizontal lines as in Fig. 5.4. The net number of crossings of a given horizontal line at height ε by levels between λ and $\lambda + \Lambda$ are counted. This number is equivalent to the difference between the number of levels below ε at $\lambda + \Lambda$ and the number of levels below ε at λ . The average over λ of the square of this number is the parametric number variance. Notice that the values of Λ are confined within intervals of λ in which the classical phase space structure does not appreciably change. The semiclassical estimate for PNV is given in the Appendix C. For classically integrable systems, we have

$$V_P(\Lambda) \approx \langle |y| \rangle n_{av} \Lambda \quad (7.2)$$

where $y = (\partial S / \partial \lambda)_\varepsilon / T$ with S the action and T the period of classical orbits. For classically totally chaotic systems, PNV is given by

$$V_P(\Lambda) \approx \begin{cases} \langle |y| \rangle n_{av} \Lambda & \Lambda \sim 0 \\ \frac{2}{\pi^2} \ln(\Lambda) + \text{constant} + O\left(\frac{1}{\langle |y| \rangle n_{av} \Lambda}\right) & \langle |y| \rangle n_{av} \Lambda \gg 1 \end{cases} \quad (7.3)$$

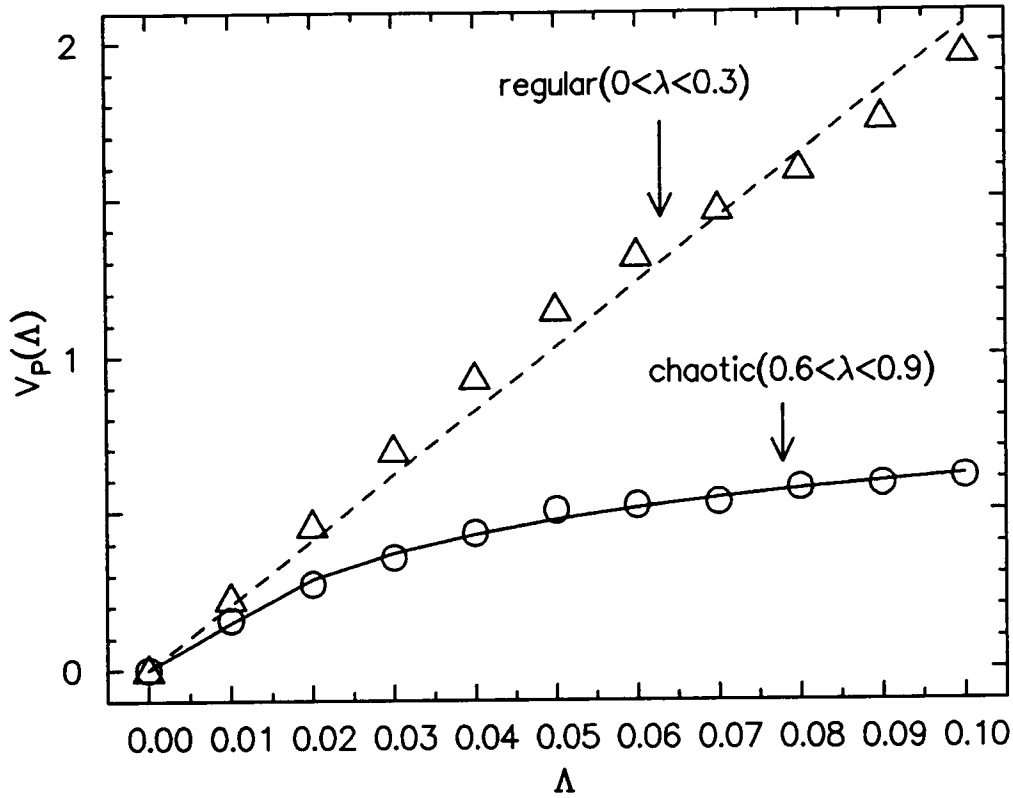


Figure 7.1: Parametric number variance for coupled Morse oscillators. triangle: integrable region ($0 < \lambda < 0.3$) and circle: chaotic region ($0.6 < \lambda < 0.9$). The dashed line is given by Eq. (7.2) and the solid line is given by (7.3) where unknown constants are determined by fitting.

Notice that in the semiclassical limit $\hbar \rightarrow 0$, $n_{av} \propto 1/\hbar^N$ is large. In the regime of $\langle |y| \rangle n_{av} \Delta \gg 1$, the behavior of PNV is sensitively dependent on the underlying classical dynamics and therefore provides a new measure of quantum chaos. Fig. 7.1 displays the PNV for coupled Morse oscillators which is described by Eqs. (7.2, 7.3) quite well. As in Chapter 6, the ensemble averages discussed in this chapter contain an interval of energy levels for the coupled Morse oscillators from the 400th to the 1000th level with energies of about 0.75 ± 0.1 in units of the dissociation energy. Q_{cl} , the fraction of the classically chaotic area on the energy hypersurface $E = 0.75$, is small ($Q_{cl} \leq 0.3$) when $\lambda \leq 0.3$, while the phase space becomes mostly chaotic ($Q_{cl} \approx 0.8$) when $\lambda \geq 0.6$. Averages will extend over the interval of $0.0 \leq \lambda \leq 0.3$ for classically mostly regular case and over the interval of $0.6 \leq \lambda \leq 0.9$ for

classically mostly chaotic case.

As discussed in Appendix C, a modification is needed for Eq. (7.3) when Λ reaches the limit of large values ($\Lambda < |y| > \geq < S/T >$). One can rewrite Eq. (7.1) as

$$V_P(\Lambda) = < (N(\varepsilon, \lambda + \Lambda) - N_{av})^2 > + < (N(\varepsilon, \lambda) - N_{av})^2 > \\ - 2 < (N(\varepsilon, \lambda + \Lambda) - N_{av})(N(\varepsilon, \lambda) - N_{av}) > \quad (7.4)$$

where $N_{av} = \varepsilon$ by the construction of the unfolded spectrum. Each of the first two terms of (7.4) is simply the number variance (see Appendix C), $\Sigma(\varepsilon)$, of the levels in the range 0 to ε . When the value of Λ is quite large, the third term vanishes for totally chaotic systems as there is no correlation between its two factors due to the multitude of overlapping avoided crossings. Thus it is expected [81] for chaotic systems

$$V_P(\Lambda) \approx 2\Sigma(\varepsilon) \quad \Lambda \rightarrow \infty. \quad (7.5)$$

7.2 Self-diffusion and the Velocity Autocorrelation Function

The motion of a tagged particle in an interacting many-body system can be described by a generalized diffusion coefficient $D(\Lambda)$ as a function of “time” Λ which is defined as the slope of the mean squared displacement $< x^2(\Lambda) >$,

$$D(\Lambda) = \frac{1}{2} \frac{d}{d\Lambda} < x^2(\Lambda) > \quad (7.6)$$

with

$$< x^2(\Lambda) > = < (\varepsilon_n(\lambda + \Lambda) - \varepsilon_n(\lambda))^2 >. \quad (7.7)$$

We denote ensemble averages by brackets $< >$ which can represent either averages over ensembles of particles at a given λ or averages over different values of the “time” λ . These averages are equivalent only if the dynamics is stationary and ergodic. In order to improve the statistics we will use both ensemble and time averages. In the limit of large Λ and in the presence of diffusive motion, Eq. (7.6) leads to the Einstein relation for the Langevin diffusion of a Brownian “tagged” particle

$$< x^2(\Lambda) > = 2D\Lambda \quad (7.8)$$

with $D = D(\Lambda \rightarrow \infty)$ the ordinary diffusion coefficient. Large Λ 's imply a "time" large compared to the average "collision" time (i.e. the interval between avoided crossings) but still small compared to the λ values where the classical phase space structure undergoes a transition from regular to chaotic motion (or vice versa). A phase transition to a glass-like system is characterized by a vanishing diffusion constant $D = 0$ and, hence, the absence of diffusive motion according to Eq. (7.8). The generalized diffusion coefficient $D(\Lambda)$ can be expressed in terms of the velocity autocorrelation function (VAF) describing the microscopic decay of the momentum correlation of the tagged particle in the many-body system

$$\psi(\Lambda) = \beta \langle p_n(\lambda + \Lambda)p_n(\lambda) \rangle \quad (7.9)$$

where β^{-1} is the mean squared momentum given by Eq. (6.2). The VAF is normalized, i.e. $\psi(\Lambda = 0) = 1$. Notice that the momentum distribution of the energy level dynamics described by the HFE (5.1) is, in general, non-Maxwellian. Only in the limit of large-scale classical chaos the momentum distribution approaches a Maxwell-Boltzmann distribution. Expressed in terms of the VAF, the generalized diffusion coefficient becomes

$$D(\Lambda) = \beta^{-1} \int_0^\Lambda d\Lambda' \psi(\Lambda') \quad (7.10)$$

and the mean squared displacement is given by

$$\langle x^2(\Lambda) \rangle = 2\beta^{-1} \int_0^\Lambda d\Lambda' (\Lambda - \Lambda') \psi(\Lambda'). \quad (7.11)$$

Eq. (7.11) allows the determination of $\langle x^2(\Lambda) \rangle$ when the diffusion constant vanishes. The properties of the VAF can be most conveniently analyzed in terms of its frequency spectrum

$$G(\omega) = \int_0^\infty d\Lambda \cos(\omega\Lambda) \psi(\Lambda). \quad (7.12)$$

The motion of the particle contains both diffusive and vibratory components. The diffusive component is characterized by a non-zero value of $G(0)$ while a vibratory component appears in $G(\omega)$ as a peak at non-zero frequency. The long-"time" behavior of $\langle x^2(\Lambda) \rangle$ is determined by $G(\omega \approx 0)$, i.e. it mainly depends on the existence of the diffusive component but is insensitive to the vibratory component. Accordingly, the diffusion coefficient is given by

$$D = \beta^{-1} G(0). \quad (7.13)$$

The VAF satisfies a generalized Langevin equation

$$\frac{d}{d\Lambda}\psi(\Lambda) = - \int_0^\Lambda d\Lambda' K(\Lambda - \Lambda')\psi(\Lambda') \quad (7.14)$$

with $K(\Lambda)$ the friction kernel containing the memory of the interaction of tagged particle with the surrounding particles. Closely related is the force correlation function

$$f(\Lambda) = \langle F_n(\lambda + \Lambda)F_n(\lambda) \rangle \quad (7.15)$$

which is given in terms of $\psi(\Lambda)$ by

$$\frac{d^2}{d\Lambda^2}\psi(\Lambda) = -\beta f(\Lambda). \quad (7.16)$$

The mean squared force in the ensemble, $\langle F_n^2 \rangle = f(\Lambda = 0)$ can be expressed in terms of the second moment of the spectrum of the VAF, $G(\omega)$, as

$$\beta f(0) = \langle \omega^2 \rangle = \frac{2}{\pi} \int_0^\infty d\omega G(\omega)\omega^2. \quad (7.17)$$

The friction kernel $K(\Lambda)$ satisfies an analogous generalized Langevin equation with the relaxation kernel playing the role of memory kernel. Eqs. (7.10), (7.11) and (7.14) are the first members of a hierarchy of equations of motion for correlation functions known as the Mori-Zwanzig projection operator formalism [82]. Simple approximations to the memory kernel for the higher order members of the hierarchy of equations of motion induce increasingly accurate approximations to the generalized diffusion coefficient and other correlation functions. Phenomenological approximations consist of choices for the memory kernel which reproduce transport coefficients such as the diffusion coefficient (Eq. (7.13)), the friction coefficient η , and frequency moments $\langle \omega^{2k} \rangle$ ($k = 1, 2, \dots$) of the VAF (Eq. (7.17)). The latter determine the short-time dynamics of the velocity correlation. Alternatively, a closed system of coupled equations of motion for a truncated set of correlation functions can be developed which can be solved self-consistently and numerically. (This approach underlies the mode-coupling approximations [83].) In the following we restrict ourselves to phenomenological approximations to the memory kernel which allow a simple analytic description of the VAF and the generalized diffusion coefficient and give direct insights into the parameter

dependence. Accurate numerical results will be generated by the molecular dynamics simulation (Eq. (5.1)).

A useful interrelation between the spectrum of the VAF and the friction kernel can be found using the Laplace transform

$$\tilde{\psi}(s) = \int_0^\infty d\Lambda \exp(-s\Lambda) \psi(\Lambda), \quad \text{Re}(s) > 0. \quad (7.18)$$

where s is the variable of the Laplace transform (not to be confused with the variable for the nearest-neighbor spacing, see Eq. (1.7)). The spectrum of the VAF is given by

$$G(\omega) = \frac{1}{2}(\tilde{\psi}(i\omega) + \tilde{\psi}(-i\omega)). \quad (7.19)$$

The generalized Langevin equation (7.14) can be solved by a Laplace transform to give

$$\tilde{K}(s) = 1/\tilde{\psi}(s) - s. \quad (7.20)$$

Furthermore, combining (7.19) and (7.20) yields for the Fourier transform of $K(\Lambda)$, $K_F(\omega)$

$$K_F(\omega) = G(\omega)/(\tilde{\psi}(i\omega)\tilde{\psi}(-i\omega)). \quad (7.21)$$

The interrelation between $K(\Lambda)$, $\tilde{\psi}(s)$ and $G(\omega)$ implies that an approximation for any of these functions uniquely determines the others, in particular the VAF, the generalized diffusion coefficient, and the mean squared displacement of the tagged particle.

7.3 Semiclassical Estimates for Correlation Functions

In this section we use general semiclassical arguments to suggest properties of the spectrum of the VAF. The choice of an approximate form of the spectrum (or equivalently, the friction kernel) of the VAF for the energy level dynamics is expected to depend on the classical dynamics of the Hamiltonian system (Eq. (2.25)). Classically regular and chaotic motion should manifest themselves in characteristic, possibly universal, properties of the spectrum of the VAF, and hence, in the self-diffusion of levels.

In establishing a correspondence one is faced with a fundamental difficulty: as described in Chapter 4, the semiclassical quantization of the classically chaotic phase space using the Gutzwiller trace formula Eq. (4.11) (or

variations thereof) for unstable periodic orbits describes fluctuations of the density of states rather than positions of individual levels. Self-diffusion of the “tagged particle”, on the other hand, is concerned with the parametric motion of individual levels and therefore with the finest scale structure of the quantum spectrum. It is therefore unlikely that a one-to-one correspondence between the spectrum of the VAF and the semiclassical limit of the quantum spectra exists. However, we conjecture that the near-zero frequency behavior of the VAF, $G(\omega \approx 0)$, is directly related to the semiclassical quantization for regular and chaotic systems. This conjecture is based on the observation that according to Eq. (7.13) the low frequency limit of the VAF determines the large “time” limit $\Lambda \rightarrow \infty$ of the self-diffusion. Only for large times can the mean squared displacement become comparable to the mean level spacing and be associated in the large scale fluctuations of the spectral density. As above, “large” Λ are restricted to intervals in which the classical phase space structure does not appreciably change. In this regime of Λ , the mean squared displacement should be proportional to the parametric number variance (Eq. (7.1))

$$\langle x^2(\Lambda) \rangle \propto \langle (N(\varepsilon_0, \lambda + \Lambda) - N(\varepsilon_0, \lambda))^2 \rangle = V_P(\Lambda) \quad (7.22)$$

with a coefficient of proportionality of the order of unity. In Eq. (7.22), ε_0 is assumed to be in the vicinity of the Brownian particle ε_n whose mean squared displacement (left hand side) is measured. Eq. (7.22) follows from the expansion of the spectral staircase function,

$$\begin{aligned} N(\varepsilon_0, \lambda) &= \frac{1}{N_0} \sum_{(n)} N(\varepsilon_n + \varepsilon_0 - \varepsilon_n, \lambda) \\ &= \frac{1}{N_0} \sum_{(n)} [n + (\varepsilon_0 - \varepsilon_n)N'(\varepsilon_n, \lambda) \cdots] \end{aligned} \quad (7.23)$$

where the sum (n) extends over N_0 energy levels (Brownian particles) in the vicinity of ε_0 and we used $N(\varepsilon_n, \lambda) = n$. The number fluctuation is therefore approximately given by

$$\begin{aligned} &N(\varepsilon_0, \lambda + \Lambda) - N(\varepsilon_0, \lambda) \\ &\approx \frac{1}{N_0} \sum_{(n)} \{ [\varepsilon_n(\lambda) - \varepsilon_n(\lambda + \Lambda)] \tilde{n}(\varepsilon_n, \lambda + \Lambda) \\ &\quad + [\varepsilon_0 - \varepsilon_n(\lambda)] [\tilde{n}(\varepsilon_n, \lambda + \Lambda) - \tilde{n}(\varepsilon_n, \lambda)] \} \end{aligned} \quad (7.24)$$

where $\tilde{n} = N'$ is the density of the unfolded spectrum. If one now approximates the spectral density $\tilde{n}$ in (7.24) by its mean value $\tilde{n}_{av} = 1$ and neglects quadratic cross correlations in $\tilde{n}$ and ε_n one arrives at (7.22). The latter is only justified when the mean squared distance the Brownian particle has travelled is comparable to the mean spacing between the levels, i.e. for large Λ . The semiclassical results of the PNV (Eqs. (7.2, 7.3)) for large values of Λ applies for the mean squared displacement (Eq. (7.22))

$$\langle x^2(\Lambda) \rangle \propto \begin{cases} \Lambda & \text{regular} \\ \ln(\Lambda) & \text{chaotic} \end{cases} \quad (7.25)$$

For the limit of $\Lambda \rightarrow \infty$, the PNV saturates for chaotic systems at a constant value (Eq. (7.5)). Accordingly,

$$\langle x^2(\Lambda) \rangle \propto 2\Sigma(\varepsilon_0) \quad \Lambda \rightarrow \infty. \quad (7.26)$$

For regular systems no such saturation is observed within the range of admissible Λ .

The semiclassical long-“time” limit of the mean squared displacement (Eqs. (7.25) and (7.26)) implies in turn for the spectrum of the VAF near zero frequency

$$G(\omega) \propto \omega^u, \quad \omega \rightarrow 0 \quad (7.27)$$

with $u = 0$ for the classically regular systems and $u = 2$ for the classically chaotic systems.

Using the semiclassical constraints (Eq. (7.27)) of the spectrum of the VAF and the properties of the molecular dynamics (HFE), it is now straightforward to construct approximate friction kernels. For the classically regular case, the molecular dynamics resembles that of a weakly interacting gas (Chapter 5). Interactions between particles proceed through hard binary collisions (i.e. narrow and isolated avoided crossings). Subsequent collisions are uncorrelated. The sequence of collisions forms a Poisson process. An approximate friction kernel is given by

$$K(\Lambda) = \eta \delta(\Lambda) \quad (7.28)$$

with the friction coefficient η

$$\eta = (D\beta)^{-1}. \quad (7.29)$$

From Eqs. (7.19) and (7.20) we find

$$G(\omega) = \frac{\eta}{\omega^2 + \eta^2} \quad (7.30)$$

which conforms with (7.27) in the classically regular region. It should be noticed that the δ peaked decay of memory (Eq. (7.28)) is an idealization which leads to an inaccurate representation of the short-time (large frequency) behavior. One consequence is the divergence of the moments, $\langle \omega^{2k} \rangle$ ($k \geq 1$) of the frequency distribution. An improved friction kernel can be derived using a narrow Gaussian friction kernel. The approximation (Eq. (7.28)) does not, however, affect the long-time limit while providing simple analytic results. The velocity autocorrelation function follows from inversion of (7.12),

$$\psi(\Lambda) = \exp(-\eta\Lambda). \quad (7.31)$$

The exponential decay of the VAF is due to poles on the imaginary frequency axis, $\omega = \pm i\eta$. For the generalized diffusion coefficient we find from Eq. (7.10)

$$D(\Lambda) = D(1 - \exp(-\eta\Lambda)) \quad (7.32)$$

and finally

$$\langle x^2(\Lambda) \rangle = 2D(\Lambda)\Lambda - 2D(\Lambda)/\eta + 2D\Lambda\psi(\Lambda), \quad (7.33)$$

which, in the limit $\Lambda \rightarrow \infty$, reproduces the Einstein relation for Brownian motion (Eq. (7.8)).

For the classically chaotic case we incorporate semiclassical result (7.27) for the spectrum of the VAF into the ansatz

$$G(\omega) = A \frac{\omega^2}{(\omega + \omega_0)^n}, \quad \omega \geq 0 \quad (7.34)$$

with the normalization constant

$$A = \frac{\pi}{4}(n-1)(n-2)(n-3)\omega_0^{n-3} \quad (7.35)$$

determined from the normalization condition $\psi(0) = 1$. The two free parameters in (7.34), ω_0 and n , can be determined from the short-time dynamics, i.e. frequency moments $\langle \omega^{2k} \rangle$ ($k = 1, 2$). Eq. (7.34) allows the analytic

determination of $\psi(\Lambda)$, $\tilde{\psi}(s)$, $D(\Lambda)$ and $\langle x^2(\Lambda) \rangle$, given in the Appendix D. In the long-time limit, $\Lambda \rightarrow \infty$, we find

$$D(\Lambda) \approx \frac{n(n-1)(n-2)(n-3)}{\beta\omega_0^4\Lambda^3} \quad (7.36)$$

and

$$\langle x^2(\Lambda) \rangle \approx \frac{(n-2)(n-3)}{\beta\omega_0^2} \left(1 - \frac{n(n-1)}{(\omega_0\Lambda)^2}\right) \quad (7.37)$$

in agreement with the semiclassical result (Eq. (7.22) and (7.26)). The friction kernel can be determined numerically from the inverse Fourier transformation

$$K(\Lambda) = \frac{2}{\pi} \int_0^\infty d\omega K_F(\omega) \cos(\omega\Lambda) \quad (7.38)$$

with $K_F(\omega)$ given by (7.21).

7.4 Comparison with Molecular Dynamics Simulations

Fig. 7.2 presents the friction kernel for both the regular and the chaotic regimes for the spectra of coupled Morse oscillators. In the classically regular case, the two parameters in the memory kernel description (Eqs. (7.28)-(7.33)), β^{-1} (Eq. (6.2)) and $G(0)$ (Eq. (7.13)), are determined from the MD calculation. In the classically (mostly) chaotic case, in addition to β^{-1} (Eq. (6.2)), the second and fourth moment, $\langle \omega^2 \rangle$ and $\langle \omega^4 \rangle$, which describe the mean-squared force and the mean-squared time-derivative of the force have been used since Eq. (7.13) is no longer well-defined. The friction kernel is approximately δ shaped for the regular motion while it displays a sharp peak at $\Lambda \approx 0$ and a long-time tail $\propto 1/\Lambda^2$ for chaotic motion which is responsible for the dramatic alteration of the long-time behavior of correlation functions.

Fig. 7.3 presents the “time” dependence of the force-correlation function for which a direct comparison with the MD experiment is possible. As expected, in the classically regular case, the force correlation rapidly decays while the classically chaotic case displays a characteristic negative “overshoot” signifying persistent (anti)correlation due to the “cage” effect in a dense interacting medium. The time-dependence of the VAF (Fig. 7.4) resembles the corresponding dependence of the force correlation function. While

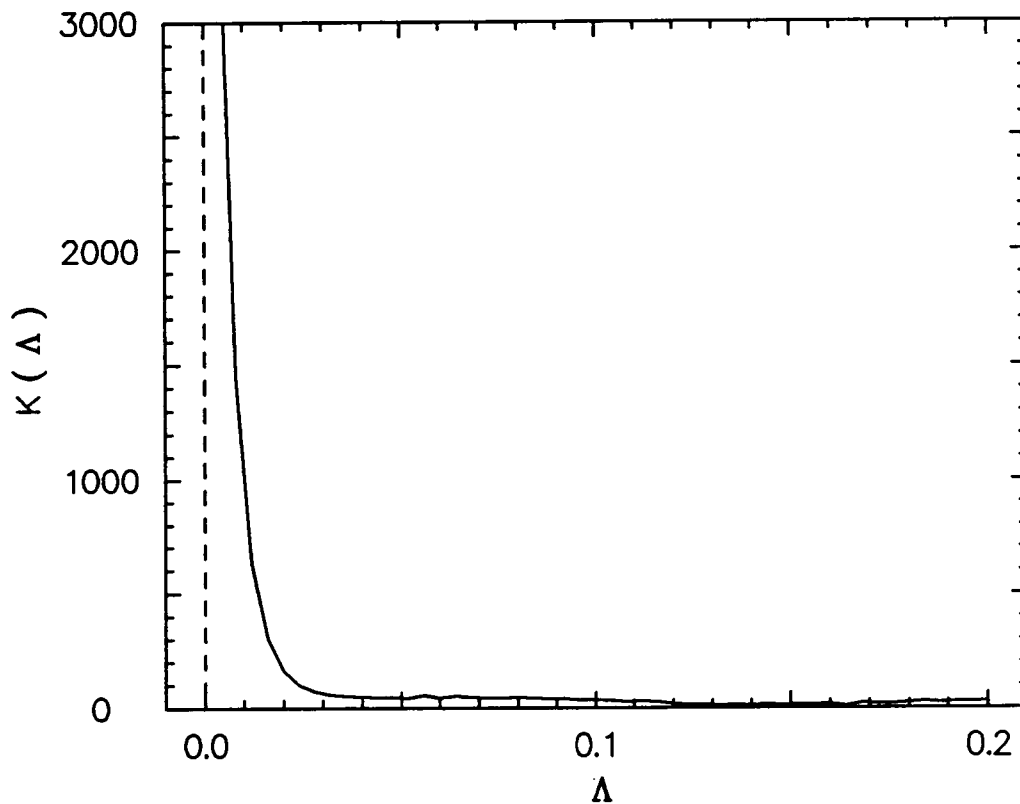


Figure 7.2: The friction kernels $K(\Lambda)$ for the classically regular regime $0.0 < \lambda < 0.3$ (Eq. (7.28), dashed line) and the classically chaotic regime $0.6 < \lambda < 0.9$ (determined from Eqs. (7.21), (7.34), and (7.38), solid line) for the vibronic energy levels for coupled Morse oscillators.

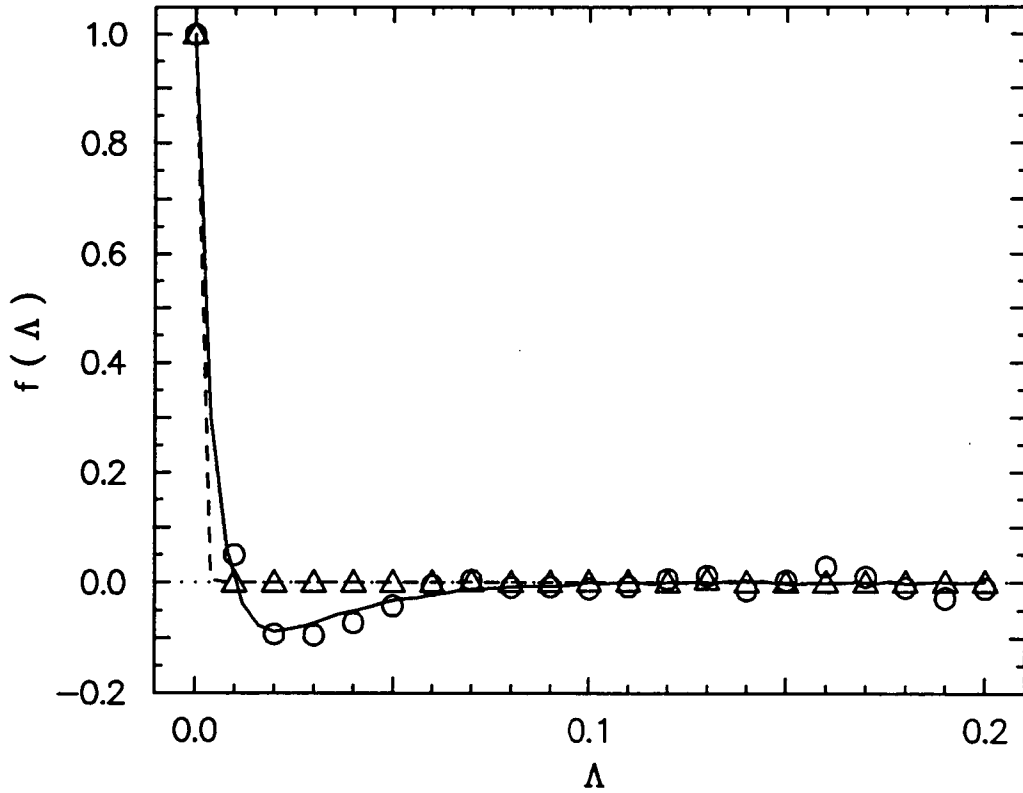


Figure 7.3: The normalized force correlation functions $f(\Lambda)$ ($f(0) = 1$) for the classically regular regime $0.0 < \lambda < 0.3$ (using the approximation Eq. (7.30), dashed line) and the classically chaotic regime $0.6 < \lambda < 0.9$ (using the approximation Eq. (7.34), solid line) compared with the results of MD simulations: $0.0 < \lambda < 0.3$, triangle; $0.6 < \lambda < 0.9$, circle.

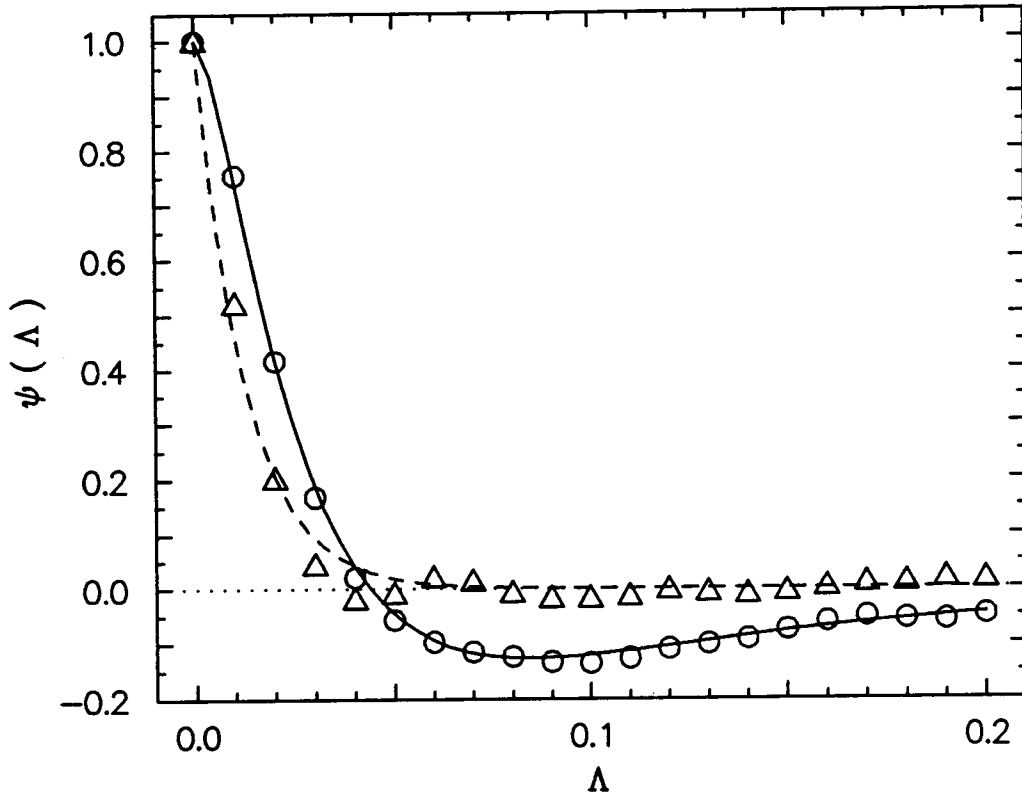


Figure 7.4: The velocity autocorrelation functions $\psi(\Lambda)$ for the classically regular regime $0.0 < \lambda < 0.3$ (using the approximation Eq. (7.30), dashed line) and the classically chaotic regime $0.6 < \lambda < 0.9$ (using the approximation Eq. (7.34), solid line) compared with the results of MD simulations: $0.0 < \lambda < 0.3$, triangle; $0.6 < \lambda < 0.9$, circle.

in the classically regular case velocity correlations decay exponentially they display a non-exponential decay pattern including negative values for the classically chaotic case. It is quite remarkable that our results for the VAF for the molecular dynamics of the pseudo-Newtonian dynamics of energy levels (Eq. (5.1)) closely resemble those of Rahman in his pioneering study of the (three-dimensional) Argon liquid [84] shown in Fig. 7.5. Another similarity of the pair correlation function between our level dynamics and real fluids was already noted in Chapter 3. One is led to the correspondence between dilute gases and classically regular systems on one hand and between liquids and classically chaotic systems on the other hand. The latter correspondence requires, however, a refinement when one investigates the long-time limit of

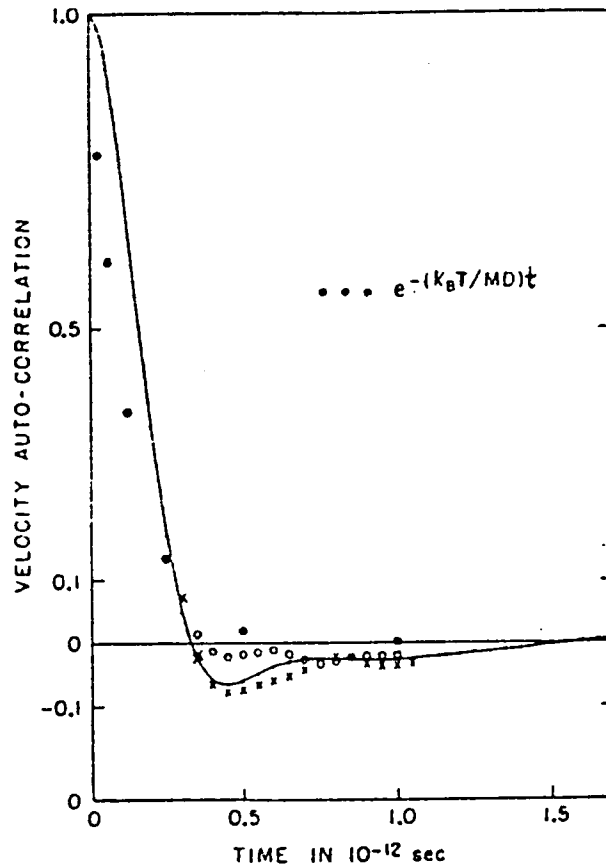


Figure 7.5: The velocity autocorrelation functions of Argon compared with the VAF of a gas (the solid circles). The continuous curve is the mean of a set of 64 curves from the calculation of Rahman. The two members of the set which have maximum departures from the mean are shown as circle and as cross. Reprinted from A. Rahman, Phys. Rev. 136, A405(1964).

diffusive motion, which is not yet apparent in Fig. 7.4. The MD results as well as the predictions of the approximate correlation functions for the generalized diffusion coefficient are presented in Fig. 7.6. While for the regular system the generalized diffusion coefficient approaches a constant value, $D(\Lambda) \rightarrow D$, it decays to zero as $\Lambda \rightarrow \infty$ for the classically chaotic case. A vanishing diffusion coefficient appears to be a signature of parametric level dynamics in classically chaotic systems. Therefore, the identification with the dynamic state of a liquid is incomplete. While the short time dynamics of $\psi(\Lambda)$ closely resembles a liquid, the long-time limit $D(\Lambda) \rightarrow 0$ corresponds to that of a glass [82]. Fig. 7.7, finally, presents the results for the mean squared displacement, $\langle x^2 \rangle$, of the energy levels. Energy levels in the classically regular

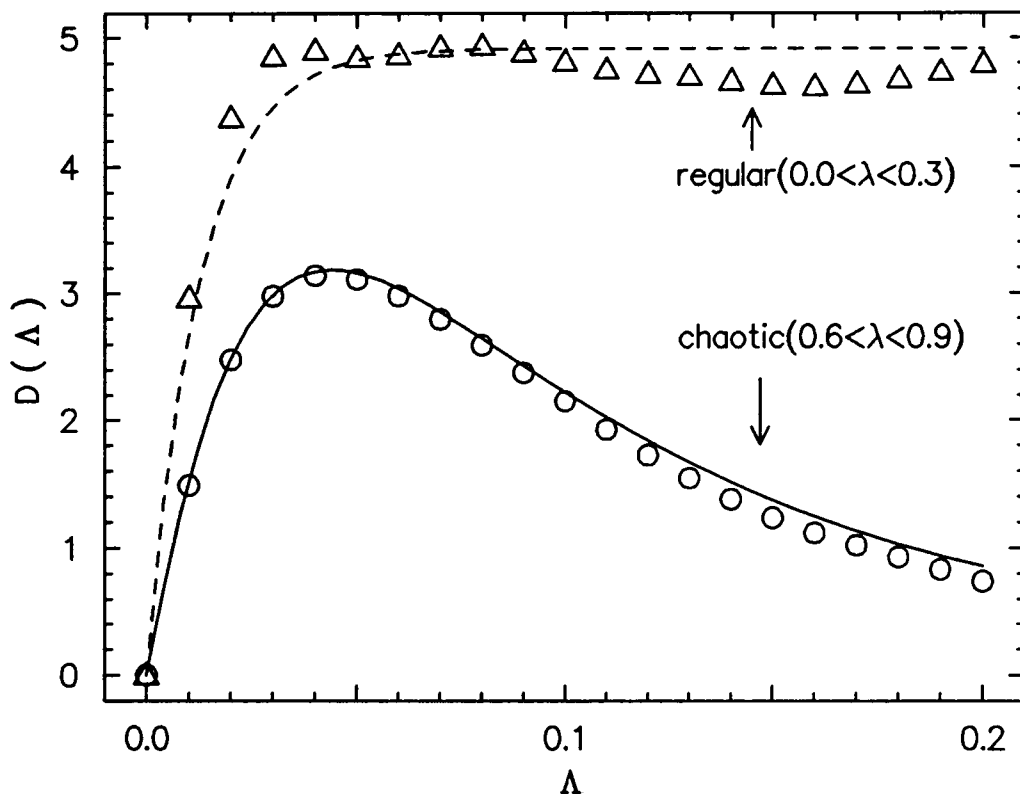


Figure 7.6: The generalized diffusion coefficients $D(\Lambda)$ for the classically regular regime $0.0 < \lambda < 0.3$ (using the approximation Eq. (7.30), dashed line) and the classically chaotic regime $0.6 < \lambda < 0.9$ (using the approximation Eq. (7.34), solid line) compared with the results of MD simulations: $0.0 < \lambda < 0.3$, triangle; $0.6 < \lambda < 0.9$, circle.

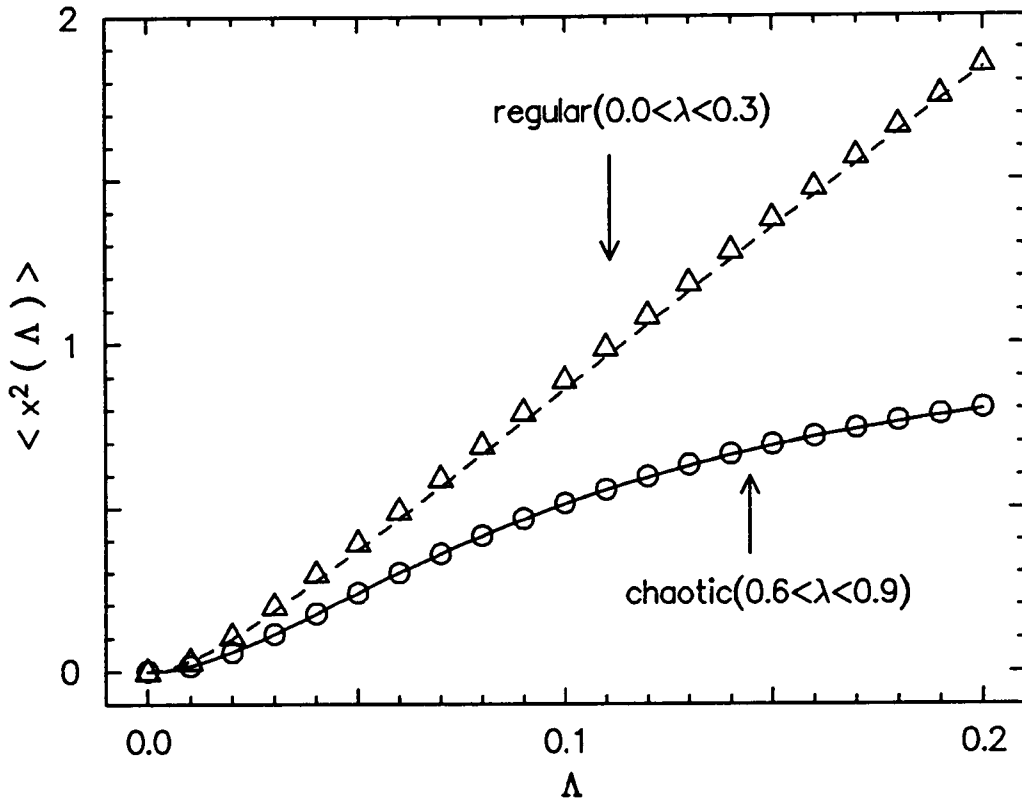


Figure 7.7: The mean-squared displacements $\langle x^2(\Lambda) \rangle$ for the classically regular regime $0.0 < \lambda < 0.3$ (using the approximation Eq. (7.30), dashed line) and the classically chaotic regime $0.6 < \lambda < 0.9$ (using the approximation Eq. (7.34), solid line) compared with the results of MD simulations: $0.0 < \lambda < 0.3$, triangle; $0.6 < \lambda < 0.9$, circle.

regime perform a Langevin diffusion satisfying an approximate Einstein relation (Eq. (7.8)). Energy levels in the classically chaotic regime show an approximately logarithmic growth of the mean squared displacement which for large Λ will ultimately saturate. Diffusive motion is suppressed due to the strong coupling of each level with many of its neighbors (i.e. due to the multitude of overlapping avoided crossings). Notice that near $\Lambda \approx 0$ no difference in $\langle x^2(\Lambda) \rangle$ between classically mostly regular and mostly chaotic regimes exists, since levels move as free particles during such short “times”, hence the behavior of $\langle x^2(\Lambda) \rangle \propto \Lambda^2$ is “ballistic”. This is a pure quantum effect and the semiclassical limit is not yet reached. It is worth noting that all MD simulations for the complete set of correlation functions and transport coeffi-

cients (Figs. 7.3-7.7) are well reproduced by single analytic approximation to the memory kernel chosen in accordance with the semiclassical limit of the parametric number variance (Eqs. (7.25) and (7.26)) and with a single set of parameters determined by the lowest frequency moments. This is particularly remarkable in view of the fact that due to the coupling of the fluctuating charges, $V_{ni}(\Lambda)$, to the parametric motion (Eq. (5.1)), the dynamics is, unlike liquids, non-Newtonian.

7.5 Some Remarks

We have found characteristic differences for the parametric motion of energy levels of a simple quantum system whose classical counterpart is chaotic. In the classically regular domain the energy levels undergo a Langevin-type diffusion resembling a gas while in the classically chaotic regime diffusion of energy levels is suppressed, characterized by a vanishing diffusion constant ($D \approx 0$) resembling a glass. In the classically regular regime the velocity autocorrelation function (VAF) displays a near-exponential decay typical for a gas. In the classically chaotic regime the VAF decays non-exponentially with a rebound characteristic for liquids. These results are consistent with the properties of the parametric number variance (PNV) for semiclassical energy level statistics. Simple approximations for the friction kernel provide a satisfactory description of the molecular dynamics data for the velocity autocorrelation functions and the generalized diffusion coefficients.

While sharp differences in the long-time behavior of transport coefficients are clearly established, an accurate quantitative determination of the leading term of the long-time behavior is complicated since the characteristic range of the control parameter λ is limited by the constraint that the classical phase space structure should be invariant. Consequently, it is difficult to accurately determine the decay law of the velocity autocorrelation function, $\psi(\Lambda) \propto \Lambda^{-\gamma}$. Furthermore, the presence of a small regular component in phase space may also alter the transport coefficients.

We like to point a possible direct observation of the diffusive motion of energy levels. It would require (a) the excitation of a group of excited states within a narrow band of energies $(x_n, \dots, x_{n+a})$, for example by a short laser pulse, and (b) the adiabatic change of the control parameter λ as a function of real time t . By mapping the pseudo-time λ of the parametric energy level motion onto the real time t adiabatically such that the wavepacket can

follow the changes of the energy levels, parameter-dependent diffusion could be measured. According to Eqs. (7.33) and (7.37) we expect a rapid spread of the energy of the wavepacket over a wide range of energies for the classically regular regime and a slower non-diffusive growth for the width of the band of energy levels in the classically chaotic domain. Such a scenario could be realized for laser or collisionly excited atoms in strong time or parameter-dependent external fields.

Chapter 8

Parametric dynamics of quantum spectrum with continuum

Strictly speaking, the HFE (5.1) are valid for bound systems only. The effects of continuum on the parametric motion of quantum levels are not a priori obvious. In this chapter, we therefore generalize the HFE to include a structureless continuum and show that the resulting parametric dynamical system is still regular. Furthermore, the parametric motion for resonances are also investigated for the first time. We demonstrate that, because resonances live in a two-dimensional manifold (i.e. position and width), the existence of the repulsion between resonances is independent of the underlying classical dynamics. Therefore, parametric correlations may play a crucial role in the identification of classical chaos.

8.1 The effects of continuum on parametric dynamics

We generalize now the HFE equations to the case of a Hamiltonian with both bound states and the continuum present [85]. We consider an autonomous system described by the Hamiltonian of Eq. (2.25) with a structureless continuum. An example for such systems is the anisotropic Kepler problem

[86]

$$H = \frac{p^2}{2} + \lambda \frac{p_z^2}{2} - \frac{1}{r}. \quad (8.1)$$

This system is totally chaotic when the energy is negative but is regular for positive energies. The case of resonances is discussed in next section. A manifold with given exact symmetry is considered so that the spectrum is nondegenerate. The bound ($|n\rangle$) and continuum ($|E\rangle$) eigenvectors form a complete orthogonal basis

$$\sum_n |n\rangle\langle n| + \int dE |E\rangle\langle E| = 1. \quad (8.2)$$

They are normalized as follows

$$\begin{aligned} \langle n|m \rangle &= \delta_{n,m} \\ \langle E|E' \rangle &= \delta(E - E') \\ \langle n|E \rangle &= 0 \end{aligned} \quad (8.3)$$

Note that the discrete eigenenergies E_n are the solutions of Schrödinger equation (Eq. (1.6)) thus are λ dependent, while the continuous eigenenergies are λ independent, i.e.

$$\frac{d}{d\lambda} E = 0 \quad (8.4)$$

Keeping this in mind and forming expectation values and differentiation with respect to λ in Eq. (1.6), we get the parametric dynamical equations for the eigenvectors

$$\frac{d}{d\lambda} |n\rangle = \sum_{m \neq n} \frac{V_{mn}}{E_n - E_m} |m\rangle + \int dE' \frac{V_{E'n}}{E_n - E'} |E'\rangle \quad (8.5)$$

$$\frac{d}{d\lambda} |E\rangle = \sum_m \frac{V_{mE}}{E - E_m} |m\rangle + \int dE' P \frac{V_{E'E}}{E - E'} |E'\rangle \quad (8.6)$$

where P denotes the principle part of the integration, $V_{\Psi\Psi'} = \langle \Psi|V|\Psi' \rangle$, and $|\Psi(\Psi')\rangle$ can be either $|n\rangle$ or $|E\rangle$. Note that the formal solution of the equation

$$Eb_{E'} = V_{E'E} + E'b_{E'} \quad (8.7)$$

where $E-E'$ may be zero is given by [87]

$$b_{E'} = P \frac{V_{E'E}}{E - E'} + Z(E)\delta(E - E'). \quad (8.8)$$

Here $Z(E)$ remains to be determined. We choose the phases of eigenvectors such that [46]

$$\langle \Psi | \frac{d}{d\lambda} | \Psi \rangle = 0. \quad (8.9)$$

The parametric dynamical equations for the eigenenergies are consequently given by

$$\begin{aligned} \frac{d}{d\lambda} E_n &= V_{nn} = p_n \\ \frac{d}{d\lambda} p_n &= 2 \left(\sum_{m \neq n} \frac{|V_{nm}|^2}{E_n - E_m} + \int dE' \frac{|V_{nE'}|^2}{E_n - E'} \right) \\ \frac{d}{d\lambda} V_{mn} &= -V_{mn} \frac{p_m - p_n}{E_m - E_n} + \sum_{k \neq m, n} V_{mk} V_{kn} \left(\frac{1}{E_m - E_k} + \frac{1}{E_n - E_k} \right) + \\ &\quad + \int dE' V_{mE'} V_{E'n} \left(\frac{1}{E_m - E'} + \frac{1}{E_n - E'} \right) \\ \frac{d}{d\lambda} V_{En} &= V_{En} \frac{p_n}{E - E_n} + \sum_{m \neq n} V_{Em} V_{mn} \left(\frac{1}{E - E_m} + \frac{1}{E_n - E_m} \right) + \\ &\quad + \int dE' V_{EE'} V_{E'n} \left(P \frac{1}{E - E'} + \frac{1}{E_n - E'} \right) \\ \frac{d}{d\lambda} V_{EE'} &= \sum_m V_{Em} V_{mE'} \left(\frac{1}{E - E_m} + \frac{1}{E' - E_m} \right) + \\ &\quad + \int dE'' V_{EE''} V_{E''E'} \left(P \frac{1}{E - E''} + P \frac{1}{E' - E''} \right) \end{aligned} \quad (8.10)$$

The parametric motions of eigenenergies and eigenvectors are completely described by Eqs. (8.5), (8.6) and (8.10) which contain obviously Pechukas' results as a special case with $V_{nE} = 0$ and $V_{EE'} = 0$.

We show now that these equations, though looking complicated and highly nonlinear, are completely regular. The regularity is not surprising since the output of the equation is connected with its initial input by a unitary transformation. We rewrite Eqs. (8.5) and (8.6) as follows

$$i \frac{d}{d\lambda} | \Psi \rangle = G | \Psi \rangle \quad (8.11)$$

with

$$\begin{aligned}
G = i[& \sum_{m,n(m \neq n)} \frac{|m\rangle\langle m|V|n\rangle\langle n|}{E_n - E_m} + \\
& + \sum_m \int dE' \left(\frac{|E'\rangle\langle E'|V|m\rangle\langle m|}{E_m - E'} + \frac{|m\rangle\langle m|V|E'\rangle\langle E'|}{E' - E_m} \right) + \\
& + \int dE' \int dE'' P \frac{|E'\rangle\langle E'|V|E''\rangle\langle E''|}{E'' - E'}]
\end{aligned} \quad (8.12)$$

where Eq. (8.3) has been used. G has two important properties: it is defined for all states and it is a Hermitian operator

$$G = G^\dagger. \quad (8.13)$$

For small change of λ , G is approximately independent of λ , and the solution of Eq. (8.11) is given by

$$\begin{aligned}
|\Psi\rangle(\lambda + \Delta\lambda) & \approx |\Psi\rangle(\lambda) - i\Delta\lambda G|\Psi\rangle(\lambda) \\
& \approx e^{-i\Delta\lambda G}|\Psi\rangle(\lambda).
\end{aligned} \quad (8.14)$$

Therefore, Eq. (8.11) is analogous to the time-dependent Schrödinger equation. For large changes of λ , $G(\lambda)$ cannot be treated as λ -independent and it is itself the solution of the equations.

G is the generator of the unitary transformation underlying Eq. (8.11) which contains all the information of Eqs. (8.5), (8.6) and (8.10). We change now our "Schrödinger representation" of parametric dynamics which is convenient for the systems with continuum spectrum to the form of the "Heisenberg representation". For any operator W , we have

$$\begin{aligned}
\frac{d}{d\lambda} \langle \Psi | W | \Psi' \rangle & = \frac{d \langle \Psi |}{d\lambda} W | \Psi' \rangle + \langle \Psi | W \frac{d | \Psi' \rangle}{d\lambda} + \langle \Psi | \frac{dW}{d\lambda} | \Psi' \rangle \\
& = \frac{1}{i} \langle \Psi | [W, G] | \Psi' \rangle + \langle \Psi | \frac{dW}{d\lambda} | \Psi' \rangle.
\end{aligned} \quad (8.15)$$

If we define a generalized matrix $\mathcal{W} = (W_{\Psi\Psi'})$ with the rule for matrix multiplication

$$(\mathcal{W}\mathcal{U})_{\Psi\Psi'} = \sum_n \mathcal{W}_{\Psi n} \mathcal{U}_{n\Psi'} + \int dE \mathcal{W}_{\Psi E} \mathcal{U}_{E\Psi'}, \quad (8.16)$$

then Eq. (8.15) can be written as

$$\frac{d}{d\lambda}\mathcal{W} = \frac{1}{i}[\mathcal{W}, \mathcal{G}] + \frac{\partial\mathcal{W}}{\partial\lambda}, \quad (8.17)$$

which is the “Heisenberg representation” of the transformation. Let $\mathcal{W}$ be $\mathcal{H}$, $\mathcal{V}$ and $\mathcal{F} = [\mathcal{H}, \mathcal{V}]$ respectively, we have

$$\frac{d}{d\lambda}\mathcal{H} = \frac{1}{i}[\mathcal{H}, \mathcal{G}] + \mathcal{V}, \quad (8.18)$$

$$\frac{d}{d\lambda}\mathcal{V} = \frac{1}{i}[\mathcal{V}, \mathcal{G}], \quad (8.19)$$

$$\frac{d}{d\lambda}\mathcal{F} = \frac{1}{i}[\mathcal{F}, \mathcal{G}]. \quad (8.20)$$

These equations are exactly in the same forms of the corresponding equations for the case of totally bound systems [88]. From Eqs. (8.18-8.20) we can derive our original set of equations (8.4) and (8.10).

By using Eq. (8.14) repeatedly, Eq. (8.11) can be solved in a completely algebraic way:

$$|\Psi > (\lambda) = U(\lambda)|\Psi > (0), \quad (8.21)$$

where $U(\lambda)$ is a unitary operator defined in terms of the time(λ)-ordering operator T_λ , i.e.

$$U(\lambda) = T_\lambda \exp[-i \int_0^\lambda d\lambda' G(\lambda')] \quad (8.22)$$

which excludes any exponential separations among initially close solutions. This regularity is another manifestation of the absence of chaos in quantum mechanics in the sense of non-vanishing Lyapunov exponents.

8.2 The parametric dynamics of resonances and measures of quantum chaos

In the real world, excited states of physical systems have a finite lifetime. An unstable state decays, for example, into open channels due to coupling to vacuum fluctuations. Therefore, in addition to the ordinary time evolution factor $\exp(-\frac{iEt}{\hbar})$, there is another factor to describe the decay of the states,

$\exp(-\frac{t}{2t_0})$, where t_0 is the lifetime of the state. Combining these two factors, the eigenenergy becomes complex, i.e.

$$E = E_R + iE_I \quad (8.23)$$

where E_R is the ordinary energy, and $E_I = -\hbar/(2t_0) \leq 0$. A state with non-zero E_I is called a resonance. Up to this point, the parametric dynamical equations Eq. (5.1) are applicable to discrete stationary levels only. The parametric dynamics for the resonances has not been investigated in detail. On the physical grounds, one would expect that the level repulsion at small distances ($\Delta E_R \leq |E_I|$, where ΔE_R is the spacing of the real energy of resonances) should be modified. In this section, the complex level dynamics for resonances will be analyzed.

Since

$$\begin{aligned} \langle \psi_1 | p \psi_2 \rangle &= \int dq \psi_1^* p \psi_2 \\ &= \int dq (p \psi_1)^* \psi_2 + \psi_1^*(q) \psi_2(q) / i |_{q \rightarrow \infty} = \langle p \psi_1 | \psi_2 \rangle + \psi_1^*(q) \psi_2(q) / i |_{q \rightarrow \infty} \end{aligned} \quad (8.24)$$

where we have used $p = \frac{d}{i dq}$ in the coordinate representation, the ordinary Hamiltonian (more precisely, the momentum operator) is Hermitian within a square-integrable Hilbert subspace where the wavefunction vanishes sufficiently fast when a coordinate approaches infinity so that the surface term of the right hand side of Eq. (8.24) vanishes. In order to get complex eigenvalues like Eq. (8.23), we need to expand the Hilbert space to include non-square-integrable basis functions which give the boundary condition for the resonances (Siegert boundary condition) [89]

$$\Psi(q) \sim \exp(ikq) \quad q \rightarrow \infty \quad (8.25)$$

where $k \propto \sqrt{E}$. Under this outgoing-wave boundary condition, the surface term of the right hand side of Eq. (8.24) is not zero, hence the Hamiltonian is not Hermitian any longer, and eigenvalues can be complex. In this standard approach, bound states and resonance states are associated with different boundary conditions. In order to derive the parametric dynamical equations for resonances, one needs to treat both bound and resonance states on the same footing. Complex rotation theory [90] provides a method for this purpose. The coordinates q are "rotated" into the complex plane by an angle θ , $0 < \theta < \pi/2$:

$$q \rightarrow q e^{i\theta} \quad (8.26)$$

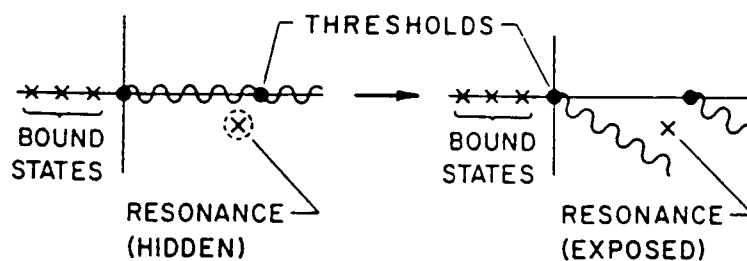


Figure 8.1: Effects of a complex rotation transformation on the spectrum. Bound states are invariant to the transformation while the continua rotate about their respective thresholds, exposing complex resonances eigenvalues in appropriate strips of the complex plan. Reprinted from C. Cerjan et al., *Int. J. Quantum Chem.* 14, 393(1978).

The original Hamiltonian is transformed into a non-Hermitian operator $H(\theta)$ by replacing q with $qe^{i\theta}$, i.e.

$$H(\theta) = -e^{-2i\theta} \frac{\nabla^2}{2} + V(qe^{i\theta}). \quad (8.27)$$

For a group of potentials ("complex rotation analytic") $V(q)$, the spectrum of the rotated Hamiltonian $H(\theta)$ contains the following elements (Aquilar-Balslev-Combes (ABC) theorem) [91].

(1). The real discrete eigenvalues of $H(\theta)$ are identical to the bound states of the original Hamiltonian H .

(2). The complex discrete eigenvalues of $H(\theta)$ correspond to the resonances of H .

(3). The scattering thresholds are invariant under this transformation.

(4). The continua of the original H are rotated around the corresponding thresholds by an angle of -2θ into the lower complex plane.

The idea is illustrated in Fig.8.1. Upon the rotation of the coordinates q , the resonance boundary condition (Eq.(8.25)) is transformed into

$$\Psi(q) \sim \exp[i(k_R \cos\theta + k_I \sin\theta)q + (k_I \cos\theta - k_R \sin\theta)q] \quad q \rightarrow \infty \quad (8.28)$$

where we have used the second part of the ABC theorem that the complex energy E (or equally k) of a resonance is unchanged under the rotation. For $\theta > \arctan(k_I/k_R)$, Eq.(8.28) becomes the boundary condition for a

bound state and the resonance is “exposed”. Therefore, $H(\theta)$ exhibits square-integrable eigenfunctions with complex eigenvalues.

Thus, the complex rotation on the Hamiltonian provides an approach to obtain the eigenvalues for both bound and resonance states via the same calculation using only square-integrable basis functions. Choosing the square-integrable basis functions to be real, Blümel and Reinhardt [92] obtained a closed set of first order differential equations for the motion of the bound and resonance eigenvalues $E_n = x_n$ of the Hamiltonian Eq. (2.25) in the complex plane

$$\begin{aligned}\frac{d}{d\lambda}x_n &= V_{nn} = p_n \\ \frac{d}{d\lambda}p_n &= 2 \sum_{i \neq n} \frac{V_{in}^2}{x_n - x_i} \\ \frac{d}{d\lambda}V_{in} &= \sum_{j \neq i, n} V_{ij}V_{jn} \left(\frac{1}{x_i - x_j} + \frac{1}{x_n - x_j} \right) - \frac{V_{in}(p_i - p_n)}{x_i - x_n}\end{aligned}\tag{8.29}$$

where $V_{in} (= |i\rangle^T V |n\rangle = V_{ni})$ is complex symmetric, and the left eigenvectors $|i\rangle^T$ are the transposed values of right eigenvectors $|i\rangle$. Eq. (8.29) has the same form as Eq. (5.1) except for the fact that the domain is complex. As for the HFE, the beauty of Eq. (8.29) is its generality. It describes the dynamics of resonances for all Hamiltonians of the form Eq. (2.25). The characteristics of a particular Hamiltonian enter only in the initial conditions.

We study now the evolution of the parametric motion in complex plane. One of the important findings is the existence of repulsion between resonances in the complex energy plane, i.e. two resonances avoid each other in their parametric motion. This situation can be analyzed with the help of a two-state approximation, since the coupling of these two states with other resonances can be neglected when two resonances (denoted by 1 and 2) become very close in the complex energy plane ($|\Delta E| = |E_2 - E_1| \rightarrow 0$). The behavior of these two resonances is described by an effective Hamiltonian

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix}.\tag{8.30}$$

Note that the effective Hamiltonian is complex symmetric after complex rotation. Solving the eigenproblem of (8.30) gives

$$\Delta E = x + iy\tag{8.31}$$

where x and y are the solutions of following equations

$$x^2 - y^2 = (H_{11}^R - H_{22}^R)^2 - (H_{11}^I - H_{22}^I)^2 + 4(H_{12}^R - H_{12}^I)(H_{12}^R + H_{12}^I), \quad (8.32)$$

$$xy = (H_{11}^R - H_{22}^R)(H_{11}^I - H_{22}^I) + 4H_{12}^R H_{12}^I. \quad (8.33)$$

Therefore, in general one needs to adjust two control parameters to get $\Delta E = 0$ ($x = y = 0$). This conclusion was obtained by von Brentano [93] using a different approach. We show now the impact of this result on the statistics of resonances. When we vary the perturbation λ , the curve $(x(\lambda), y(\lambda))$ in general does not cross the origin ($x = y = 0$), and two resonances avoid each other even though one of the two components of the force may become attractive. If the curve cross y (or x) axis the real (or imaginary) parts of two complex energy cross each other while the imaginary (or real) parts avoid each other. Following the similar argument of Berry [68] for the NNS distribution of bound system, the resonance spacing distribution in the limit of small $|\Delta E|$ can be expressed by

$$P(|\Delta E|) = \int dx dy W(x, y) \delta(|\Delta E| - \sqrt{x^2 + y^2}) \quad (8.34)$$

where $W(x, y)$ is the distribution function of x and y . By simply rescaling the integration variables in Eq. (8.34), one obtains

$$P(|\Delta E|) = |\Delta E| \int dx dy W(|\Delta E|x, |\Delta E|y) \delta(1 - \sqrt{x^2 + y^2}) \quad |\Delta E| \rightarrow 0. \quad (8.35)$$

The statement of genericity of Hamiltonian H requires $W(x, y)$ to be a smooth function without singularities. Because W in (8.35) depends on $|\Delta E|$ (~ 0) very weakly, we find the interesting result

$$P(|\Delta E|)_{|\Delta E| \rightarrow 0} \propto |\Delta E|. \quad (8.36)$$

It is important to notice that Eq. (8.36) is valid for both integrable and chaotic systems, because the integrable systems are the limiting cases of $H_{12} = 0$, while $H_{12} = 0$ does not lead to x (or y) identical to zero. Therefore, Eq. (8.31) and Eq. (8.36) are still valid. This means that the existence of resonance repulsion is independent of the underlying classical dynamics. We show now, by using a result obtained by Hertz about 100 years ago, that this “repulsion” for integrable systems is due to the fact that the resonance energy “live” on a two-dimensional manifold. The fact that $H_{12} \rightarrow 0$ implies that

the parametric motion of the resonance energies for the integrable systems resembles the motion of two-dimensional ideal gas. Hertz [94] showed that the nearest-neighbor spacing distribution for an ideal gas in an N -dimensional coordinate space is given by

$$P_N(r) = n_{av} \frac{dv_N(r)}{dr} \exp[-n_{av}v_N(r)] \quad (8.37)$$

where n_{av} is the coarse-grained number density and $v_N(r)$ is the volume of a N -dimensional sphere of diameter r . It is well-known that

$$v_N(r) = \frac{\pi^{N/2}}{\Gamma(N/2 + 1)} \left(\frac{r}{2}\right)^N. \quad (8.38)$$

Some examples are $v_1(r) = r$, $v_2(r) = r^2\pi/4$, $v_3(r) = r^3\pi/6$. It is now remarkable that after “unfolding” the spacing

$$s = n_{av}^{1/N} r, \quad (8.39)$$

Eqs. (8.37) and (8.38) lead to the Brody distribution (Eq. (3.22)) with Brody parameter $\kappa = N - 1$. Hence, in one dimension $P_{N=1}(s) = \exp(-s)$ is the Poisson distribution (Eq. (3.12)) which shows particle clustering while in two dimension $P_{N=2}(s) = \pi/2 s \exp(-\pi s^2/4)$ gives a Wigner distribution (Eq. (3.17)) which shows particle repulsion. Therefore, we conclude that repulsion between resonances can be simply a consequence of the dimensionality of the problem. We call such repulsion “geometric repulsion”. In particular, geometric repulsion can produce the same effects as dynamical repulsion. We conclude that, in the limit of small spacing, the dynamical repulsion ($H_{12} \neq 0$) is “buried” by the geometric repulsion. Therefore the NNS distribution is not sensitive to the underlying dynamics for resonances, unlike for bound states. For isolated resonances, the NNS distribution becomes more sensitive to the underlying dynamics since Eq. (8.36) is valid only in the range of $|\Delta E| \ll |E_I|$.

For the case of overlapping resonances ($|\Delta E| \sim |E_I|$), we need to find other measures to diagnose the properties of classical dynamics. Here the parametric correlations may play crucial roles to distinguish classical regular and chaotic motion. The condition that the system “forgets” its initial conditions after an interval of λ and reaches a thermal equilibrium state is the existence of strong and complicated couplings between resonances. This is a purely dynamical condition. Therefore, a well-defined temperature and a Maxwell-Boltzmann distribution for the single particle’s momentum of the system (Eq. (8.29)) is conjectured as the manifestation of classical chaos.

8.3 Example: the parametric motion of resonances for hydrogen atom in a strong electric field

Besides insights into the dynamics of the resonances, Eq. (8.29) also provides a numerical method to the problem. In general, numerical solutions for large numbers of resonances are much more complicated than the similar problem of bound states. This is not only due to the complex domain which needs more computing time and space, but is also due to the delicate coupling to the continuum which is essential for resonances. Compared with other methods, the major advantage of parametric dynamics approach lies in the fact that a single solution provides “en route” the resonances for all parameters in the integration interval. Therefore, each resonance can be easily identified in contrast to other methods when the density of resonances is high and resonances begin to overlap. Using this equation, we determine the parametric motion of resonances for a hydrogen atom in a strong electric field. While the system of a hydrogen atom in a magnetic field plays the role of paradigm for the study of quantum chaos, hydrogen in an electric field is a prototype of a classically integrable atomic system and has attracted considerable attention [95]. However, many interesting questions remain to be answered [96]. The purpose of the investigation is two-fold. One is to test the numerical applicability of Eq. (8.29), and the other is to gain more physical understanding of this prototype quantum system, especially in terms of classical mechanics.

For the sake of simplicity, we consider the system in one dimension, i.e. the Hamiltonian of the system is given by (in atomic units)

$$H = \frac{p^2}{2} - \frac{1}{z} - \lambda z \quad z \geq 0 \quad (8.40)$$

where λ is the strength of the electric field. The reason for this approximation is that, in a strong electric field, the radial part of an excited state of hydrogen atom approaches the limit of a one-dimensional state closely resembles the Schrödinger equation of the one-dimensional model [97]. Therefore, the one-dimensional model Eq. (8.40) should catch the essence of the three-dimensional physics. The EBK quantization (Eq. (4.15)) gives

$$\frac{1}{\pi} \int_0^a \sqrt{2(E + \frac{1}{z} + \lambda z)} dz = n + 1/2 \quad (8.41)$$

with the turning point at $a = \frac{1}{2\lambda}(|E| - \sqrt{E^2 - 4\lambda})$. If we scale

$$\tilde{E}_n = E_n n^2, \quad \tilde{\lambda} = \lambda n^4 \quad (8.42)$$

then $\tilde{E}_n$ depends on n through the variable $(1 + \frac{1}{2n})$. i.e. the EBK quantization implies that $\tilde{E}_n$ is independent of n for highly excited states. We use these scaled quantities to plot our results of full quantum calculations.

Fig. 8.2 displays the scaled complex energy of excited states ($n = 7-11$) as a function of the scaled electric field together with the value of the potential barrier. One striking feature is that the semiclassical scaling law is well satisfied in the domain of strong electric fields indicating the validity of the EBK quantization. Another striking feature is that while the real part of energy passes the barrier continuously, the width (imaginary part of the energy) behaves very differently. When the energy lies below the barrier, the width is negligible as expected from the tunnelling. In this regime, the state can be treated as a bound state and perturbation theory is valid. When the state lies above the barrier, the width becomes significantly large and grows with an algebraic law of λ^γ , where γ is close to but slightly smaller than 1. In this regime, perturbation theory breaks down and the state is short lived. The dramatic change of the behavior of resonances around the barrier is an example of a quantum system following the corresponding classical dynamics. The classical trajectory is totally bounded when energy is below the potential barrier while it becomes totally unbounded when energy is above the barrier. The approximately linear dependence on the electric field of the width above the barrier is also observed [98] in the problem of three-dimensional hydrogen atom in an electric field. This behavior can be qualitatively understood by a classical argument. The time for the electron travelling from the origin ($z_0 = 0$) to the saddle point ($z_s = 1/\sqrt{\lambda}$) is determined by

$$\Delta t = \int_0^{1/\sqrt{\lambda}} \frac{dz}{\sqrt{2(E + 1/z + \lambda z)}} \propto (1/\lambda)^{3/4} \quad \lambda \rightarrow \infty. \quad (8.43)$$

By the uncertainty principle for energy and time, the width (imaginary part) of the energy should be proportional to $1/\Delta t$. Therefore, classical theory predicts $\gamma = 3/4$ which is close to 1.

Fig. 8.3 shows the trajectories of resonances of excited states ($n = 7-11$) in the complex energy plane. The resonances move essentially on a one-dimensional manifold embedded in the two-dimensional complex plane. Therefore, the system is far from generic and the unfolding procedure of the

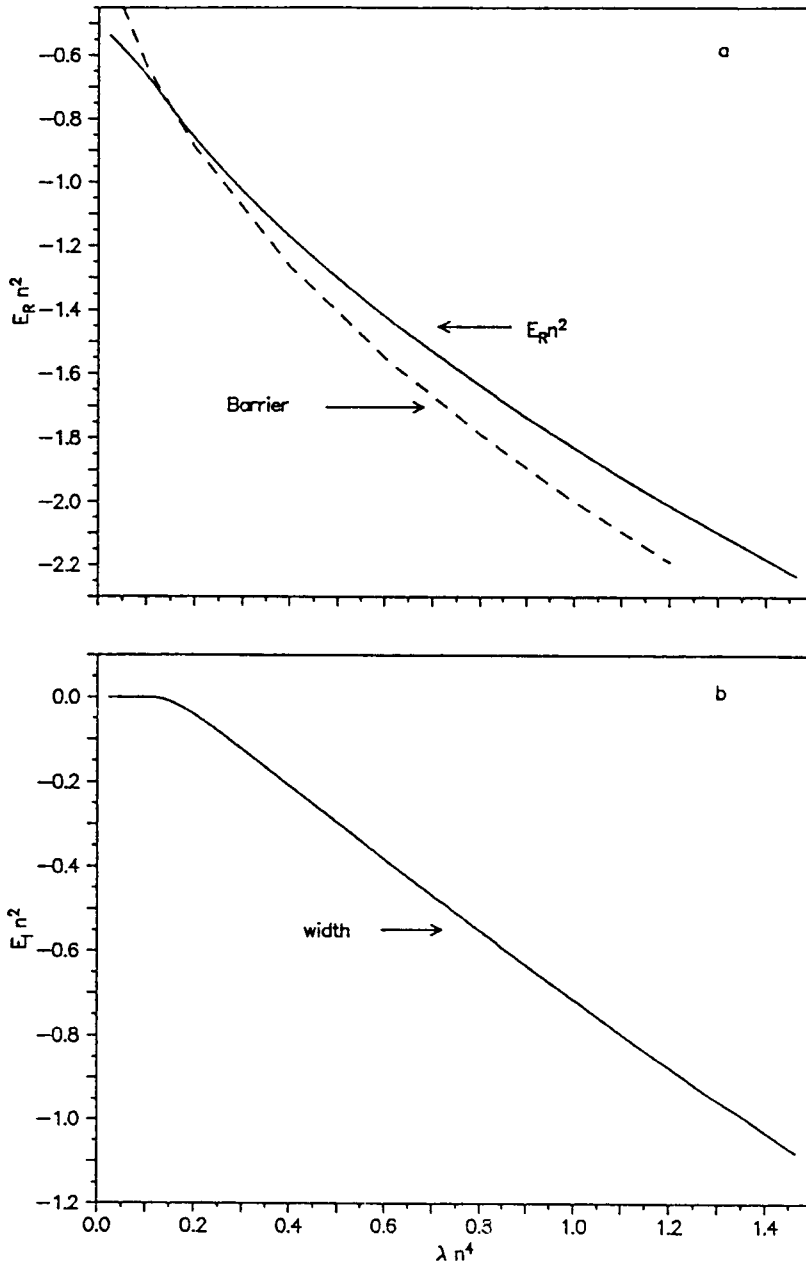


Figure 8.2: Complex energy of excited states ($n = 7 - 11$) as a function of the electric field where the dashed line represents the value of the barrier.

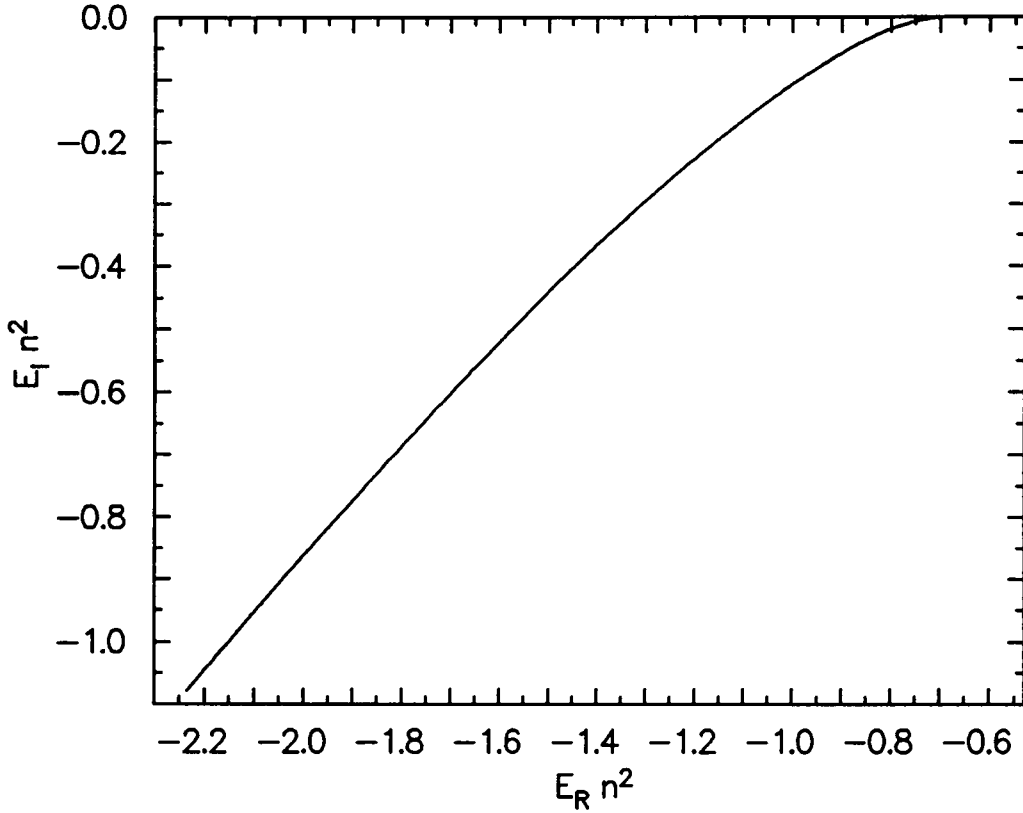


Figure 8.3: The trajectories of resonances of excited states ($n = 7 - 11$) in the complex energy plane.

eigenvalues should follow Eq.(3.2) instead of Eq.(8.39). For a given value of λ , E_n is a function of the quantum number n . In the vicinity of n_0 , the semiclassical limit is given by $(n - n_0)/n_0 \rightarrow 0$ (see equivalent condition Eq.(3.1)). Hence $E_n \approx E_{n_0} + (n - n_0)dE_{n_0}/dn$ and the NNS distribution is

$$P(s) = \delta(s - 1) \quad (8.44)$$

as predicted for one-dimensional systems in Appendix B.

Fig.8.4 displays the scaled momentum of resonances of excited states ($n = 7 - 11$). As the energy itself, the momentum obeys the semiclassical scaling law and displays changes around the barrier. Notice that $|\tilde{p}^I|$ decreases slightly with $\tilde{\lambda}$, confirming that $\gamma < 1$. If we use the classical approximation $\gamma = 3/4$, then $E_n^I \propto n\lambda^{3/4}$. Therefore $p_n^I \propto n$ and the distribution of momentum p_n^I is far from a Maxwell-Boltzmann distribution as expected for a one-dimensional non-generic system.

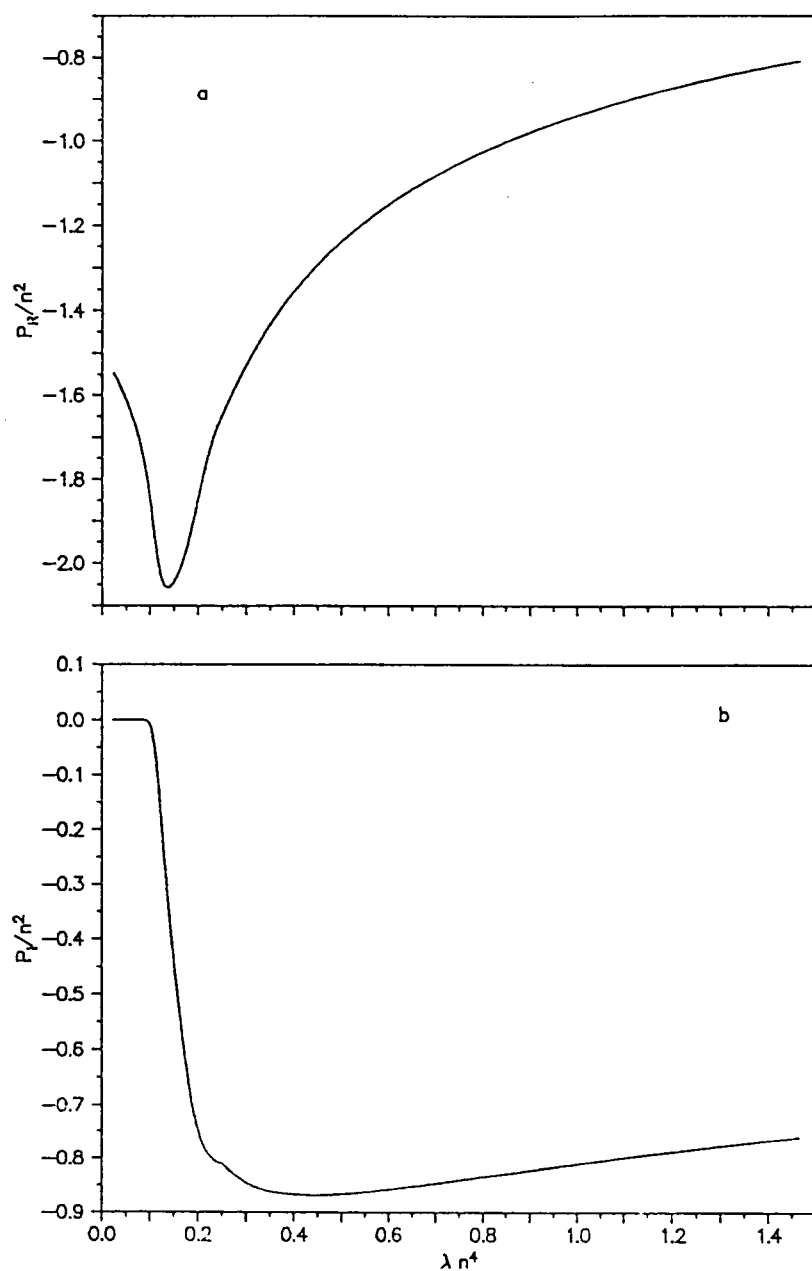


Figure 8.4: The scaled momentum of resonances of excited states ($n = 7-11$) as function of electric field.

Chapter 9

Conclusions

We have investigated the parametric motion of quantum spectra for classically chaotic systems. It is shown that the classical transition from predominantly regular motion to global chaos is accompanied by a transition from a nonequilibrium state to an equilibrium state in the parametric motion of quantum energy levels. The equilibrium distribution function provides an explanation of the Wigner-type NNS distribution for classically totally chaotic systems. The microscopic mechanism for the transition from a nonequilibrium state to an equilibrium state is the existence of avoided crossings. The width distribution of avoided crossings is closely related to the fraction of the accessible classical phase space in which the motion is chaotic. The overlapping of avoided crossings is a fingerprint of classical chaos. The study of relaxation processes in the parametric motion of energy levels reveals that the parametric correlation functions are sensitively dependent on the underlying classical dynamics, and the transition from classically regular to chaotic motion manifests itself in the disappearance of parametric diffusion in quantum spectrum. The discussion of the parametric motion of resonances indicates that due to the existence of geometric repulsion, the nearest-neighbor spacing distribution is not sensitive to the underlying dynamics for resonances. Instead, the parametric correlations may play a crucial role in the identification of classical chaos. We suggest that the transition to the thermal equilibrium state in the parametric motion of resonances is the signature of classical chaos. Therefore, besides providing a new numerical method for calculating spectra, the parametric dynamics approach connects the quantum eigenproblem with both equilibrium and nonequilibrium statistical mechanics and molecular dynamics. In this way, it is not only capable of confirming

the universality of fluctuations in quantum spectra for classically chaotic systems but also reveals rich structure in the parametric motion of energy levels itself.

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Appendices

Appendix A

Solution of the stability matrix near the integrable limit

The stability matrix of a Hamiltonian system obeys the differential equation

$$\frac{d}{dt}M = J \frac{\partial^2 H}{\partial x^2} M \quad (\text{A.1})$$

with initial conditions $M(0) = 1$, where J is given by Eq. (2.6).

We discuss now the solutions of the stability matrix for those periodic trajectories which are continuously deformed from the integrable limit. Therefore, we can use perturbation theory

$$\begin{aligned} I &\approx I_0 + \lambda I' \\ \theta &\approx \theta_0 + \lambda \theta' \\ M &\approx M_0 + \lambda M' \end{aligned} \quad (\text{A.2})$$

where the action-angle variables are exploited so that $\nabla_\theta H_0 = 0$. Because of Eq. (2.32), we only need to solve Eq. (A.1) within one period. To the first order in λ we get

$$M(T) = \exp\left(J \frac{\partial^2 H_0}{\partial x^2} T\right) (1 + \lambda T A) \quad (\text{A.3})$$

where $\frac{\partial^2 H_0}{\partial x^2}$ is a $2N \times 2N$ matrix with elements $\frac{\partial^2 H_0}{\partial x_i \partial x_j}$ and A is another $2N \times 2N$ matrix

$$A = \left\langle \exp\left(-J \frac{\partial^2 H_0}{\partial x^2} t\right) J \frac{\partial^2}{\partial x^2} [I'(t) \cdot \nabla_{I_0} H_0 + V] \exp\left(J \frac{\partial^2 H_0}{\partial x^2} t\right) \right\rangle \quad (\text{A.4})$$

where $\langle \rangle$ denotes time average over one period.

Note that from Eq. (2.39) the largest eigenvalue of the stability matrix $M(T)$ is always larger than 1 ($\zeta_1 > 1$) for the unstable case. Thus the periodic trajectory appears as a hyperbolic fixed point [10] in the Poincaré surface of section, i.e. a nearby trajectory stays on a single branch of a hyperbola in the Poincaré surface of section. The inverse-hyperbolic case ($\zeta_1 < -1$), i.e. the points of a nearby trajectory in the Poincaré surface of section appear alternatively on both branches of a hyperbola [10], is excluded because the trajectory is not continuously deformed under the perturbation.

Appendix B

Unfolding of the spectra of one-dimensional single-well potential systems

We discuss the unfolding of one-dimensional systems

$$H = p^2/2 + V(q) \quad (\text{B.1})$$

where $V(q)$ can be any single-well potential as illustrated in Fig. B.1.

Unfolding can be performed via

$$\varepsilon_n = \mathcal{N}_{av}(E_n). \quad (\text{B.2})$$

where $\mathcal{N}_{av}$ is the averaged integrated density of the physical energy levels (Eq. (4.25)). Eq. (B.2) is equivalent to Eq. (3.2) when levels are contained in an energy interval as defined by Eq. (3.1) so that we can expand the averaged integrated density of states

$$\mathcal{N}_{av}(E_n) \approx \mathcal{N}_{av}(E) + \mathcal{N}'_{av}(E_n - E). \quad (\text{B.3})$$

Notice that $\mathcal{N}'_{av} = n_{av} = 1 / \langle \Delta E \rangle$, then Eq. (B.2) leads to

$$\varepsilon_n = E_n / \langle \Delta E \rangle + \text{constant} \quad (\text{B.4})$$

which is equivalent to Eq. (3.2).

The averaged integrated density of states, Eq. (4.25), is

$$\mathcal{N}_{av}(E) = \frac{1}{2\pi\hbar} \int_{E \geq p^2/2 + V(q)} dp dq$$

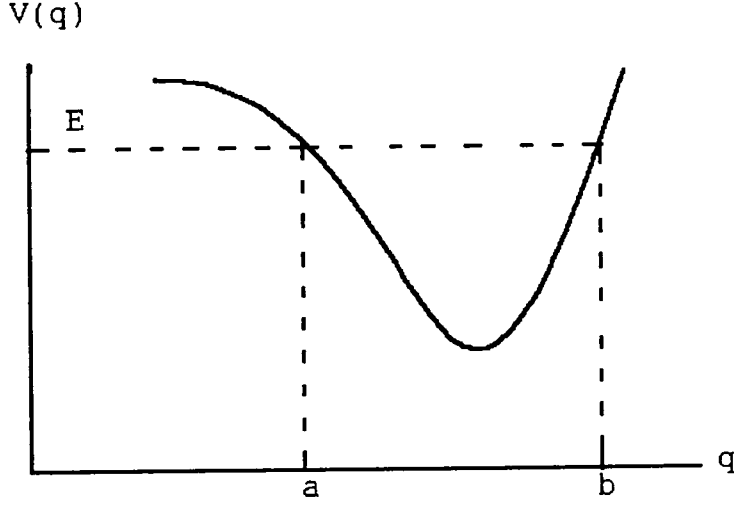


Figure B.1: One-dimensional single-well potential with two turning points a and b .

$$\begin{aligned}
 &= \frac{2}{2\pi\hbar} \int_a^b \sqrt{2(E - V(q))} dq \\
 &= \frac{2}{2\pi\hbar} \int_a^b p dq = I(E)/\hbar
 \end{aligned} \tag{B.5}$$

where a and b are the turning points and $I(E)$ is the action variable (Eq. (2.21)). The unfolded spectrum is given by

$$\varepsilon_n = \mathcal{N}_{av}(E_n) = I(E_n)/\hbar. \tag{B.6}$$

Inverting the EBK quantization (Eq. (4.15)) for a one-dimensional single-well potential, we have

$$I(E_n) = (n + \frac{1}{2})\hbar. \tag{B.7}$$

Here we have used fact that there are two turning points, so $\alpha = 2$. Therefore

$$\varepsilon_n = n + \frac{1}{2}. \tag{B.8}$$

We see that after unfolding, the spectra of one-dimensional single-well potential systems form a universality class of the harmonic oscillator type irrespective of the anharmonicity and the presence of the continuum. The NNS distribution is then

$$P(s) = \delta(s - 1) \quad (\text{B.9})$$

Notice that several well-known spectra, e.g. the spectrum of one-dimensional hard-square potential, the spectrum of one-dimensional Coulomb potential and therefore the spectrum of three-dimensional Coulomb problem within a given subspace of angular momentum (l and L_z) belong to this class.

Appendix C

Semiclassical relations between the number variance and the parametric number variance

The correlations between consecutive level spacings are probed by the number variance

$$\Sigma(L) = \langle (m(L) - L)^2 \rangle \quad (\text{C.1})$$

where $m(L)$ is the number of the unfolded levels $\{\varepsilon_n\}$ in the interval $(\varepsilon - L/2, \varepsilon + L/2)$, and, by the definition of unfolding,

$$\langle m(L) \rangle = L. \quad (\text{C.2})$$

Random matrix theory [22] predicts for a Poisson sequence

$$\Sigma_{\text{poisson}}(L) = L, \quad (\text{C.3})$$

and for the GOE systems

$$\Sigma_{\text{GOE}}(L) \approx \frac{2}{\pi^2} (\ln L + \ln 2 + \gamma + 1 - \frac{\pi^2}{8}) \quad (L \gg 1) \quad (\text{C.4})$$

where γ is Euler's constant.

Using the semiclassical trace formula (Eq. (4.11)) one finds [99]

$$\Sigma(L) = \frac{8}{\hbar^{2\mu}} \int_0^\infty dT \times$$

$$\left(\frac{\sin(LT/(2\hbar n_{av}))}{T} \right)^2 < \sum_{\nu, \xi}^+ A_\nu A_\xi \cos\left(\frac{S_\nu - S_\xi}{\hbar}\right) \delta\left(T - \frac{T_\nu + T_\xi}{2}\right) > \quad (C.5)$$

and the similar result [81] for the parametric number variance

$$V_P(\Lambda) = \frac{8}{\hbar^{2\mu}} \int_0^\infty \frac{dT}{T^2} < \sum_{\nu, \xi}^+ A_\nu A_\xi \cos\left(\frac{S_\nu - S_\xi}{\hbar}\right) \delta\left(T - \frac{T_\nu + T_\xi}{2}\right) \sin^2\left(\frac{T y_{\nu\xi} \Lambda}{2\hbar}\right) > \quad (C.6)$$

where $y_{\nu\xi} = (y_\nu + y_\xi)/2$ and $y_\nu = (\partial S_\nu / \partial \lambda)_\epsilon / T_\nu$. We derive now a semiclassical relation between $\Sigma(L)$ and $V_P(\Lambda)$. In the semiclassical limit ($\hbar \rightarrow 0$), factors of the form $\cos(\frac{S_\nu - S_\xi}{\hbar})$ eliminate the contributions from those pairs with $(S_\nu - S_\xi) > \hbar$ hence the main contributions are from the pairs with $(S_\nu - S_\xi) < \hbar$. Therefore $A_\nu A_\xi \cos(\frac{S_\nu - S_\xi}{\hbar}) \delta(T - \frac{T_\nu + T_\xi}{2})$ is smooth while $\sin^2(T y_{\nu\xi} \Lambda / (2\hbar))$ is a fast oscillating factor which thus can be replaced by its average value

$$\sin^2\left(\frac{T y_{\nu\xi} \Lambda}{2\hbar}\right) \rightarrow \int_{-\infty}^\infty dy \rho(y) \sin^2\left(\frac{T y \Lambda}{2\hbar}\right) \quad (C.7)$$

where $\rho(y)$ is the probability distribution function of y . Substituting (C.7) into Eq. (C.6) and comparing with Eq. (C.5), we get

$$V_P(\Lambda) = \int_{-\infty}^\infty dy \rho(y) \Sigma(|y| n_{av} \Lambda). \quad (C.8)$$

Substitution of the results of the random matrix theory (Eqs. (C.3) and (C.4)) into Eq. (C.8) leads to Eqs. (7.2) and (7.3). We note that Goldberg et al. [81] did not discuss the PNV for integrable systems and their approximation of the PNV for chaotic systems differs from our Eqs. (7.2, 7.3). Our result is, however, within the numerical uncertainty, consistent with the numerical results of Ref. [81] for the hydrogen in a magnetic field as well as the present results for the coupled Morse oscillators, as shown in Fig. 7.1.

Note that the derivation of Eq. (C.6) assumes that

$$S \gg |(\partial S / \partial \lambda)_\epsilon| \Lambda. \quad (C.9)$$

The values of Λ in quantum calculations are confined within the intervals of λ in which the classical phase space structure does not appreciably change.

Within these values ($\Lambda < 0.2$ for the coupled Morse oscillators), the condition (C.9) is satisfied for classically regular systems because S is a smooth function of the perturbation strength λ . On the other hand, it may not be valid for chaotic systems when Λ reaches the limit of large values since the action S becomes sensitively dependent upon the perturbation and $|(\partial S/\partial \lambda)_\epsilon|$ can be large. In this limit, a modification for the semiclassical estimate Eq. (7.3) is needed and is given by Eq. (7.5).

Appendix D

Measures of parametric diffusion for chaotic systems

We give in this appendix explicit expressions for the velocity autocorrelation function (VAF), $\psi(\Lambda)$, its Laplace transform, $\hat{\psi}(s)$, the generalized diffusion coefficient $D(\Lambda)$, and the mean squared displacement $\langle x^2(\Lambda) \rangle$ for the classically chaotic regime. All expressions are determined from the approximation (Eq. (7.34)) to spectrum of the VAF.

We can express $\psi(\Lambda)$ in terms of $G(\omega)$ by inverting Eq. (7.12)

$$\psi(\Lambda) = \frac{2}{\pi} \int_0^\infty d\omega G(\omega) \cos(\omega\Lambda). \quad (\text{D.1})$$

Substitution of Eq. (7.34) into the above equation gives

$$\psi(\Lambda) = \frac{2A}{\pi} \frac{d^2}{d\Lambda^2} H(\omega_0, \Lambda, n) \quad (\text{D.2})$$

with A is given by Eq. (7.35) and

$$\begin{aligned} H(\omega_0, \Lambda, n) &= - \int_0^\infty d\omega \frac{\cos(\omega\Lambda)}{(\omega + \omega_0)^n} \\ &= - \frac{1}{\Lambda(n-1)!} \left(-\frac{d}{d\omega_0}\right)^n U(\omega_0\Lambda). \end{aligned} \quad (\text{D.3})$$

$U(z)$ is defined by

$$U(z) = \int_0^\infty dt \frac{\sin(t)}{t+z} = \int_0^\infty dt \frac{\exp(-zt)}{t^2+1}$$

$$= Ci(z)\sin(z) - (Si(z) - \pi/2)\cos(z) \quad (D.4)$$

where $Si(z)$ and $Ci(z)$ are the sine and cosine integrals, respectively. It is straightforward to get $D(\Lambda)$, $\langle x^2(\Lambda) \rangle$ and $\tilde{\psi}(s)$ by substitution $\psi(\Lambda)$ into Eqs. (7.10), (7.11) and (7.18):

$$D(\Lambda) = \frac{2A}{\beta\pi} \frac{d}{d\Lambda} H(\omega_0, \Lambda, n), \quad (D.5)$$

$$\langle x^2(\Lambda) \rangle = \frac{4A}{\beta\pi} \left(H(\omega_0, \Lambda, n) + \frac{1}{(n-1)\omega_0^{n-1}} \right) \quad (D.6)$$

and

$$\begin{aligned} \tilde{\psi}(s) = & \frac{As^2}{\pi i} \left(\frac{1}{(\omega_0 + is)^n} (\ln(s/\omega_0) - i\frac{\pi}{2}) - \frac{1}{(\omega_0 - is)^n} (\ln(s/\omega_0) + i\frac{\pi}{2}) \right. \\ & + \frac{1}{(n-1)} \left(\frac{1}{(\omega_0 + is)^{n-1}} \left(\frac{1}{\omega_0} - \frac{1}{is} \right) - \frac{1}{(\omega_0 - is)^{n-1}} \left(\frac{1}{\omega_0} + \frac{1}{is} \right) \right) \\ & + \frac{1}{(n-1)(n-2)} \sum_{k=0}^{n-4} \frac{k+1}{\omega_0^{n-3-k}} \left(\frac{1}{(\omega_0 + is)^{k+2}} \left(\frac{1}{\omega_0} + \frac{k+2}{(n-3-k)(\omega_0 + is)} \right) \right. \\ & \left. \left. - \frac{1}{(\omega_0 - is)^{k+2}} \left(\frac{1}{\omega_0} + \frac{k+2}{(n-3-k)(\omega_0 - is)} \right) \right) \right), \quad (D.7) \end{aligned}$$

where s is the variable of the Laplace transform.

Curriculum Vitae

Xiazhou Yang was born on June 23, 1954 in Kunming city of Yunnan province, P. R. China. He has one older brother and one older sister. He spent his childhood with much love from his family and the beauty of the nearby Dianchi lake, the biggest mountain lake in southeast Asia.

In 1966, the Cultural Revolution began. He was moved from one village to another with his parents in the remote mountainous areas of the province until 1972, when he fortunately had a chance to enter the most prestigious high school in the province, the high school affiliated with Kunming Normal University, where teachers were teaching sciences under the risk of being classified as the "enemy of the people". After graduation from high school in 1973, he worked on a farm and then in a factory. When the Cultural Revolution was over and universities reopened, he passed the first entrance exams in eleven years, and in 1978, he became a freshman of Yunnan University. He obtained the B.S. in the spring of 1982 and entered Beijing University as a graduate student majoring in particle physics. Beijing University is the center of science and democracy in China and has had great impact on China's history. Xiazhou Yang graduated with his M.S. in 1984 under the guidance of Professor Chongshou Gao. Then he joined the theoretical high energy physics group of Professor Benhao Sa in the Institute of Atomic Energy, the largest national laboratory in China. Two years later, introduced by Professor Yongshou Chen of the Institute, he became a graduate student of Professor Joachim Burgdörfer at the department of physics, University of Tennessee. He is working on the theory of quantum chaos and expects to receive his Ph. D. in August 1993.