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Review of quantum mechanics.

1.1 Classical mechanics.

Classical and quantum mechanics begin by defining elementary notions of state and physical quantity. However, very different mathematical objects are assigned to these concepts in the two theories. We will begin with the more familiar notions of classical mechanics in the Hamiltonian formulation.

1.1.1 States, physical quantities, instruments and operations

Definition.
A classical state, \( P(q_1, q_2, \ldots, q_n, p_1, p_2, \ldots, p_n) \) is positive, real valued, integrable function (with norm one in \( L^1 \)) on an even dimensional sympletic manifold, the phase space.

The normalisation is
\[
\int_{-\infty}^{\infty} dq^n dp^n P(q_i, p_i) = 1 \tag{1.1}
\]

Technical note: States are elements of the positive cone, \( V^+ \) of the Banach space \( L^1 \), where
\[
V^+ = \{ x \in L^1 : x \text{ is a positive function} \} \tag{1.2}
\]

A symplectic manifold is a manifold endowed with a particular differential two-form,
\[
\gamma = dp_i \wedge dq^i \tag{1.3}
\]

(there is a sum over the repeated index). Here \( dq, dp \) are differential one forms. Let \( f, g \) be two real valued functions on phase space. Real valued
functions define flow vectors by
\[ v_f(q,p) = \left(-\frac{\partial F}{\partial q^i}, \frac{\partial F}{\partial p_i}\right) \] (1.4)

The canonical two form is then defined by its action on these vectors,
\[ \gamma[v_f, v_g] = -\{f, g\} \] (1.5)

where \( \{f, g\} \) is the Poisson bracket
\[ \{f, g\} = \left(\frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q^i} \frac{\partial f}{\partial p_i}\right) \] (1.6)

In fact we need to consider a more general class of functions to represent states which includes delta functions, because of the following definition.

**Definition.**
A completely specified state is a pure state and is given by
\[ P(q,p|q_0,p_0) = \delta^{(2n)}(q - q_0, p - p_0) \] (1.7)

A pure state corresponds to a single point in phase space. A completely specified state means that we know everything there is to know about the state. There is no uncertainty in the specification. (Note we have suppressed the dependence on all the \( 2n \) canonical variables and use just the symbols \( q, p \) to denote the full set of coordinates for the sympletic manifold.

We now turn to the definition of physical quantities.

**Definition.**
A physical quantity is a real valued function \( A(q,p) \) on the symplectic manifold.

Technical note: physical quantities are the positive elements of \( L^\infty \), the dual to the space \( L^1 \) of states. The Banach space \( L^\infty \) is the space of functions \( f(q,p) \) on phase space such that \( |f(q,p)| < \infty \). In fact the space of physical quantities is the positive cone of an Abelian \( C^* \) algebra, where the involution is complex conjugation*.

Note that in this case we do mean regular differentiable functions, not delta functions. Examples are:

- kinetic energy \( T = p^2/(2m) \)

* See for example *An invitation to \( C^* \) algebras*, W. Arveson, Graduate texts in Mathematics, 39 (Springer, 1976)
• potential energy $V(q)$
• total energy (Hamiltonian) $H = T + V$
• angular momentum $\vec{L} = \vec{q} \times \vec{p}$

Definition.
The moments of a physical quantity $A$ in the state $P$ is given by

$$\langle A \rangle_P = \int_{-\infty}^{\infty} dq dp A(q, p) P(q, p) \quad (1.8)$$

Technical note: the moment defined by a state $P$ is a bounded positive linear functional on the space $L^\infty$ of physical quantities. We may thus identify states with positive linear functionals, with unit norm, on the set of physical quantities. In the theory of $C^*$ algebras, positive linear functionals of unit norm are called states. The origin of this designation should be clear enough.

States in classical mechanics admit an ignorance interpretation. By this we mean that if a system is in a state $P$, that is not a pure state, then we interpret this as reflecting our lack of knowledge of the actual pure state of the system. (This interpretation is not possible in quantum theory of physical states). We imagine that, given enough effort, we could resolve this ignorance by a more careful specification of the system. That is to say, there is some measurement that will tell us the actual state of the system as a pure state.

To make this idea a little more precise let us write a general state $P(q, p)$ as a convolution over pure states

$$P(q, p) = \int dq' dp' P(q - q', p - p') \delta(q', p') \quad (1.9)$$

In this form it is compelling to interpret the state $P(q, p)$ as resulting from an average over the a priori pure states, $\delta(q, p)$ with respect to the conditional probability distribution

$$P(q, p|q', p') = P(q - q', p - p') \quad (1.10)$$

which we can say represents our lack of ability to resolve a pure state.

Equation (1.9) suggests a generalisation:

$$P_{\text{obs}}(q, p) = \int dq' dp' P(q, p|q', p') P(q', p') \quad (1.11)$$

which we interpret by saying that the a priori state of the system is $P(q, p)$, however, due to finite resolving power of the instrument (represented mathematically by the conditional probability $P(q, p|q', p')$) that
1.1 Classical mechanics.

we use to determine the state, the observed state is $P_{\text{obs}}(q,p)$. With this interpretation $P(q,p|q',p')$ is the conditional probability for the instrument to record the values $(q,p)$ given that the system is in the pure state $\delta(q',p')$. It is easy to show that Eq.(1.11) defines a linear operator on state space, that is, it is a positive linear operator from states to states.

**Exercise 1.1** Prove this last statement.

We shall refer to the conditional probability $P(q,p|q',p')$ as an instrument or as an effect.

We are now led to ask a very natural question: if we use the instrument $P(q,p|q',p')$ on the a priori state, $P(q,p)$, what is the state of the system conditioned on a particular measurement result $(\bar{q},\bar{p})$? In other words, what is the a postiori state given a particular outcome? The answer is a straightforward application of Baye’s theorem:

$$P'(q,p|\bar{q},\bar{p}) = \frac{P(\bar{q},\bar{p}|q,p)P(q,p)}{P_{\text{obs}}(\bar{q},\bar{p})}$$

(1.12)

where the prime reminds us that this is the a postiori state. The transformation from a priori state to a postiori state is called an operation. Note that this is a nonlinear transformation as $P_{\text{obs}}(\bar{q},\bar{p})$ depends on the prior distribution.

**Exercise 1.2** Gaussian states are defined by

$$P(q,p) = (2\pi|\det\sigma|)^{-1/2} \exp\left[-\frac{1}{2}(q - q_0, p - p_0)\sigma^{-1}(q - q_0, p - p_0)^T\right]$$

(1.13)

where

$$(q,p)_P = (q_0,p_0)$$

(1.14)

and $\sigma$ is the covariance matrix. Likewise a Gaussian instrument is defined by

$$P(q,p|q',p') = (2\pi|\det\Delta|)^{-1/2} \exp\left[-\frac{1}{2}(q - q', p - p')\Delta^{-1}(q - q', p - p')^T\right]$$

(1.15)

Show that in this case the operation transforms a priori Gaussian states to a postiori Gaussian states.

1.1.2 Dynamics

There are two pictures to specify the dynamics. We can consider equations of motion for the physical quantities themselves, with states held independent of time. This is the Hamilton picture. Alternatively we
can consider the evolution of states and hold physical quantities fixed in
time. This is the Liouville picture. Both pictures give the same results
for moments of physical quantities as we now show.

In the Hamilton picture, the evolution of physical quantities is given by
Hamilton’s equations,
\[
\frac{dA}{dt} = -\{H, A\} + \frac{\partial A}{\partial t}
\]
where the last term accounts for an explicit time dependence in the function
\(A(q,p,t)\), which typically we will not consider. The \(\{ , \}\) is the usual
Poisson bracket.

In the Liouville picture, we seek an evolution equation for the phase
space probability density \(P(q,p,t)\), which specifies the state at time \(t\). A
phase space function of the form \(F(q,p,t)\) may change in time due to the
implicit dependence of the canonical variables on time and there may be
an explicit time dependence. The total time derivative is then
\[
\frac{dF}{dt} = \frac{dq}{dt} \frac{\partial F}{\partial q} + \frac{dp}{dt} \frac{\partial F}{\partial p} + \frac{\partial F}{\partial t}
\]
\[
= \{F,H\} + \frac{\partial F}{\partial t}
\]
We can think of the dynamics of the density \(P(q,p,t)\) like the flow of
a fluid. Imagine that the density describes an ensemble of particles at
different points in phase space, all moving according to Hamilton’s
equations. The total derivative is then the rate of change of the density with
time as we follow the flow. The partial derivative however is evaluated
at fixed \(q,p\), and corresponds to sitting at a particular point in the phase
plane and monitoring the density. The functions \(q(t), p(t)\) which specify
the canonical coordinates as time changes are generated by Hamilton’s
equations and thus constitute canonical transformations. Such transfor-
mations do not change phase space volume. This means that \(P(q,p)\)
behaves like a density for an incompressible fluid flow on phase space.
This implies that the total derivative \(\frac{dP}{dt} = 0\). We thus find that
\[
\frac{\partial P}{\partial t} = \{H,P\}
\]
This is Liouville’s equation and it describes the dynamics in the Liouville
picture.

**Exercise 1.3** Show that the evolution of moments of physical quantities
are the same in both pictures.

An important point to note here is that the Liouville equation is a
linear partial differential equation with only first order derivatives. This
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has the important consequence that two nearby states will remain nearby under evolution, regardless of whether or not the dynamics is regular or chaotic. There are a number of ways to see this. A interesting path was first given by Koopman in the early part of last century.

To be more specific we need to state precisely what we mean by ‘nearby’. We will use a statistical notion of nearby that arises in classical mathematical statistics. In what sense can two probability distributions $P_1$ and $P_2$ be considered close to each other? We cannot measure a probability, we can only measure $q, p$ and thus sample the distribution. In a long run of experiments on identically prepared systems we can then try and estimate the probability distribution based on the relative frequency of observations. If two distributions are very close it may not be possible for sampling of this kind to distinguish them. In mathematical statistics considerations such as this led to the development of a notion of statistical distance. We can specify this either as an infinitesimal distance $ds^2$ or as a global metric, $d(P_1, P_2)$. A infinitesimal metric may be consistent with more than a single global metric. The infinitesimal distance is defined by considering a parametric family of states $P_\theta(q, p)$ and then ask for the statistical distance between $P_\theta$ and $P_{\theta+d\theta}$. This is given in terms of the Fisher information, $F_\theta$,

$$ds^2 = \langle \left(\frac{\partial \ln P}{\partial \theta} \right)^2 \rangle d\theta^2$$

$$= \int dq dp P_\theta(q, p) \left(\frac{\partial \ln(P_\theta(q, p))}{\partial \theta} \right)^2$$

$$= F_\theta d\theta^2$$

Or we can use the Kullback information which, while not a metric, does give a measure of statistical distinguishability,

$$L(P_1, P_2) = \int_{-\infty}^{\infty} P_1(x) \log \left(\frac{P_1(x)}{P_2(x)}\right) dx$$

**Exercise 1.4** Show that the statistical distance does not change in time under Hamiltonian evolution.

Show that the Kullback information of two states does not change under Hamiltonian evolution.

In classical mechanics the state of a single particle in three dimensions is given by a probability distribution on a six dimensional real manifold, with a sympletic structure (ie a Poisson bracket), called the phase space. Three coordinates give the position of the particle and three give the

† See Asher Peres, *Quantum Theory*, (Kluwer, 1995)
momenta. The dimension of the phase space for two such particles is simply the \textit{Cartesian product} of the two phase spaces for each particle, which has twelve dimensions. In the case of $k$ particles the phase space is of dimension $6k$, that is, it increases linearly with the number of sub systems.

\section*{1.2 Quantum Mechanics.}

In quantum mechanics we also define physical states, physical quantities and dynamics, but the mathematical structure assigned to the definitions is very different from classical mechanics.

\textbf{Definition.}

The \textit{state} of a physical system is specified by a positive trace class operator, $\rho$, of trace one acting on Hilbert space $L^2$. The operator $\rho$ is called the \textit{density} operator.

\textbf{Definition.}

The physical quantities are given by self adjoint operators, $A$, on the Hilbert space.

\textbf{Definition.}

The \textit{moments} of physical quantities are given by

$$\langle A \rangle = \text{tr}(A\rho) \quad (1.21)$$

We now pause to note some curious differences between quantum and classical mechanics. First we note that there is as yet no reference to a phase space at all. This immediately raises the question of how quantum and classical mechanics can be compared at all. Second we note that it is not at all clear how to connect the quantum notion of a state with what is actually done in a real experiment. Typically an experiment is specified by a preparation procedure which may involve setting various devices, cooling the system, turning on and off interactions between component systems etc., and a measurement procedure in which various outcomes are recorded. Both preparation and registration procedures can be specified by strings of numbers, possibly coded in binary form. An analysis of the experiment then compares the strings specifying the preparation procedure to those specifying the measurement results, and interesting correlations reported. As it stands however we have made no mention of how quantum mechanics describes the results of a particular experiment. The hint on how to do this is contained in the definition of physical moments, $\langle A \rangle = \text{tr}(A\rho)$. 
1.2 Quantum Mechanics.

The self-adjoint operator $A$ on Hilbert space may be written in terms of its spectral decomposition

$$A = \sum_a a|a\rangle\langle a|$$ (1.22)

for operators with a discrete spectrum and

$$A = \int d\mu(a)|a\rangle\langle a|$$ (1.23)

for some measure $d\mu(a)$, for operators with a continuous spectrum.‡

The average of the physical quantity represented by $A$ may now be written as

$$\langle A \rangle = \text{tr}(A\rho)$$

$$= \text{tr} \left( \sum a|a\rangle\langle a| \rho \right)$$

$$= \sum a \text{tr}(|a\rangle\langle a| \rho)$$

$$= \sum aP(a)$$

where

$$P(a) = \text{tr}(|a\rangle\langle a| \rho)$$ (1.24)

As $\rho$ and $|a\rangle\langle a|$ are both positive operators, bounded by unity under a trace norm it is not difficult to see that $0 < P(a) \leq 1$ and thus it is possible to interpret $P(a)$ as a probability§. In that case Eq.(1.24) is clearly in the form of a standard statistical average over measurement results. We can thus interpret the eigenvalues of $A$ as the possible results of a measurement of this physical quantity and $P(a) = \text{tr}(|a\rangle\langle a| \rho)$ gives the probability distribution over the measurement results.

The density operator is the most general representation of a quantum state and encodes all of the physical meaningful information about the preparation of the system. This is in fact the content of Gleason’s theorem[2] which says that for Hilbert spaces of dimension not less than 3, every probability measure on the set of projection operators can be written as

$$P(\pi = 1) = \text{tr}(\hat{\rho}\hat{\Pi})$$ (1.25)

where $\hat{\Pi}$ is a projection operator on the Hilbert space, $\pi = 0, 1$ are the eigenvalues of the projection operator, and $\rho$ is a positive bounded, trace class operator of trace one.

‡ We are using Dirac notation here. A more careful treatment can be found texts such as that of Reed and Simon.....

§ Strictly we need to check a few more properties before we make this leap, but they all work out OK
In fact even the restriction to projection operators turns out to be an unnecessary. The most general way to represent probability distributions in quantum mechanics is

$$P(a) = \text{tr} (F(a) \rho)$$

where $F(a)$ is a positive operator (ie it has positive eigenvalues) and satisfies $\sum_a F(a) = 1$. We call $F(a)$ a positive operator valued measure (POVM). Almost any realistic measurement is described in terms of the POVMs rather than projection operators (see Milburn and Wise-man, *Quantum Measurement and Control*, Chap. 1). We shall return to this point when we consider how a phase space description of a quantum system can be given.

A general quantum state can give a non zero variance for every physical quantity. However there are a special class of states for which there is at least one physical quantity that is certain, that is to say, a physical quantity for which the outcome of the measurement is certain. Such states are called pure states.

**Definition.**
A state for which $\rho^2 = \rho$ is a pure state.

Pure states are thus projection operators onto a one dimensional subspace of Hilbert space. We write such a state as $\rho = |\psi\rangle\langle\psi|$. In this case the probability distributions are given by

$$P(a) = |\langle a|\psi\rangle|^2$$

We call the complex function $\langle a|\psi\rangle$, the *probability amplitude* for the measurement result to take the value $a$. We see that probabilities are not primary in quantum physics but determined at a deeper level by probability amplitudes, which are not necessarily positive, not even real. Every state that is not pure is called mixed. A mixed state can always be written as a convex combination of pure states,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

Thus

$$P(a) = \sum_i P_i(a)$$

where $P_i(a) = |\langle a|\psi_i\rangle|^2$.

Pure states are the quantum analogue of classical states represented by delta function distributions on phase space. In classical mechanics a pure state means that all measurement results for physical quantities
are certain, i.e. dispersion free. Quantum pure states however are not like this at all. For a pure quantum state, for which there is at least one physical quantity that is certain, simultaneously there is always at least one physical quantity which is completely uncertain. This is the consequence of Heisenberg uncertainty principle. Quantum states are irreducibly random; a puzzling but well verified experimental fact. Even when we know everything there is to know about a quantum state, there remain quantities that are totally uncertain.

We now need to consider how quantum mechanics deals with dynamics. This is given by a simple rule. If a state at time zero has a definite value of energy, that is an energy eigenstate, $|E\rangle$, then at a later time $t$ the state is just a rotation in Hilbert space $e^{-iEt/\hbar}|E\rangle$. For an arbitrary initial state $|\psi(0)\rangle$ we can expand in the eigenstates of energy as

$$|\psi(0)\rangle = \sum_E c_E |E\rangle$$

Thus at a later time

$$|\psi(t)\rangle = \sum_E c_E e^{-iEt/\hbar} |E\rangle$$

In differential form,

$$\frac{d|\psi(t)\rangle}{dt} = -\frac{i}{\hbar} \hat{H} |\psi(t)\rangle$$

where $\hat{H}$ is the energy operator. We postulate that the energy operator is a function of the position and momentum operators as

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

In the case of probability amplitude for position measurements we find

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + V(x)\psi(x,t)$$

In the case of a general quantum state, we find that

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [\hat{H}, \rho]$$

which is the quantum analogue of the classical Liouville equation. There is a quantum analogue of the statistical distance between quantum states. The proof is not so simple as we need to find a definition that works for all possible probability distributions that result from positive operator valued measures. However the conclusion is that an appropriate quantum
version of the statistical distance is [See Nielsen and Chuang, *Quantum computation and quantum information*, CUP, 2000].

\[ d(\rho_1, \rho_2) = \arccos F(\rho_1, \rho_2) \]  

(1.36)

where the fidelity, \( F(\rho_1, \rho_2) \) is given by

\[ F(\rho_1, \rho_2) = \text{tr} \left( \sqrt{\rho_1^{1/2} \rho_2 \rho_1^{1/2}} \right) \]  

(1.37)

It does not look particularly symmetric...but it is. It is then easy to show that under Hamiltonian evolution, this quantity is invariant, which is the quantum analogue of the result for the classical statistical distance.

**Exercise**

Prove that the Fidelity is invariant under Schrödinger dynamics.

A comment is called for at this point. It is often said that there cannot be a quantum analogue of chaos because the linearity of the quantum evolution equation enforces the invariance of the statistical distance between states as a function of time. This is clearly nonsense as the same result holds for the quantum statistical distance between states. While it is true that quantum and classical non integrable dynamics are very different, the difference has nothing to do with the linearity of the Schrödinger equation.

### 1.2.1 Quantum Mechanics and Phase Space

Consider an operator \( \hat{Q} \) having the real line as its spectrum. This could represent the position of a particle, for example. Because of its continuous spectrum, the eigenstates \( |q \rangle \) of \( \hat{Q} \) are not normalizable. That is, it is not possible to have \( \langle q | q \rangle = 1 \). The usual convention is to choose the scaling for the states such that

\[ \int_{-\infty}^{\infty} dq |q\rangle \langle q| = 1. \]  

(1.38)

Squaring the above equation implies that the normalization for these states is

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

(1.39)

The quantum state \(|\psi\rangle\) in the position representation is often represented as

\[ \psi(q) = \langle q | \psi \rangle, \]  

(1.40)
and called the wavefunction. The probability density to find the particle at position \( q \) is \(|\psi(q)|^2\), and this integrates to unity. The state \(|\psi\rangle\) is recovered from the wavefunction as follows:

\[
|\psi\rangle = \int dq |q\rangle \langle q|\psi\rangle = \int dq \psi(q) |q\rangle.
\]

(1.41)

Here we are using the convention that the limits of integration are \(-\infty\) to \(\infty\) unless otherwise indicated.

If \( \hat{Q} \) does represent the position of a particle, then its momentum is represented by another operator with the real line as its spectrum, \( \hat{P} \). Using \( \hbar = 1 \), the eigenstates for \( \hat{P} \) are related to those for \( \hat{Q} \) by

\[
\langle q|p\rangle = (2\pi)^{-1/2}e^{ipq}
\]

(1.42)

Here the normalization factor is chosen so that

\[
\int dp |p\rangle\langle p| = 1, \quad \langle p|p'\rangle = \delta(p - p').
\]

(1.43)

Equation 1.43 is the a key postulate from which the quantum description of particle mechanics follows. It should be seen as a kinematical postulate to accompany the dynamical postulate introduced above.

**Exercise 1.5** Show these, using the position representation and the result that \( \int dy e^{iyx} = 2\pi \delta(x) \).

The momentum representation wavefunction is simply the Fourier transform of the position representation wavefunction:

\[
\psi(p) = \langle p|\psi\rangle = (2\pi)^{-1/2} \int dq e^{-ipq} \psi(q)
\]

(1.44)

This is very different from the classical case where the marginal distributions, while given by integration over states with respect to \( q \) or \( p \), are otherwise unrelated.

From the above it is easy to show that in the position representation, \( \hat{P} \) acts on a wavefunction identically to the differential operator \(-i\frac{\partial}{\partial q}\). First,

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

(1.45)

\[
= (2\pi)^{-1} \int dp \int dq' pe^{ip(q-q')} \psi(q').
\]

(1.46)

Now \( pe^{ip(q-q')} = i\frac{\partial}{\partial q'} e^{ip(q-q')} \), so using integration by parts, and assuming that \( \psi(q) \) vanishes at \( \pm\infty \) (as required by normalization if it is a well-behaved function) we obtain

\[
\langle q|\hat{P}|\psi\rangle = -i(2\pi)^{-1} \int dp \int dq' e^{i\frac{p}{\hbar}(q-q')} \frac{\partial}{\partial q} \psi(q')
\]

(1.47)
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\[ = -i \frac{\partial}{\partial q} \psi(q'). \quad (1.48) \]

It is now easy to find the commutator between \( \hat{Q} \) and \( \hat{P} \):

\[ \langle q | [\hat{Q}, \hat{P}] | q' \rangle \int dq' \psi(q') = q(-i)\frac{\partial}{\partial q} \psi(q) - (-i)\frac{\partial}{\partial q} q \psi(q) = i\psi(q). \quad (1.49) \]

Since \( \psi(q) \) is arbitrary, it follows that

\[ [\hat{Q}, \hat{P}] = i. \quad (1.50) \]

The assumption that \( \psi(q) \) is “well-behaved” can be made more precise. It turns out that we require that all \( \psi(q) \) belong to the set \( L^2(\mathbb{R}) \). That is, the integral (technically, the Lebesgue integral) of \( |\psi''(q)|^2 \) from \( -\infty \) to \( \infty \) must be finite. Although the space \( L^2(\mathbb{R}) \) is infinite, it is actually countably infinite. That is, the number of basis states for the Hilbert space \( \mathcal{H} = L^2(\mathbb{R}) \) is countable. The continuum in the spectrum of \( \hat{Q} \) does not require a continuum of Hilbert space dimensions. The apparent continuum of states \( \{ |q\rangle \} \) or \( \{ |p\rangle \} \) does not contradict this: these “states” are not normalizable and so are not actually in the Hilbert space. They exist as limits of true states, but the limit lies outside \( \mathcal{H} \).

1.2.2 Minimum Uncertainty States

From the above commutation relation it follows that the variances in \( Q \) and \( P \) must satisfy

\[ \langle (\Delta P)^2 \rangle \langle (\Delta Q)^2 \rangle \geq \frac{1}{4} \quad (1.51) \]

(Remember we have set \( \hbar = 1 \).) The states which saturate this are known as minimum uncertainty states (MUSs). It can be shown that these are Gaussian states. By this we mean they are states with a Gaussian wavefunction. They are parametrized by three real numbers. Below, we take these to be \( q_0, p_0 \) and \( \sigma \).

The position probability amplitude (i.e. wavefunction) for a MUS takes the form

\[ \psi(q) = (\pi\sigma^2)^{-1/4} \exp \left[ +ip_0(q - q_0) - (q - q_0)^2 / 2\sigma^2 \right]. \quad (1.52) \]

Here we have chosen the overall phase factor to give \( \psi(q) \) a real maximum at \( q = q_0 \). It is then easily verified that the moments for \( X \) are

\[ \langle Q \rangle = q_0 \quad (1.53) \]

\[ \langle (\Delta Q)^2 \rangle = \sigma^2 / 2. \quad (1.54) \]

Note the factor of two in the variance, because \( \varphi(q) = |\psi(q)|^2 \).
1.2 Quantum Mechanics.

The Fourier transform of a Gaussian is also Gaussian, so in the momentum representation
\[ \psi(p) = \left(\frac{\pi}{\sigma^2}\right)^{-1/4} \exp \left[ -i q_0 p - (p - p_0)^2 \sigma^2 / 2 \right]. \] (1.55)

From this it is easy to show that
\[ \langle \hat{P} \rangle = p_0 \] (1.56)
\[ \langle (\Delta \hat{P})^2 \rangle = 1 / 2 \sigma^2 \] (1.57)

The saturation of the Heisenberg bound (1.51) follows.

### 1.2.3 The Harmonic Oscillator

So far there is nothing that sets a natural length (or, consequently, momentum) scale for the system. The simplest dynamics which does so is that generated by the harmonic oscillator Hamiltonian
\[ \hat{H} = \frac{\hat{P}^2}{2m} + \frac{m \omega^2 \hat{Q}^2}{2}. \] (1.58)

Here \( m \) is the mass of the particle, and \( \omega \) the oscillator frequency. This Hamiltonian applies to any mode of harmonic oscillation, such as a mode of a sound wave in a condensed matter system, or a mode of the electromagnetic field. In the latter case, \( \hat{Q} \) is proportional to the magnetic field, and \( \hat{P} \) to the electric field.

Classically the harmonic oscillator has no characteristic length scale, but quantum mechanically it does, namely
\[ \sigma = \sqrt{\hbar / m \omega} \] (1.59)

where we have temporarily restored \( \hbar \) to make its role apparent. If we define
\[ \hat{a} = \frac{1}{\sqrt{2}} \left( \frac{\hat{Q}}{\sigma} + i \frac{\sigma \hat{P}}{\hbar} \right) \] (1.60)

then we can rewrite the Hamiltonian as
\[ H = \hbar \omega (\hat{a} \hat{a}^\dagger + \hat{a}^\dagger \hat{a}) / 2 = \hbar \omega (\hat{a} \hat{a} + \frac{1}{2}). \] (1.61)

Now from the commutation relations of \( \hat{Q} \) and \( \hat{P} \) we can show that
\[ [\hat{a}, \hat{a}^\dagger] = 1. \] (1.62)

Also, we can show that the state \( |\psi_0\rangle \) with wavefunction
\[ \psi_0(q) = \langle q | \psi_0 \rangle \propto \exp(-q^2 / 2\sigma^2) \] (1.63)

is an eigenstate of \( \hat{a} \) with eigenvalue 0.
Exercise 1.6 Show this using the position representation of $\hat{P}$ as $-i\hbar \frac{\partial}{\partial q}$.

Thus it is also an eigenstate of the Hamiltonian (1.61), with eigenvalue $\hbar \omega / 2$. Since $\hat{a}^\dagger \hat{a}$ is obviously a non-negative operator, this is the lowest eigenvalue of the Hamiltonian. That is, we have shown that the quantum harmonic oscillator has a ground state that is a minimum uncertainty state with $q_0 = p_0 = 0$ and a characteristic length $\sigma$ given by Eq. (1.59).

1.2.4 Number States

From the above it is easy to show that the eigenvalues of $\hat{a}^\dagger \hat{a}$ are the non-negative integers, as follows. From the commutation relations (1.62) it follows that (for integer $k$)

$$[\hat{a}^\dagger, (\hat{a}^\dagger)^k] = \hat{a}^\dagger [\hat{a}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k.$$  \hspace{1cm} (1.64)

Exercise 1.7 Show this.

**Hint:** Start by showing it for $k = 1$ and $k = 2$ and then find a proof by induction.

Then, if we define an unnormalized state $|\psi_n\rangle = (\hat{a}^\dagger)^n |\psi_0\rangle$ we can easily show that

$$\langle \hat{a}^\dagger \hat{a} \rangle |\psi_n\rangle = (\hat{a}^\dagger \hat{a})(\hat{a}^\dagger)^n |\psi_0\rangle = \left[ n(\hat{a}^\dagger)^n + (\hat{a}^\dagger)^n (\hat{a}^\dagger \hat{a}) \right] |\psi_0\rangle = n(\hat{a}^\dagger)^n |\psi_0\rangle = n |\psi_n\rangle.$$  \hspace{1cm} (1.65)

which establishes the result and identifies the eigenstates.

Thus we have derived the eigenvalues of the harmonic oscillator as $\hbar \omega \left( n + \frac{1}{2} \right)$. The corresponding unnormalized eigenstates are $|\psi_n\rangle$, which we will denote $|n\rangle$ when normalized. If the Hamiltonian (1.58) refers to a particle, these are states with an integer number of elementary excitations of the vibration of the particle. They are therefore sometimes called *vibron* number states, that is, states with a definite number of vibrons. If the harmonic oscillation is that of a sound wave, then these states are called *phonon* number states. If the oscillator is electromagnetic field, they are called *photon* number states. Especially in this last case, the ground state $|0\rangle$ is often called the vacuum state.

Because $\hat{a}^\dagger$ raises the number of excitations by one, with

$$|n\rangle \propto (\hat{a}^\dagger)^n |0\rangle,$$  \hspace{1cm} (1.66)

it is called the creation operator. Similarly, $\hat{a}$ lowers it by one, and is called the annihilation operator. To find the constants of proportionality, we must require that the number states to be normalized, so that

$$\langle n | m \rangle = \delta_{nm}.$$  \hspace{1cm} (1.67)
1.2 Quantum Mechanics.

Now since $|n\rangle$ is an eigenstate of $a^\dagger a$ of eigenvalue $n$,

$$\langle n|a^\dagger a|n\rangle = n\langle n|n\rangle = n.$$ \hspace{1cm} (1.68)

However we also have

$$\langle n|\hat{a}^\dagger \hat{a}|n\rangle = \langle \psi|\psi\rangle,$$ \hspace{1cm} (1.69)

where $|\psi\rangle = \hat{a}|n\rangle \propto |n-1\rangle$. Therefore the constant of proportionality must be

$$|\psi\rangle = \hat{a}|n\rangle = e^{i\phi}\sqrt{n}|n-1\rangle$$ \hspace{1cm} (1.70)

for some phase $\phi$. We choose the convention that $\phi = 0$, so that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle.$$ \hspace{1cm} (1.71)

Similarly it can be shown that

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle$$ \hspace{1cm} (1.72)

**Exercise 1.8** Show this, and show that the above two relations are consistent with $|n\rangle$ being an eigenstate of $\hat{a}^\dagger \hat{a}$.

Note that $\hat{a}$ acting on the vacuum state $|0\rangle$ produces nothing, a null state.

**Exercise 1.9** Show that the normalized number state is $|n\rangle = (n!)^{-1/2}(\hat{a}^\dagger)^n|0\rangle$.

1.2.5 Coherent States

No matter how large $n$ is, a number state $|n\rangle$ never approaches the classical limit of an oscillating particle (or oscillating field amplitude). That is because for a system in a number state the average value of $Q$ and $P$ is always zero.

**Exercise 1.10** Show this.

For this reason, it is useful to consider a state for which there is a classical limit, the coherent state. This state is defined as an eigenstate of the annihilation operator

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$$ \hspace{1cm} (1.73)

where $\alpha$ is a complex number (because $\hat{a}$ is not an Hermitian operator).

There are no such eigenstates of the creation operator $\hat{a}^\dagger$.

**Exercise 1.11** Show this. Assume that there exists states $|\beta\rangle$ such that $\hat{a}^\dagger|\beta\rangle = \beta|\beta\rangle$ and consider the inner product $\langle n|(\hat{a}^\dagger)^{n+1}|\beta\rangle$. Hence show that the inner product of $|\beta\rangle$ with any number state is zero.
It is easy to find an expression for $|\alpha\rangle$ in terms of the number states as follows. In general we have

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle.$$  \hfill (1.74)

Since $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ we get

$$\sum_{n=0}^{\infty} \sqrt{n} c_n |n-1\rangle = \sum_{n=0}^{\infty} \alpha c_n |n\rangle.$$  \hfill (1.75)

Equating the coefficients of the number states on both sides we get the recursion relation

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}} c_n.$$  \hfill (1.76)

so that $c_n = \frac{\alpha^n}{\sqrt{n!}} c_0$. Choosing $c_0$ real and normalizing the state, we get

$$|\alpha\rangle = \exp \left(-|\alpha|^2/2\right) \sum_{n} \frac{\alpha^n}{\sqrt{n!}} |n\rangle.$$  \hfill (1.77)

The state $|\alpha:=0\rangle$ is the same state as the state $|n:=0\rangle$. For $\alpha$ finite the coherent state has a non-zero mean photon number:

$$\langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle = \alpha^* \langle \alpha | \alpha \rangle = |\alpha|^2.$$  \hfill (1.78)

The number distribution (the probability for measuring a certain excitation number) for a coherent state is a Poissonian distribution of mean $|\alpha|^2$:

$$P_n = |\langle n | \alpha \rangle|^2 = e^{-|\alpha|^2} \frac{(|\alpha|^2)^n}{n!}.$$  \hfill (1.79)

This distribution has the property that the variance is equal to the mean. That is,

$$\langle (\hat{a}^\dagger \hat{a})^2 \rangle - \langle \hat{a}^\dagger \hat{a} \rangle^2 = |\alpha|^2.$$  \hfill (1.80)

**Exercise 1.12** Verify this, either from the distribution (1.79) or directly from the coherent state using the commutation relations for $\hat{a}$ and $\hat{a}^\dagger$.

Setting $\hbar = 1$, it is simple to show that

$$\langle \alpha | \hat{Q} | \alpha \rangle = \sqrt{2} \sigma \text{Re}[\alpha]$$  \hfill (1.81)

$$\langle \alpha | \hat{P} | \alpha \rangle = (\sqrt{2} / \sigma) \text{Im}[\alpha]$$  \hfill (1.82)

$$\langle \alpha | (\Delta \hat{Q})^2 | \alpha \rangle = \sigma^2 / 2$$  \hfill (1.83)

$$\langle \alpha | (\Delta \hat{P})^2 | \alpha \rangle = 1 / 2 \sigma^2$$  \hfill (1.84)

$$\langle \alpha | \Delta \hat{Q} \Delta \hat{P} + \Delta \hat{P} \Delta \hat{Q} | \alpha \rangle = 0$$  \hfill (1.85)
That is, a coherent state is a minimum uncertainty state as defined in Sec. 1.2.2.

Because $\hat{a}$ is not an Hermitian operator, the coherent states are not orthogonal. In fact it can be shown that

$$|(\alpha|\alpha')|^2 = \exp(-|\alpha - \alpha'|^2). \quad (1.86)$$

If $\alpha$ and $\alpha'$ are very different (as they would be if they represent two macroscopically distinct fields) then the two coherent states are very nearly orthogonal. Another consequence of their nonorthogonality is that the coherent states form an overcomplete basis. Whereas for number states we have

$$\sum_n |n\rangle\langle n| = \hat{1}, \quad (1.87)$$

the identity, for coherent states we have

$$\int d^2\alpha |\alpha\rangle\langle\alpha| = \pi \hat{1}. \quad (1.88)$$

**Exercise 1.13** Show this using the expansion (1.77). The result $n! = \int_0^{\infty} dx x^n e^{-x}$ may be useful.

Unlike number states, coherent states are not eigenstates of the Hamiltonian. However, they have the nice property that they remain coherent states under the harmonic oscillator Hamiltonian

$$\hat{H} = \omega \hat{a}^\dagger \hat{a} \quad (1.89)$$

Here we have dropped the $1/2$ from the Hamiltonian (1.61) as it has no physical consequences (at least outside of general relativity). The amplitude $|\alpha|$ of the states remain the same; only the phase changes at rate $\omega$ (as expected):

$$\exp(-iHt/\hbar)|\alpha\rangle = |e^{-i\omega t}\alpha\rangle \quad (1.90)$$

**Exercise 1.14** Show this, using Eq. (1.77).

This form-invariance under the harmonic oscillator evolution is why they are called coherent states.

### 1.3 Semiclassical quantum mechanics

Prior to the discovery of quantum mechanics by Schrödinger, Heisenberg and others, a version of the quantum theory was constructed by Bohr, Einstein and Sommerfeld using an ad hoc combination of classical mechanics of point particles and wave theory. We now know that this
approach gives a powerful insight into the quantum mechanics of states which are semiclassical in the sense that the average action for such states is large compared to Plank’s constant. We now review semiclassical approaches to quantum mechanics. However it is worth noting the reason why Einstein and others abandoned the semiclassical approach to develop a general quantum theory: they could see no way to extend it to describe classically non integrable systems. It is interesting that quantum chaos considerations were central to the development of the quantum theory.

Consider a system with one degree of freedom and energy given by

$$E = \frac{p^2}{2m} + V(x)$$  \hspace{1cm} (1.91)

Suppose we know only the energy of this system. Its motion is then defined by a phase space curve;

$$p^{(cl)}(x) = p(x; E) = \pm \sqrt{2m(E - V(x))}$$  \hspace{1cm} (1.92)

We can specify the state of this system with a classical probability distribution, $W^{(cl)}(x, E)$. We expect this distribution to be small where the velocity of the particle is large and large where the velocity of the particle is small. Thus we propose that

$$W^{(cl)}(x) = \frac{1}{2} N^2 \frac{1}{p^{(cl)}(x)}$$  \hspace{1cm} (1.93)

This distribution diverges at the turning points, $q_1, q_2$ of the classical motion. The normalisation is fixed by

$$\int_{q_1}^{q_2} dx W^{(cl)}(x; E) = 1$$  \hspace{1cm} (1.94)

which gives

$$1 = \frac{1}{2} N^2 \int_{q_1}^{q_2} \frac{dx}{p^{(cl)}(x; E)} = N^2 \frac{T}{2m} \int_0^{T/2} dt = \frac{N^2 T}{4m}$$

where $T$ is the period of the motion. Thus

$$N = 2 \left( \frac{m}{T} \right)^{1/2}$$  \hspace{1cm} (1.95)
The states of definite energy, in the position representation \( u(x) \), are given in the quantum theory as solutions of

\[
\frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} \left( E - V(x) \right) = 0 \tag{1.96}
\]

If the potential was a constant, \( V_0 \), then the solution would simply be

\[
u(x) = N \cos \left[ \frac{1}{\hbar} \int_x^{q_2} dp_0 \right] - \alpha \tag{1.97}
\]

where \( p_0 = \sqrt{2m(E - V_0)} \) and \( N, \alpha \) are integration constants. So let us try the ansatz

\[
u^{(\text{wave})} = \cos \left[ \frac{1}{\hbar} \int_x^{q_2} dx p(x; E) - \alpha \right] \tag{1.98}
\]

which satisfies the equation,

\[
\left[ \nu^{(\text{wave})} \right]' + \left\{ \left( \frac{p}{\hbar} \right)^2 - \left( \frac{p'}{\hbar} \right) \tan \left[ \frac{1}{\hbar} \int_x^{q_2} dx p(x; E) - \alpha \right] \right\} u^{(\text{wave})} = 0 \tag{1.99}
\]

If we could neglect the term in square brackets this begins to look like the Schrödinger equation. However we also need to satisfy a correspondence principle: we expect that the probability density \( |u(x)|^2 \) should be the same as the classical expression \( W^{(cl)}(x; E) \) in some limit. However this ansatz looks nothing like the classical distribution. So let us try the modified ansatz

\[
u^{(WKB)}(x) = u^{(cl)}(x) u^{(\text{wave})}(x) \tag{1.100}
\]

where

\[
u^{(cl)}(x) = \frac{N}{\sqrt{p(x; E)}} \tag{1.101}
\]

where WKB stands for Wentzel, Kramers, and Brillouin. This satisfies the equation

\[
\left[ u^{(WKB)}(x) \right]' + \left\{ \left( \frac{p}{\hbar} \right)^2 \left( \frac{1}{\sqrt{p}} \right) \right\} u^{(WKB)} = 0 \tag{1.102}
\]

The resulting probability density is

\[
W^{(WKB)} = |u^{(cl)}|^2 |u^{(\text{wave})}|^2 \tag{1.103}
\]

which begins to look a bit more like the classical distribution, apart from the oscillations. In the limit these oscillations develop a very small wavelength.
and most experiments would find it difficult to resolve such fine scale structure. We thus are led to an average over these oscillations:

\[ \tilde{W}^{(WKB)} = \frac{\mathcal{N}^2}{p(x)} \frac{1}{q_1 - q_0} \int_{q_0}^{q_1} dx \frac{1}{2} \left[ 1 + \cos \left( 2 \int_x^{q_1} dp(x) - \alpha \right) \right] \]

\[ \simeq \frac{1}{2} \frac{\mathcal{N}^2}{p(x)} = W^{(cl)}(x) \]

The range of validity of the WKB amplitude is

\[ p^2 >> \sqrt{p} \left| \frac{1}{\sqrt{p}} \right| ^{''} h^2 \]  

or

\[ \frac{h^2}{2m} \left| \frac{5}{16} (V'(x))^2 + \frac{1}{4} \frac{V''(x)}{(E - V(x))^3} \right| << 1 \]

The approximation requires slowly varying potentials...no sharp edges. In addition the approximation breaks down at the classical turning points, \( q_0, q_1 \).

We can deal with the apparent divergence at the turning points using Maslov’s method[1]. To implement this method we write the WKB amplitude more generally as a complex amplitude,

\[ \psi(x) = \frac{\psi_0}{\sqrt{|p(x)|}} \exp \left( \frac{i}{\hbar} \int_x^{q_1} p(x) dx - i\alpha \right) \]

The essential idea is that although the position amplitude may be a poor approximation in some places, the momentum amplitude may be better, and vice versa.

The momentum probability amplitude is given by

\[ \tilde{\psi}(p) = \frac{1}{\sqrt{2\pi \hbar}} \int dx \psi(x) \exp \left( \frac{i}{\hbar} xp \right) \]

\[ = \frac{\psi_0}{\sqrt{2\pi \hbar}} \int \frac{dx}{\sqrt{|p(x)|}} \exp \left[ \frac{i}{\hbar} \left( \int_x^{q_1} p(x) dx - xp \right) \right] \]

Integrals in the form

\[ I = \int dx A(x) \exp \left( \frac{i}{\hbar} \Phi(x) \right) \]

can be approximated using the method of stationary phase. The basic ideas is that as \( \hbar \to 0 \) the exponential oscillates rapidly except near those
points, \(x_s\), where the phase \(\Phi(x)\) varies least rapidly, \(\Phi'(x_s) = 0\), i.e. is stationary. Expanding around the stationary phase point we have

\[
\Phi(x) = \Phi(x_s) + \frac{(x - x_s)^2}{2\Phi''(x_s)}
\]  
(1.110)

The integral is then approximated by

\[
I \simeq A(x_s) \exp \left( \frac{i}{\hbar} \Phi(x_s) \right) \int \exp \left[ \frac{i}{\hbar} \frac{(x - x_s)^2}{2\Phi''(x_s)} \right] dx
\]

(1.111)

We may now use the result (Fresnel)

\[
\int_{-\infty}^{\infty} e^{iax^2} dx = \sqrt{\frac{\pi}{|a|}} \exp \left[ i\pi \frac{\text{sgn}(a)}{4} \right]
\]

(1.112)

Then

\[
I \simeq \sqrt{\frac{2\pi\hbar}{|\Phi''(x_s)|}} A(x_s) \exp \left[ \frac{i}{\hbar} \Phi(x_s) + \frac{i\pi}{4} \text{sgn}[\Phi''(x_s)] \right].
\]

(1.113)

If we use the phase convention \(\sqrt{i} = e^{i\pi/4}\), the integral becomes

\[
I \simeq \sqrt{\frac{2\pi i\hbar}{|\Phi''(x_s)|}} A(x_s) \exp \left[ \frac{i}{\hbar} \Phi(x_s) \right]
\]

(1.114)

The stationary phase approximation may be extended to d-dimensions,

\[
I \simeq \frac{(2\pi i\hbar)^d/2}{\sqrt{|\partial^2 \Phi/\partial x_n \partial x_m|}} A(x_s) \exp \left[ \frac{i}{\hbar} \Phi(X_s) \right]
\]

(1.115)

Using the stationary phase approximation we find the momentum amplitude is given by

\[
\tilde{\psi}(p) = \frac{\psi_0}{\sqrt{|p(x_s)p'(x_s)|}} \exp \left\{ \frac{i}{\hbar} \left[ \int_{q_1}^{x_s} p(x) dx - px_s \right] + \frac{i\pi}{4} \text{sgn}[p'(x_s)] \right\}
\]

(1.116)

Let us now try to follow the phase of the probability amplitude on a complete orbit around the trajectory in phase space. Consider the phase space orbit shown in figure (1.1)

Between points 1 and 2 the position amplitude is

\[
\psi(x) = \frac{\psi_0}{\sqrt{|p(x)|}} \exp \left[ \frac{i}{\hbar} \int_{q_1}^{x} p(x) dx \right]
\]

(1.117)
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1. Review of quantum mechanics.

Fig. 1.1. Phase portrait of a typical one-dimensional oscillator.

At point 2 we transform to the momentum representation

\[ \tilde{\psi}(p) = \psi_0 \sqrt{\frac{|x'(p)|}{p}} \exp \left\{ \frac{i}{\hbar} \left[ \int_{q_1}^{x(p)} p(x)dx - px(p) \right] - \frac{i\pi}{4} \right\} \quad (1.118) \]

Note that \( x_s \) has been written as a function \( x(p) \) to indicate that \( x_s \) is a function of \( p \). Also \( x'(p) \) is negative in the lower left quadrant. This representation is invalid where the trajectory crosses the \( p \) axis, we transform back to position space at point 3.

\[ \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dp \tilde{\psi}(p) \exp \left( \frac{i}{\hbar} px \right) \]
\[ = \frac{\psi_0}{\sqrt{2\pi\hbar}} \int dp \sqrt{\frac{|x'(p)|}{p}} \exp \left\{ \frac{i}{\hbar} \left[ \int_{q_1}^{x(p)} p(x)dx - px(p) + px \right] - \frac{i\pi}{4} \right\} \]

We now use the method of stationary phase:

\[ \Phi(p) = \frac{1}{\hbar} \left[ \int_{q_1}^{x(p)} p(x)dx - px(p) + px \right] \]
\[ \Phi'(p) = x - x(p) \]
\[ \Phi''(p) = x'(p) \]
Repeating the same steps as above we find the position probability amplitude is

$$\psi(x) = \frac{\psi_0}{\sqrt{|p(x)|}} \exp \left( i \frac{\hbar}{\hbar} \int_{q_1}^{x} p(x) dx - i \frac{\pi}{2} \right)$$  \hspace{1cm} (1.119)$$

We thus see from Eq.(1.117) that in passing through the turning point a phase shift of $\pi/2$ has occurred. In this way we see that after a complete orbit we find a phase shift of

$$\Delta \Phi = \frac{1}{\hbar} S - \frac{\nu \pi}{2}$$  \hspace{1cm} (1.120)$$

where the action on the orbit is

$$S = \oint p(x) dx$$  \hspace{1cm} (1.121)$$

and $\nu$ is called the Maslov index. If the amplitude is not to be multi valued on a complete orbit we need

$$S - \frac{\nu \pi}{2} = 2\pi n \hspace{1cm} n = 1,2,\ldots$$  \hspace{1cm} (1.122)$$

Apart from the Maslov index this is equivalent to the Bohr Sommerfeld quantisation condition of early quantum mechanics.

**Exercise 1.15** Evaluate the action on the orbit of a harmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$$  \hspace{1cm} (1.123)$$

and show that Eq.(1.122) implies the energy quantisation condition $E_n = \hbar \omega (n + 1/2)$. Note that the Maslov index is required to get the ground state energy correct.

**Exercise 1.16** In the WKB approximation show that the mean kinetic energy for a bound state $|\psi_n\rangle$ of a potential $V(x)$ is given by

$$\langle \psi_n | \hat{T} | \psi_n \rangle = \frac{1}{2} \left( n + \frac{1}{2} \right) \frac{dE_n}{dn}$$  \hspace{1cm} (1.124)$$

**Exercise 1.17** With the ansatz $\psi(x,t) = \phi(x,t)e^{iS(x,t)/\hbar}$ show that in the limit $\hbar \to 0$, $S$ obeys the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V(x) = 0$$  \hspace{1cm} (1.125)$$
1.4 Phase space quasi-probability distributions.

The description of classical mechanics as a flow of probability density on phase space is such an appealing geometric picture that many attempts have been made to find some quantum version. We will only consider two such methods; the Wigner function and the Husimi function (also called the Q-function). These methods generally go by the name of quasi-probability methods to make it clear that these are special ways to characterise quantum states in terms of phase space. In the case of the Wigner function, the resulting densities are not even positive for some quantum states! While in the case of the Husimi function, delta functions cannot occur.

1.4.1 The Wigner function.

The Wigner function, $W(x, p)$ was the first attempt to develop a phase space representation of quantum states. The function is constructed in such a way that the marginal distributions reproduce the quantum position and momentum probability distributions. The price one pays for this requirement is that the resulting Wigner functions are not necessarily positive and thus have no interpretation as true probability distributions on phase space.

The Wigner function for a quantum state $\rho$ is

$$W(x, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ipy/\hbar} \langle x - \frac{y}{2} | \rho | x + \frac{y}{2} \rangle$$  \hspace{1cm} (1.126)

**Exercise 1.18** Show that the Wigner function uniquely determines the density operator by inverting Eq.(1.126) to obtain $\langle x | \rho | x' \rangle$.

The marginal distributions of the Wigner function are given by

$$\int_{-\infty}^{\infty} dp W(x, p) = \langle x | \rho | x \rangle$$ \hspace{1cm} (1.127)

$$\int_{-\infty}^{\infty} dx W(x, p) = \langle p | \rho | p \rangle$$ \hspace{1cm} (1.128)

The average of a quantum operator is given by

$$\text{tr}(\hat{A}\rho) = \int_{-\infty}^{\infty} dxdp W(x, p) A(x, p)$$ \hspace{1cm} (1.129)

where the function $A(x, p)$ is the Wigner-Weyl symbol for the operator $\hat{A}$. The Wigner symbol of an operator is given by

$$A(x, p) = \int dy (x - \frac{y}{2}) \langle x - \frac{y}{2} | \hat{A} | x + \frac{y}{2} \rangle e^{ipy/\hbar}$$ \hspace{1cm} (1.130)
1.4 Phase space quasi-probability distributions.

We now consider taking averages in the other direction, that is forming averages over the Wigner phase space variables. If we try and form moments of the Wigner function we do not always reproduce the corresponding quantum average. In fact the Wigner function moments correspond to quantum averages of symmetrically ordered operator products. This is called the Wigner-Weyl correspondence.

A little reflection shows that the Wigner function may be written as the Fourier transform of a characteristic function,

$$W(x, p) = \frac{1}{(2\pi \hbar)^2} \int dy \int dk e^{i(py - kx)/\hbar} \text{tr}(\rho e^{i(k\hat{x} - \hat{p} y)/\hbar})$$

(1.131)

where the Wigner characteristic function is

$$\chi^w(y, k) = \text{tr}(\rho e^{i(k\hat{x} - \hat{p} y)/\hbar})$$

(1.132)

The characteristic function of a probability distribution is used as a moment generating function. In this case the characteristic function generates the symmetrically ordered averages as

$$\text{tr}(\rho (\hat{x}^n \hat{p}^m)_s) = \frac{\partial^{n+m}}{\partial k^n \partial y^m} \chi^w(y, k)|_{y=k=0}$$

(1.133)

where \((ab)_s\) means the symmetrically ordered product. Thus we find

$$\text{tr}(\rho (\hat{x}^n \hat{p}^m)_s) = \int_{-\infty}^{\infty} dx dp W(x, p) x^n p^m$$

(1.134)

The fact that the moments of the Wigner function do not directly give the quantum averages, but must be augmented by an operator ordering rule is a typical feature of quasi probability distributions.

**Exercise 1.19** Calculate the Wigner function for an energy eigenstate of a simple harmonic oscillator. Show that for certain energies it may be negative.

The Wigner function itself does not have a physical interpretation, but the square of the Wigner does[3].

The Wigner function inherits an evolution equation from the Schrödinger equation. The result is

$$\frac{\partial W}{\partial t} = \{H^{(cl)}, W\}_PB + \sum_{n \geq 1} \frac{\hbar(-1)^n}{2^{2n}(2n + 1)!} \partial_x^{2n+1} V(x) \partial_p^{2n+1} W(x, p)$$

(1.135)

The first term is the classical Liouville equation and \(H^{(cl)}\) is just the classical Hamiltonian function. Note that if the potential is no more than a
quadratic function of position, the Wigner function equation corresponds to the classical Liouville equation. In all other cases the Wigner function dynamics can be very different. Under some circumstances however the higher order derivatives may be neglected at least for short times. Unfortunately these circumstances certainly do not include classical chaotic systems. We shall return to this point in part B.

**Exercise 1.20** Derive the Wigner function evolution equation for the anharmonic oscillator

\[ H = \frac{p^2}{2m} + ax^2 + bx^4 \]  

(1.136)

1.4.2 The Husimi function.

In elementary introductions to quantum mechanics, the probability distribution for the measured values of a physical quantity, such as position, are given by a projection valued measure

\[ P(q) dq = \text{tr}(\rho |q\rangle \langle q| dq) \]  

(1.137)

It turns out that this is a special case. More generally we need measurements described by positive operator valued measures \( \hat{E}(q) \) such that

\[ P(q) dq = \text{tr}(\rho \hat{E}(q) dq) \]  

(1.138)

It is possible to define a positive operator valued measure which corresponds to the simultaneous measurement of position and momentum. The statistics are of course given by a true probability density on phase space. However the moments of this distribution do not directly give the quantum averages. An extra rule needs to be supplied which essentially adds to the moments a small amount of noise which arises from the attempt to measure position and momentum simultaneously.

The model of Arthurs and Kelly consists of two meters which are allowed to interact instantaneously with the system. The interaction couples one of the meters to position and the other to momentum, encoding the results of the measurement in the final states of the meters. Projective measurements are then made on each of the meter states separately. These measurements can be done simultaneously as the position and momentum operators for distinct meters commute. For appropriate meter states this measurement forces the conditional state of the system into a Gaussian state. We assume some appropriate length scale such that the positions and momenta are dimensionless, and satisfy \( [\hat{X}, \hat{P}] = i \).

The appropriate unitary interaction is

\[ \hat{U} = \exp \left[ -i \left( \hat{X} \hat{P}_1 + \hat{P} \hat{P}_2 \right) \right]. \]  

(1.139)
Here the subscripts refer to the two detectors, initially in minimum uncertainty states $|d_1\rangle$ and $|d_2\rangle$ respectively. In the position representation these are

$$\langle x_j|d_j\rangle = (\pi\Delta_j^2)^{-\frac{1}{4}} \exp \left(-\frac{x_j^2}{2\Delta_j^2}\right)$$

where $\Delta_1$ and $\Delta_2$ quantify the position dispersion in each of the meters. For simplicity we will assume that the length scale has been chosen so that $\Delta_1 = \Delta_2 = 1$. This gives equal variances for position and momentum of $1/2$.

After the interaction, the detectors are measured in the position basis. The measurement result is thus the pair of numbers $(X_1, X_2)$. Following the theory given above, the measurement operator for this result is

$$\hat{M}(x_1, x_2) = \langle x_1|\langle x_2|\hat{U}|d_2\rangle|d_1\rangle$$

With a little effort it is possible to show that $\hat{M}(x_1, x_2)$ is proportional to a projection operator:

$$\hat{M}(x_1, x_2) = \frac{1}{\sqrt{2\pi}}|\langle x_1, x_2 \rangle|.$$  \hspace{1cm} (1.142)

Here the state $|x_1, x_2\rangle$ is a Gaussian minimum uncertainty state with a position probability amplitude distribution

$$\langle x|\langle x_1, x_2 \rangle = (\pi)^{-1/4} \exp \left[i xx_2 - \frac{1}{2} (x - x_1)^2\right]$$

This is a state with mean position and momentum given by $x_1$ and $x_2$ respectively, and with the variances in position and momentum equal to $1/2$.

**Exercise 1.21** Verify Eq.(1.142).

The corresponding probability density for the observed values, $(x_1, x_2)$, is found from the effect density

$$\hat{E}(x_1, x_2)dx_1dx_2 = \frac{1}{2\pi}|\langle x_1, x_2 \rangle|dx_1dx_2.$$  \hspace{1cm} (1.144)

**Exercise 1.22** Show that

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \hat{E}(x_1, x_2) = 1$$

From this positive operator valued measure (POM) we can show that

$$E[X_1] = \langle \hat{X} \rangle, \quad E[X_1^2] = \langle \hat{X}^2 \rangle + \frac{1}{2},$$

$$E[X_2] = \langle \hat{P} \rangle, \quad E[X_2^2] = \langle \hat{P}^2 \rangle + \frac{1}{2}.$$  \hspace{1cm} (1.146)
where $\langle \hat{A} \rangle = \text{Tr}[\hat{A}\rho]$ is the quantum expectation, while $E$ is a classical average computed by an integral over the probability density, $\varphi(x_1,x_2)$. Thus the readout variables $X_1$ and $X_2$ give, respectively, the position and momentum of the system with additional noise.

It is more conventional to denote the state $|(x_1,x_2)\rangle$ by $|\alpha\rangle$, where the single complex parameter, $\alpha$, is given by $\alpha = (x_1 + ix_2)/\sqrt{2}$. In this form the states are known as coherent states. The corresponding effect density is $F(\alpha) = |\alpha\rangle\langle\alpha|/\pi$ and the resulting probability density $\varphi(\alpha)d^2\alpha = \text{Tr}\left[F(\alpha)\rho\right] d^2\alpha$. This is known as the $Q$-function in quantum optics. For different initial pure states for the detectors, the more general probability density for observed results is known as the Husimi function.

**Exercise.**
Prove that the Husimi function is positive and bounded and thus delta function Husimi functions are not possible.

**Exercise.**
Prove that the Husimi function uniquely determines the density operator, and find the inversion formula.

**Exercise.**
Find the characteristic function (the Fourier transform) for the $Q$ function and express it as an average of a characteristic operator.

**Exercise.**
Prove that there are physical states for which the Husimi function has zeros.

The Husimi function inherits a dynamics from the Schrödinger equation in a similar fashion to the Wigner dynamics. As for the Wigner function, the evolution equation may be a partial differential equation with infinitely many derivatives. Even if the equation truncates to only second order derivatives it does not take the form of a legitimate Probability density evolution equation. See G.J. Milburn, “Quantum and classical Liouville mechanics of the anharmonic oscillator”, Phys.Rev. A 33, 674-685, (1986).

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*In fact apart from two constants, the $Q$ function is uniquely determined by its zeros. This is a consequence of the Wierstrass theorem for entire analytic functions of order two.*
2
Atoms in optical potentials

The material in this and the next chapter is adapted from the PhD thesis of Dr S. Dyrting.

We will be concerned with a particular type of interaction between light and matter: the resonant interaction of laser light with neutral atoms. The atom is neutral, so there is no net force associated with a charge. The interaction is due to the effective dipole moment arising from the spatial distribution of electrons and protons within the atom. Even though the dipole moment is a well defined classical quantity the resonant interaction between light and atoms is an inherently quantum mechanical effect because the internal energy of the atom can only take on certain well defined values. The resonant interaction is particularly strong because it is inversely proportional to the frequency difference between the light and the atomic transition. To investigate the resonant interaction of light with neutral atoms one needs a source of light with a well defined frequency and a reasonable intensity. This light is produced by lasers.

Light carries energy, linear momentum, and angular momentum. These properties of electromagnetic radiation are not measured directly but are inferred from its interaction with matter. If spectroscopy can be thought of as the study of the energy transferred from light to the atom then atom optics is the natural extension of spectroscopy to include the transfer of linear and angular momentum. Linear momentum is transferred to the atom by virtue of the fact that in general the intensity of light will change depending on the atom’s position. The spatial properties of laser light can be one of two forms. First there is the spatial change of the beam in the direction of beam propagation. This change occurs over distances of the order of an optical wavelength. Then there is also the transverse profile of the laser beam which is determined by the mode of the laser.
cavity that is excited. It is not our purpose to investigate the effect of the transverse variation of the field.

The laser beam is not the only mode of the radiation field that the atom interacts with. Light can be scattered into a vacuum mode by the process of spontaneous emission. There are an infinite number of vacuum modes into which the light can be scattered, with only a very small probability of the quanta being reabsorbed. Therefore spontaneous emission can be treated as a stochastic process using a density operator to represent the quantum mechanical and statistical state of the atom. The effect of spontaneous emission is to damp the excited state of the atom and to give random kicks to its center-of-mass momentum. More importantly for our investigation of the quantum dynamics of a two-level atom, spontaneous emission disrupts the coherent evolution embodied by Schrödinger’s equation.

The strength of the interaction between light and the electronic dipole is conveniently quantified by the Rabi frequency, the average interaction energy, divided by Planck’s constant. It is proportional to the dipole moment of the transition and the electric field strength at the atom. The most common way of reducing the effect of spontaneous emission is to tune the frequency of the laser so that the difference between the laser and the atomic transition frequency $\Delta = \omega_L - \omega_0$ is large compared to the Rabi frequency $\Omega$. When the atom is excited by the electric field it makes a virtual transition to a higher energy state and is then de-excited back to the ground state after a time $\delta t$. From the energy-time uncertainty relation the time spent in the virtual state is of the order $\delta \tau \approx 1/\Delta$. Thus if $\Delta$ is large the atom will probably make a stimulated transition before it has time to spontaneously emit.

Although the combined scattering process has had no effect on the internal state of the atom it can affect the center-of-mass momentum. The longitudinal periodicity of the laser field means that the momentum of the atom changes by units of $\hbar k$ every time it makes a coherent transition between its internal states. Imagine that the atom is initially in the ground state with momentum $p$ and after being excited it absorbs a unit of momentum $\hbar k$. If the atom re-emits a quanta of momentum $\hbar k$ then the net change in momentum is zero. But if the atom emits a momentum $-\hbar k$ then the net change in momentum is $2\hbar k$. In this chapter we will spend some time developing the equations of motion, and discussing their method of solution.

### 2.1 The dynamics for large detunings

In this section we outline the derivation of the evolution equation in the limit of large detuning. The center-of-mass dynamics of the atom along
the axis defined by the laser beam can be described in terms of the position and momentum operators $\hat{x}$ and $\hat{p}_x$. Although the atom has many electronic energy levels we will assume that the atom can be approximated by a two-state system. This is not as crazy as it sounds: because the light has a well defined frequency only a relatively small number of levels are involved in the interaction. If we use linearly or circularly polarized light tuned to a transition where the ground state angular momentum is $j_a = 0$ and the excited states angular momentum is $j_b = 1$ then the atom can only make transitions between two Zeeman sublevels. In this way we can restrict our description to the two states that are resonant with the light and which obey the magnetic quantum number selection rules $\Delta m = 0$ for linearly polarized light and $\Delta m = \pm 1$ for circularly polarized light. Let $|a\rangle$ and $|b\rangle$ denote the ground and the excited states. Then the internal dynamics can be described by internal population inversion operator $\hat{\sigma}_3 = |b\rangle\langle b| - |a\rangle\langle a|$, and the internal lowering operator $\hat{\sigma} = |a\rangle\langle b|$. The coherent coupling between the internal and center-of-mass variables is through the position dependent Rabi frequency $\Omega(\hat{x}) = \frac{d \cdot E(x)}{\hbar}$ where $d$ is the dipole matrix element for the internal states $E(x)$ is the classical electric field vector at position $x$ and $\cdot$ the scalar product of two vectors. We can write the Rabi frequency in the general form

$$\Omega(x) = \Omega f(kx, t). \quad (2.1)$$

$k = c/\omega_L$ is called the wavenumber and $\omega_L$ is the frequency of the laser. $\Omega$ is a measure of the intensity of the field and without loss of generality it can be chosen to be real. The function $f(s, \tau)$ describes the spatial variation of the Rabi frequency. The symbol $\tau$ is meant to remind us that this function can be explicitly time-dependent. For example, the light produced by a single continuous laser is called a traveling wave and in this case $f(s, \tau) = e^{is}$.

The mode function for two counter propagating traveling waves is

$$f(s, \tau) = \sin(s). \quad (2.2)$$

If the detuning is large enough the spontaneous emission may be ignored and we obtain the equations for a two-level atom coherently interacting with a far-off-resonance laser. To see this consider the hamiltonian for the simpler case of a two level atom, with resonant frequency $\omega_0$ interacting with a laser field at frequency $\omega_L$:

$$H = \hbar \frac{\omega_0}{2} \hat{\sigma}_3 + (\hat{\sigma} \Omega e^{-i\omega_L t} + \hat{\sigma}^\dagger \Omega^* e^{-i\omega_L t}) \quad (2.3)$$

We now transform to the interaction picture by the unitary transformation

$$U_0(t) = \exp[-i\omega_0 t/2]$$

$$U_0(t) = \exp[-i\omega_0 t/2] \quad (2.4)$$
The interaction Hamiltonian is then given by the time dependent form
\[ H_I(t) = \hat{\sigma} \Omega(x) e^{-i\Delta t} + \hat{\sigma}^\dagger \Omega(x)^* e^{-i\Delta t} \tag{2.5} \]
where the detuning is given by \( \Delta = \omega_L - \omega_0 \). The corresponding unitary operator for the dynamics in the interaction picture is then given by the series
\[ U_I(t) = 1 + \left( \frac{-i}{\hbar} \right) \int_0^t dt_1 H_I(t_1) + \left( \frac{-i}{\hbar} \right)^2 \int_0^t dt_1 \int_0^{t_2} dt_1 H_I(t_2) H_I(t_1) + \ldots \tag{2.6} \]
If we now assume that we are only interested in times such that \( \Delta t \gg 1 \), we may approximate this equation as
\[ U_I(t) \simeq 1 + \left( \frac{-i}{\hbar} \right) \frac{|\Omega(x)|^2}{2\Delta} \hat{\sigma}_3 \tag{2.7} \]
which arises from an effective Hamiltonian of the form
\[ H_{\text{eff}} = \frac{|\Omega(x)|^2}{2\Delta} \hat{\sigma}_3 \tag{2.8} \]
From this we see that if the atom starts in the ground state it will stay there (as \( |a\rangle \) is the \(-1\) eigenstate of \( \hat{\sigma}_3 \)). This is only an approximation and there is a finite probability that the atom will be excited from the ground state. If that happened then there is a chance that the atom would spontaneously emit and recoil in a random direction. Fortunately the probability of this happening scales as \( \gamma/\Delta^2 \) where \( \gamma \) is the spontaneous emission rate. Thus for large enough detuning spontaneous emission this can be neglected, and the atom stays in the ground state.

We want to look at time dependent Rabi frequencies because then the classical motion is non-integrable. We can achieve this if the Rabi frequency is time dependent and periodic, but with a period that is small compared to \( \Delta^{-1} \). In that case we can simply substitute the time dependent rabi frequency directly into Eq.(2.8) The two cases we will examine will be periodic in time with a driving frequency \( \omega \) and are the standing wave with modulated intensity
\[ f(s, \tau) = \left[ 1 - 2\epsilon \cos(\omega \tau) \right] \sin(s), \tag{2.9} \]
and the standing wave with oscillating nodes
\[ f(s, \tau) = \sin [s - \lambda \sin(\omega \tau)/2]. \tag{2.10} \]
Following Ref. [7] we introduce the dimensionless variables for convenience: \( \hat{\kappa} = \frac{\hbar k_x^2}{m\omega}, \ \kappa = \frac{\hbar k_x^2 \Omega^2}{2m\omega^2}, \ t = \omega \tau, \ q = 2kx, \text{ and } p = \frac{2kp_x}{m\omega}. \) The operators \( \hat{q} \) and \( \hat{p} \) satisfy the commutation relation
\[ [\hat{q}, \hat{p}] = i\hat{\kappa}. \tag{2.11} \]
In other words $\kappa$ plays the role of a dimensionless Planck’s constant and $\hat{q}$ and $\hat{p}$ are the rescaled position and momentum. The center-of-mass observables are fully described by the total density operator

$$\hat{\rho} = \hat{\rho}_a + \hat{\rho}_b. \tag{2.12}$$

In the limit of large detuning and without spontaneous emission the internal states are constants of the motion as discussed above. Recall that the detuning is $\Delta = \omega_L - \omega_0$. This can be negative (red detuning) or positive (blue detuning). We will assume red detuning here. The light field induces a shift in the energy of the internal states

$$V(\hat{q}, t) = \pm 2\kappa f(\hat{q}/2, t)\dagger f(\hat{q}/2, t). \tag{2.13}$$

where $+$ is for atoms in the ground state and $-$ is for atoms in the excited state. To the center-of-mass dynamics this light shift acts like an optical potential: the ground state $|a\rangle$ moves in a potential $+V(\hat{q}, t)$, and the excited state $|b\rangle$ moves in the potential $-V(\hat{q}, t)$. Notice that for standing waves the optical potential is $2\pi$-periodic. This implies that the Hamiltonian operators $\hat{H}_a$ and $\hat{H}_b$ commute with $\hat{S}_{2\pi} = \exp (2\pi i \hat{p}/\kappa)$, the generator of $2\pi$-translations in $q$:

$$[\hat{H}_a, \hat{S}_{2\pi}] = [\hat{H}_b, \hat{S}_{2\pi}] = 0. \tag{2.14}$$

### 2.2 Integrating the classical equations

If the atom is initially in its ground state $|a\rangle$ and if we ignore spontaneous emission and set $\gamma = 0$ then the center-of-mass motion will be conservative. The total center-of-mass density operator has a dynamics generated by the hermitian operator $\hat{H}_a$. The motion of the atom is the quantization of the motion of the classical quantities $q$ and $p$ given by the classical Hamiltonian

$$H = \frac{p^2}{2} + V(q, t), \tag{2.15}$$

through Hamilton’s equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = p, \tag{2.16}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\frac{\partial}{\partial q}V(q, t). \tag{2.17}$$
Here $V(q,t)$ is the optical potential which in this thesis will take one of the following forms

$$
V(q,t) = \begin{cases} 
2\kappa \sin^2(q/2), & \text{stationary standing wave} \\
2\kappa (1 - 2\epsilon \cos t) \sin^2(q/2), & \text{modulated intensity} \\
2\kappa \sin^2[(q - \lambda \sin t)/2], & \text{oscillating nodes}.
\end{cases}
$$

Of particular importance for us will be the property that for different choices of $f(q,t)$ and the parameters $\epsilon$ and $\lambda$ the solutions of these equations will be integrable, near-integrable or globally chaotic. Throughout this thesis we will examine the classical motion of the atom and then see how this motion is altered when the center-of-mass variables $q$ and $p$ are quantized and when spontaneous emission is included. Except for the case of the stationary standing wave we cannot solve Hamilton’s equations exactly. Because the classical equations can show a range of behavior from regular to chaotic we must use a numerical integration routine that is robust enough to handle all of these situations efficiently. Both of the routines we will use are fourth order in the incremental time step $\delta t$. The first is the fourth order Runge-Kutta method and the second is a fourth-order symplectic integrator.

For our Runge-Kutta routines we consulted the excellent book *Numerical Recipes* by Press, Teukolsky, Vetterling and Flannery [8]. This routine was initially used because of its stability and because faster integrators like the Bulirsch-Stoer routine based on Richardson extrapolation could not handle the nonlinear equations (2.16) and (2.17). The Runge-Kutta routine is so well known that we simply refer the reader to [8] for further details. Most of the classical numerical calculations we have done will use this method. The powerful method of symplectic integrators can also be used if the Hamiltonian structure of the equations of motion needs to be preserved.

Hamiltonian evolution represents a very special class of transformations of phase space onto itself: it preserves the Poisson bracket. Let $f(q,p)$ and $g(q,p)$ be two functions from phase space to the set of real numbers, then the Poisson bracket of $f$ and $g$ is

$$
\{f,g\}_{q,p} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}.
$$

If $q$ and $p$ are regarded as functions on phase space then they satisfy the fundamental Poisson bracket relation

$$
\{q,p\}_{q,p} = 1.
$$

The Poisson bracket can be given a deeper significance in differential geometry where it is thought of as a symplectic 2-form. Therefore we say
that Hamiltonian dynamics preserves the symplectic structure of phase space. It is acknowledged that symplectic were first discovered by the mathematician René de Vogalaère in the 1950’s. He had the idea of using numerical integrators that explicitly preserved the symplectic nature of Hamilton’s equations. Unfortunately he failed to get his ideas accepted for publication. It was not until the 1980’s that they resurfaced again when people who designed particle accelerators wanted to numerically track the evolution of a cloud of particles in a storage ring. To test the long term stability of the dynamics the particles must be tracked over millions of cycles, and any numerical errors may cause the system to be unstable or at least unphysical. One answer is to make the time increment $\delta t$ small enough, but this can lead to programs that take a prohibitively long time to run.

The crucial observation made by Ruth in 1983 [9] was that Hamiltonian evolution preserves the Poisson bracket relation

$$\{q(t), p(t)\}_{q,p} = 1 ,$$  \hspace{1cm} (2.21)

but the fourth order Runge-Kutta method only preserves it up to fourth order in $\delta t$. As a result Runge-Kutta routines can give unphysical behavior such as a spurious gain or loss in energy of the system. Ruth [9] wanted to find integrators that were explicit and which intrinsically preserved the Poisson bracket relation. Since this rediscovery of symplectic integrators people have used Lie algebra techniques to construct efficient high order routines. The routine which we used for some of our calculations was proposed by Forest and Berz [10]. The routine they gave was for time independent systems but we have changed it to include time dependent systems using the extended phase space technique. The mapping $T$ from $(q(t), p(t))$ to $(q(t + \delta t), p(t + \delta t))$ is given by the composition

$$T = M_1(s_1) \circ M_2(d_1) \circ M_1(s_2) \circ M_2(d_2) \circ M_1(s_2) \circ M_2(d_1) \circ M_1(s_1) ,$$  \hspace{1cm} (2.22)

where $M_1(s)$ and $M_2(d)$ are the following elementary maps on $(q, p, t)$

$$\begin{align*}
(q, p, t) & \xrightarrow{M_1(s)} (\bar{q}, \bar{p}, \bar{t}) , \\
\bar{q} & = q + ps , \\
\bar{p} & = p , \\
\bar{t} & = t + s ,
\end{align*}$$  \hspace{1cm} (2.23 - 2.26)

$$\begin{align*}
(q, p, t) & \xrightarrow{M_2(d)} (\bar{q}, \bar{p}, \bar{t}) , \\
\bar{q} & = q , \\
\bar{p} & = p - d \frac{\partial}{\partial q} V(q, t) , \\
\bar{t} & = t ,
\end{align*}$$  \hspace{1cm} (2.27 - 2.30)
and $s_i$ and $d_i$ are given by

\begin{align*}
    s_1 &= \frac{\delta t}{2(2 - \beta)}, \\
    s_2 &= \frac{(1 - \beta)\delta t}{2(2 - \beta)}, \\
    d_1 &= \frac{\delta t}{2 - \beta}, \\
    d_2 &= -\frac{\beta\delta t}{2 - \beta}, \\
    \beta &= \sqrt{2}.
\end{align*}

(2.31) \quad (2.32) \quad (2.33) \quad (2.34) \quad (2.35)

This routine is just as efficient as fourth order Runge-Kutta but is much more stable.

### 2.3 Integrating the quantum equations

Our first step in investigating the quantum mechanical motion of the atom will be to see how the coherent dynamics changes after quantization. If the atom starts in its ground state and if the pumping process can be neglected then the motion of the atom will be entirely coherent. It then follows that if the density operator is initially in a pure state $\hat{\rho}(0) = |\psi(0)\rangle\langle\psi(0)|$ then it will always remain in a pure state $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$ and the state $|\psi(t)\rangle$ evolves according to Schrödinger’s equation

\[ i\hbar \frac{d}{dt} |\psi\rangle = \hat{H}_a |\psi\rangle. \]

(2.36)

In this section I will describe how Schrödinger’s equation was solved numerically. It is traditional to approach the Schrödinger equation from the position representation. For the simplest case of motion in a stationary standing wave this has the rather forbidding form

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2} \frac{\partial^2 \psi}{\partial q^2} + 2\kappa \sin^2(q/2)\psi. \]

(2.37)

To integrate such a differential equation one would usually use a routine that would approximate the partial derivative with respect to position by a difference quotient and then treat the resulting differential-difference equation as a single vector differential equation. From a numerical and physical point of view this is not a good way to solve this problem. As has already been explained the elementary process by which light acts on the atom is through quantized momentum exchanges with the classical light field. Therefore we have more physical insight when we write
2.3 Integrating the quantum equations

Schrödinger’s equation in the momentum representation:

\[ i\hbar \frac{\partial}{\partial t} \psi(p) = \frac{p^2}{2} \psi(p) + a(t)\psi(p + \hbar) + 2\kappa a(t)^*\psi(p - \hbar). \] (2.38)

In Eq. (2.38) I have dropped the c-number terms from the Hamiltonian operator. The function \(a(t)\) is the time-dependent amplitude for the atom to absorb a quanta of momentum from the classical field and it depends on which type of standing wave the atom is in. For the three types we will consider it is given by

\[
a(t) = \begin{cases} 
\kappa, & \text{stationary standing wave} \\
\kappa (1 - 2\epsilon \cos t), & \text{modulated intensity} \\
\kappa \exp (i\lambda \sin t), & \text{oscillating nodes}.
\end{cases}
\] (2.39)

Notice that the complex amplitude \(\psi(p)\) is only coupled to \(\psi(p + m\hbar)\) for \(m\) an integer. This means that the field equation can be exactly represented by a continuum of ordinary differential equations labeled by a momentum variable \(p\) which varies continuously in the interval \([−\hbar/2, \hbar/2]\). This reflects the energy band structure arising from the translational symmetry of the atom-light interaction. In practice, for bounded motion the bands are so narrow that at most two values will be needed in our calculations: \(p = 0\) and \(p = −\hbar/2\). Note also that in practice the infinite vector \(\psi(p + m\hbar)\) is truncated for \(|m| < M\). In all our examples KAM curves bound the classical chaotic dynamics to a region \(|p| < p_{\text{max}}\) and so \(M\) is chosen so that \(\hbar M > p_{\text{max}}\). For the coherent dynamics these equations were integrated using a multi-variable Bulirsch-Stoer method which gives high accuracy combined with excellent speed and stability.

In some sections of this work we will diagonalize the stationary Hamiltonian operator for the nonlinear pendulum and the Floquet operator for the driven pendulum. The stationary Hamiltonian is real-symmetric in the momentum representation and so was diagonalized using a NAG routine for real-symmetric matrices. Using the time-reversal and parity symmetries one can show that the Floquet operator for the case of a modulated intensity is symmetric and its eigenstates real in the momentum representation. This property was useful in diagonalizing the Floquet operator.

In the following lectures the atom is initially in a pure state. It starts off in the ground state, \(a\), with a center-of-mass wavefunction in the momentum representation

\[
\langle p|\psi(0)\rangle = (2\pi\delta)^{-1/4} \exp \left[ \frac{(p - p_0)^2}{4\delta} - iq_0 \frac{p}{\hbar} \right].
\] (2.40)

This is a minimum uncertainty state with means \(\langle \hat{p} \rangle = p_0, \langle \hat{q} \rangle = q_0\) and a momentum variance of \(\delta\). Using pure states has the advantage that in
our simulations we only have to track a single center-of-mass state. In order to take account of the band structure our calculations have been done in the momentum representation with momentum separated by $\hbar/2$, half the width of the Brillouin zone.
Before we examine the motion of the two level atom when the optical potential is time-dependent we will see what happens when the light field is the usual stationary standing wave. For the case of arbitrary detuning the center-of-mass and internal dynamics of the atom become entangled in a very complicated way, so that one must usually make approximations when treating it theoretically. The large-detuning condition is sufficiently weak that we still retain important features of the interaction between the center-of-mass and internal states.

Our study of the stationary standing wave in this chapter will serve several purposes. In the previous chapter we derived the general equations of motion together with a summary of their numerical solution. In this chapter we will introduce some of the analytic techniques which can be brought to bear on the classical and quantum motion, techniques which will be built upon in subsequent chapters. The general theme of this chapter will be regular as opposed to chaotic dynamics of the atom. But regular does not mean boring. There are some surprising features in the quantum motion of the atom where the corresponding classical motion is regular but nonlinear.

In the first section of this chapter we will study the classical coherent motion of the atom and introduce the basic ideas of nonlinearity, integrability and Louville dynamics in phase space. In the second section we will study the coherent quantum dynamics and start off by discussing the important changes in our understanding as exemplified by the eigenstates and eigenvalues of the Hamiltonian operator. This discussion will then flow over to our review of the WKB approximation. Both of these topics can be seen as discussions on the meaning of integrability in quantum mechanics. We will then go on to explain the meaning of quantum nonlinearity and to show how it causes the classical and quantum mechanical dynamics to be very different.
3 Regular Motion

3.1 Regular classical motion

3.1.1 phase space

The stationary standing wave has a sinusoidal mode function and in the limit of large detuning the optical potential is \( V(q,t) = 2\kappa \sin^2(\frac{q}{2}) \). Notice that the strength of the potential is proportional to \( \Omega^2 \) but inversely proportional to \( \Delta \), so that when experiments are performed in the limit of large detuning the laser intensity is usually very high. The time scale of the motion when the atom is bound in the light potential well is determined by the frequency parameter \( \sqrt{\kappa} \). Another important frequency variable is \( \eta \), the rate of incoherent stimulated transitions of the atom from the ground to the excited state. If we use the typical parameters \( \kappa \sim 1, \eta \sim 10^{-3} \) then we can estimate their relative size,

\[
\frac{\sqrt{\kappa}}{\eta} \sim 10^3 \gg 1, \tag{3.1}
\]

so that a ground state atom will undergo many periods of oscillation in the cosine potential before making an incoherent transition. Therefore, for times \( t < 1/\eta \) the dynamics is effectively coherent. In the classical approximation to the dynamics we replace the position and momentum operators \( \hat{q} \) and \( \hat{p} \) by c-number variables \( q \) and \( p \) and assume that the state of the atom evolves according to the Hamiltonian for a classical point particle in a real potential \( V(q,t) = 2\kappa \sin^2(\frac{q}{2}) \). Its essential features are that it is \( 2\pi \)-periodic in \( q \) and is zero at the standing wave nodes and maximum at the anti-nodes. The maximum energy of the bounded motion is \( V_{\text{max}} = 2\kappa \). Dropping constant terms, which corresponds to shifting the zero point of the total energy, the Hamiltonian becomes

\[
H = \frac{p^2}{2} - \kappa \cos q. \tag{3.2}
\]

The Hamiltonian for an atom in a standing wave looks just like the Hamiltonian for a nonlinear pendulum, but there is one important difference between the motion of the atom and the dynamics of a pendulum: For a pendulum \( q \) would correspond to the angle made by the bob with respect to the vertical and is thus restricted to the interval \( q \in [0, 2\pi] \), but for an atom \( q \) may take on values over the entire real line. Of course these two models are equivalent if the atom is bound around the potential minimum, and in general the motion of the atom can be mapped into the pendulum via the transformation \( q \rightarrow q \mod 2\pi \). This is not a canonical transformation but rather a mapping from the phase space of the atom (the plane) to the phase space of the pendulum (the cylinder). Under this transformation of phase space \( p \) becomes the angular momentum of the pendulum. This equivalence only holds for the classical approximation.
When the quantum mechanical motion is taken into account we shall see that the atom is not equivalent to the quantum pendulum.

For the time being imagine that somehow we were able to initially localize the atom at a well defined position and momentum. The atom would then follow a trajectory in phase space given by a solution to Hamilton’s equations, as discussed in the previous chapter. In Fig. 3.1 we show a series of trajectories for different initial conditions. The starting point for each trajectory has been marked with a cross. Notice that the trajectory of the atom follows a one dimensional curve in phase space. This means that there is a constant of the motion which is constraining the dynamics. This of course is just the total energy

\[ E = \frac{p^2}{2} - \kappa \cos q \, . \]  

But the existence of conserved quantities is more significant than just this. If a Hamiltonian system has as many independent conserved quantities as it has co-ordinates the motion is exactly solvable by quadratures and for the case of periodic motion there is a continuous map from the old variables to canonical variables which parameterize a torus. These new variables are called action-angle variables. These systems are said to be integrable or regular.

### 3.1.2 action and angle variables

A classical Hamiltonian system is said to be periodic if \( q \) and \( p \) are both periodic functions of time (libration) or if \( p \) is a periodic function of \( q \) (rotation), which is certainly the case for the classical motion of an atom in a stationary standing wave where \( p = \pm \sqrt{2(E + \kappa \cos q)} \). For the case of the nonlinear pendulum the Hamiltonian is trivially separable. This means that one can define a canonical transformation to new position and momentum variables \( \bar{q} \) and \( \bar{p} \) such that the new Hamiltonian \( \bar{H} \) is just \( \bar{H} = g(\bar{p}) \), where \( g(\bar{p}) \) is any function of \( \bar{p} \) we would like to choose. This transformation is defined in terms of a generating function \( S(q, \bar{p}) \) as follows

\[ p = \frac{\partial S}{\partial q} \, , \]  

\[ \bar{q} = \frac{\partial S}{\partial \bar{p}} \, . \]  

If the transformation function is not explicitly time-dependent then the new Hamiltonian at the new co-ordinates is equal to the old Hamiltonian at the old co-ordinates. \( S(q, \bar{p}) \) is found by substituting for \( p \) using
Eq. (3.4) and using the fact that we want the new Hamiltonian to have a particular form. We then find that $S(q, \bar{p})$ satisfies
\[
\frac{1}{2} \left( \frac{\partial S}{\partial q} \right)^2 - \kappa \cos q = g(\bar{p}) .
\] (3.6)

Because the new Hamiltonian is a function of $\bar{p}$ only it follows from Hamilton’s equations that $\bar{p}$ is a constant of the motion, and that the rate of change of $\bar{q}$ with time is just
\[
\frac{d\bar{q}}{dt} = \frac{dg}{d\bar{p}} .
\] (3.7)

If $T$ is the period of the classical motion then the change in $\bar{q}$ over one period is
\[
\Delta \bar{q} = \frac{dg}{d\bar{p}} T .
\] (3.8)

Now the trick in mapping to action-angle variables is to choose $g$ so that the change in the new position over one period is just equal to $2\pi$, then $dg/d\bar{p}$ will be the frequency of the nonlinear motion. We can also calculate the change in the new position co-ordinate by integrating over the old
3.1 Regular classical motion

The symbol $\oint$ denotes a line integral taken over the trajectory traced out over one period $T$. It follows from this equation that the new momentum is just

$$\vec{p} = \frac{1}{2\pi} \oint \frac{\partial S}{\partial q} dq,$$

which is called the action integral. The action is significant because it is an adiabatic constant of the motion: If a time-dependent Hamiltonian is slowly varying then the action will be approximately conserved. Since $\vec{q}$ changes by $2\pi$ every period it is called the angle variable. Because of the importance of the action and angle variables they are usually given the special symbols $J$ and $\Theta$ respectively. The transformation to action-angle variables is given by the two integrals

$$J(E) = \frac{1}{2\pi} \oint p(E, q) dq,$$

$$\Theta(q, E) = \left(\frac{dJ}{dE}\right)^{-1} \int_0^q \frac{dp}{dE} dq,$$

which for the nonlinear pendulum can be evaluated in terms of elliptic integrals [11] and are found to be

$$J = \sqrt{\frac{8}{\kappa}} \pi \left\{ \begin{array}{l} E(N) - (1 - N^2)K(N), \quad N < 1 \\ \frac{1}{4N}E(N^{-1}), \quad N > 1 \end{array} \right.$$

$$\Theta = \frac{\pi}{2} \left\{ \begin{array}{l} K^{-1}F(\zeta, N), \quad N < 1 \\ 2K(N^{-1})^{-1}F(q/2, N^{-1}), \quad N > 1 \end{array} \right.$$

Here $2N^2 = 1 + E/\kappa$, $N \sin \zeta = \sin(q/2)$. $E$ and $K$ are the complete elliptic integrals of the first and second kind [11] and $F$ is the incomplete integral of the first kind.

Notice that there are different functional forms for the action-angle variables depending on whether the motion of the atom is bounded ($N < 1$) or unbounded ($N > 1$). From the expression for the action of the atom one can calculate the frequency of motion as a function of the total energy $E$,

$$\omega_d(E) = \left(\frac{dJ}{dE}\right)^{-1} = \frac{\pi}{2} \sqrt{\kappa} \left\{ \begin{array}{l} 1/K(N), \quad N < 1 \\ 2N/K(N^{-1}), \quad N > 1 \end{array} \right.$$

In Fig 3.2 I have plotted the frequency as a function of energy. Notice that it decreases monotonically with energy and rapidly falls to zero as bounded motion approaches the separatrix $E_s$, after which the frequency begins to increase again when the motion is unbounded.
3.1.3 dynamics of a classical distribution

Up until now we have imagined that the atom was initially prepared at some well-defined position and momentum. The cooling of atoms in phase space is a very active area of research where the aim is to cool many atoms in a very small volume so that co-operative effect such as Bose condensation might be observed. However, the uncertainty principle limits the extent to which confinement in phase space can be achieved. The appropriate description of atomic dynamics is using probability distributions on phase space. We define a classical state to be a probability measure on phase-space of the form $Q(q, p) \, dq \, dp$ where $Q(q, p)$ is the joint probability density. The density then obeys the Liouville equation

$$ \frac{\partial Q}{\partial t} = -\{H, Q\}_{q,p} = -p \frac{\partial Q}{\partial q} + \kappa \sin q \frac{\partial Q}{\partial p}, \quad (3.16) $$

where $\{ , \}_{q,p}$ is the usual Poisson bracket. This equation can be solved by the method of characteristics [14]. Let us choose the initial state, $Q_0(q, p)$, to be a bivariate gaussian centered on $(q_0, p_0) = (-1.5, 0)$ with position variance $\sigma_q = 0.18$ and momentum variance $\sigma_p = 0.33$

$$ Q_0(q, p) = \frac{1}{2\pi \sqrt{\sigma_q \sigma_p}} \exp \left[ \frac{(p - p_0)^2}{2\sigma_p} \right] \exp \left[ \frac{(q - q_0)^2}{2\sigma_q} \right], \quad (3.17) $$

Fig. 3.2. The frequency of atomic motion as a function of total energy.
3.1 Regular classical motion

Fig. 3.3. The effect of nonlinear dynamics on the state of the atom represented as a classical distribution in phase space. $\kappa = 1.2$, and the initial distribution has the mean co-ordinates $(q_0, p_0) = (-1.5, 0)$, and the variances $\sigma_q = 0.18$, $\sigma_p = 0.33$. (a) Initially the atom is localized in the region of bounded motion; (b) After just ten classical periods the distribution of the atom is sheered over the trajectories on which it has support.

The solution to Eq. (3.16) then is

$$Q(q,p,t) = Q_0 \left[ \bar{q}(q,p,-t), \bar{p}(q,p,-t) \right],$$

(3.18)

where $(\bar{q}(q,p,t), \bar{p}(q,p,t))$ is the trajectory generated by Hamilton’s equations. If the initial density is localized in a region of bounded motion, it will not remain localized but undergo a rotational shearing. This shearing occurs because points at larger energies (further from the origin in phase-space) oscillate with lower frequencies. This is the typical behavior of nonlinear systems, where the frequency of oscillation varies with the classical action. The resulting pattern is referred to as a ‘whorl’[12]. In Fig. 3.3 we show the effect of nonlinearity on a phase space distribution for an atom moving classically. The distribution for the atom is initially localized in phase space but after just ten classical periods it has become sheered over the trajectories on which it has support.

An estimate of the shearing rate can be found by assuming that the classical frequency decreases linearly within the region of bounded motion. This is a good approximation provided the atom is not too close to the separatrix. If the initial localized distribution for the atom has support on an action interval $\Delta J$ centered on the trajectory $J$ then it is sheared over the trajectory when the difference in the angle variable across the distribution is approximately $2\pi$. This takes a time $T_{col}$, which we call the collapse time, given by

$$T_{col} = T_{cl} \left( \frac{d\omega_{cl}}{dE} \right)^{-1}.$$

(3.19)
Fig. 3.4. The effect of nonlinear dynamics on the momentum statistics of the atom. A plot of the classical momentum statistics as a function of strobe number. (a) the mean momentum, $\langle p \rangle$, rapidly collapses to zero due to the sheering action of the nonlinear motion; (b) the momentum variance, $V(p)$, rapidly rises to its steady state.

The reason why we call it the collapse time can be seen in Fig. 3.4 where we graph the momentum mean and variance as a function of time. These statistics were calculated by tracking 2000 points in phase space initially distributed with a density given by Fig. 3.3(a). Since we are not interested in the variation over one classical period, but rather the long time evolution, we have plotted the statistics at times $t = 2\pi s$, with $s$ integer. For obvious reasons $s$ is referred to as the strobe number. We see that over the collapse time the mean is rapidly damped and the variance rises to a constant value.

### 3.2 Regular quantum motion

So far we have assumed that the coherent motion of the atom can be approximated classically. How does this approximation emerge from the underlying quantum mechanical equations of motion? This is a non-trivial question but one which we will not attempt to answer in a rigorous way. I will approach this question from the point of view that the atom is best described by a distribution in phase space since this is how atoms are prepared at the moment. Now a classical distribution will have a continuous range of energies associated with the continuous range of trajectories that intersect it in phase space. The energy of the quantum
mechanical distribution can be complicated and is given by the spectrum of the Hamiltonian operator. First I will discuss the limitations of the classical approximation through an examination of the spectrum of the quantum mechanical Hamiltonian operator.

You will have heard many times that quantum mechanics is a linear theory because the Schrödinger equation is linear. The fundamental difference between classical and quantum mechanics is more subtle than this for in the sense of phase space densities the Liouville equation is also linear. The concept of nonlinearity as defined in terms of the classical frequency can be transported to quantum mechanics in the following way. The harmonic oscillator is a linear classical system with a quantization that is well known. Loosely speaking we can think of the nonlinearity of a quantum system in terms of how much its dynamics differs from the quantum harmonic oscillator. We will see how this quantum mechanical definition of nonlinearity is connected with our classical definition when we come to consider the distribution of the quantum mechanical energy spacings. The important result of this section will be to show that for long times when the dynamics cannot be approximated classically we no longer see the continuous shearing of the atomic distribution of the previous section: Quantum nonlinear dynamics implies fractional revivals of the initial wave packet on a time scale much larger than the classical collapse time.

3.2.1 eigenstates and eigenvalues

The quantum mechanical optical potential is periodic. This means that the translation operator $\hat{S}_{2\pi} = \exp(-2\pi \hat{p}/\hbar)$ commutes with the ground state Hamiltonian $\hat{H}_a = \hat{p}^2/2 + 2\kappa \sin^2(\hat{q}/2)$. The quantum mechanics of Hamiltonians with periodic potentials arises naturally when considering systems with spatial periodicity. Up until the birth of atom optics most of these studies were in solid state physics, where one considers the motion of an electron in the potential arising from a periodic lattice of atoms.

It is known [13] that the spectrum of a periodic Hamiltonian consists of a countable number of intervals called energy bands. Each band is labeled by an integer $n$ called the band number. Since the operator of $2\pi$ translations in position commutes with the ground state Hamiltonian it is possible to choose the eigenstates of $\hat{H}_a$ to be eigenstates of $\hat{S}_{2\pi}$ as well. The translation operator has eigenvalues $\exp(2\pi \hat{p}/\hbar)$ parameterized by the momentum-like variable $p$ called the quasi-momentum. For the quantum pendulum, states must be physically unchanged when rotated by $2\pi$ radians about its axis. This means that eigenstates of the pendulum are restricted to the case $p = m\hbar$, where $m$ is an integer. This restriction does not apply to the motion of an atom, and in this case the quasi-
momentum may take on any value. The quantum motion of the atom is therefore not equivalent to the quantum pendulum.

The eigenstates $|E_n, p\rangle$ which diagonalize both $\hat{H}_a$ and $\hat{S}_2\pi$ are called Bloch states. Likewise we can use $n$ and $p$ to parameterize the energy through the eigenvalue problem

$$\hat{H}_a|E_n, p\rangle = E_n(p)|E_n, p\rangle .$$

(3.20)

Notice that the optical potential does not change when $q$ is transformed to $-q$. This implies that both $\hat{H}_a$ and $\hat{H}_b$ are invariant under a parity operation. Let $\hat{P}$ be the parity operator with the action, $\hat{P}|p\rangle = |-p\rangle$ on the momentum eigenstates. This implies that the momentum operator transforms as $\hat{P}\hat{p}\hat{P} = -\hat{p}$, and that the translation operator is reversed: $\hat{P}\hat{S}_2\pi\hat{P} = \hat{S}_{-2\pi}$. This means that the states $|E_n, p\rangle$ and $|E_n, -p\rangle$ have the same energy.

If we define $u_{n,p}(q)$ to be the wavefunction of $|E_n, p\rangle$ in the position representation then Schrödinger’s equation reads

$$-\frac{k^2}{2} \frac{d^2 u_{n,p}}{dq^2} + 2\kappa \sin^2(q/2) u_{n,p} = E_n(p)u_{n,p} .$$

(3.21)

This second-order differential equation is called Mathieu’s equation. We are fortunate that there is a great deal about this equation in the mathematical literature [11]. The wavefunction $u_{n,-p}$ is a second solution to this equation, and for quasi-momenta $p \neq m\hbar/2$ where $m$ is an integer it will be linearly independent from $u_{n,p}$ because they have different eigenvalues of $\hat{S}_2\pi$. Eigenstates differing in quasi-momentum by an amount $\hbar$ must have the same energy and the same translation eigenvalue, and, since there are only two solutions of Mathieu’s equation because it is second order in $q$, translated Bloch states states must be equal up to multiplication by a complex number. Hence the energy and the Bloch functions repeat themselves in quasi-momentum space. For uniqueness $p$ is usually restricted to the interval $[\hbar/2, -\hbar/2)$. This region is called the first Brillouin zone [15]. For the quasi-momenta $p = -\hbar/2$ and $p = 0$, $u_{n,p}$ and $u_{n,-p}$ have the same translational eigenvalues so they may no-longer be linearly independent. In fact there is only one physical solution at these two quasi-momenta because the other is not normalizable.

If $u_{n,p}$ is a Bloch wavefunction then we can multiply it by an arbitrary function of the quasi-momentum and still get a Bloch function. Therefore we can assume that $u_{n,p}$ is a continuous function of $p$. The Bloch states are complete and their normalization can be chosen in different ways, and following Slater [17]we shall take it to be box normalization. For the atom in the stationary standing wave the energy bands don’t overlap so that we also have orthogonality between bands. The completeness, normalization,
and orthogonality conditions can be expressed in terms of the Bloch state wavefunction as follows:

\[
\begin{align*}
\sum_{n=1}^{\infty} \int_{\frac{k}{2}}^{\frac{k}{2}} u_{n,p}(q')^* u_{n,p}(q) \, dq &= 2\pi \delta(q' - q) \quad \text{(completeness)}, \\
\int_{-\frac{k}{2}}^\frac{k}{2} |u_{n,p}(q)|^2 \, dq &= 1 \quad \text{(normalization)}, \\
\int_{-\infty}^{\infty} u_{n',p'}(q)^* u_{n,p}(q) \, dq &= 2\pi \delta_{n',n} \delta(p' - p) \quad \text{(orthogonality)}.
\end{align*}
\]

(3.22)

The Bloch states are eigenstates of the translation operator and this means that they are delocalized in the position representation. This makes it difficult to use them directly to analyze the motion of an atom bound around a single potential minimum. A more useful basis of states are the Wannier states \( |W_{n,m}\rangle \) found by integrating over the Bloch states in the \( n \)th band [17]

\[
|W_{n,m}\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\frac{k}{2}}^{\frac{k}{2}} \exp \left(-\frac{2\pi i m p}{k}\right) |E_{n,p}\rangle \, dp. \quad (3.23)
\]

The Wannier state \( |W_{n,m}\rangle \) is localized at the point \( q = 2\pi m \) and it is easy to verify that it satisfies the translation identity, \( \hat{S}_{2\pi} |W_{n,m}\rangle = |W_{n,m + 1}\rangle \). Eq. (3.23) can be inverted to express the Bloch states in terms of the Wannier states

\[
|E_{n,p}\rangle = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} \exp \left(\frac{2\pi i m p}{k}\right) |W_{n,m}\rangle. \quad (3.24)
\]

Physically this relation tells us that the relative probability of finding a Bloch state atom localized around the site \( q = 2\pi m \) is \( |\exp \left(\frac{2\pi i m p}{k}\right)|^2 = 1 \) which confirms our statement that the Bloch states are delocalized. By virtue of the corresponding Bloch state relations the Wannier states are orthonormal and complete. If \( a_{n,m}(q) \) is the Wavefunction of the Wannier state \( |W_{n,m}\rangle \) in the position representation, the normalization and completeness relations are

\[
\begin{align*}
\int_{-\infty}^{\infty} a_{n',m'}(q)^* a_{n,m}(q) \, dq &= \delta_{n',n} \delta_{m',m} \quad \text{(normalization)}, \\
\sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} a_{n,m}(q')^* a_{n,m}(q) &= \delta(q - q') \quad \text{(completeness)}.
\end{align*}
\]

(3.25)

There is one further property of the Wannier states which makes them very useful for studying systems with translational symmetry. Since the Bloch wavefunctions are periodic up to a phase factor they can be expanded in a Fourier series

\[
u_{n,p}(q) = \sum_{m=-\infty}^{\infty} v_n(p + m\frac{k}{2}) \exp \left[i(p + m\frac{k}{2}) q\right]. \quad (3.26)
\]
The Fourier coefficients \( v_n(p + m\hat{k}) \) determine all of the Bloch states and together with the dispersion relation \( E_n(p) \) they fully characterize the dynamics of the atom. Using the relation Eq. (3.24) we see that the function \( v_n(p) \) is the wavefunction of the Wannier states centered on \( q = 0 \) in the momentum representation i.e.

\[
v_n(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a_{n,0}(q) \exp(-ipq/\kappa) \, dq \quad (3.27)
\]

Therefore to completely determine the dynamics of the atom all we have to find is the \( m = 0 \) Wannier states in the momentum representation and the energy dispersion relation.

One way of finding the energy is to express the eigenvalue problem Eq. (3.20) in the momentum representation and solve the resulting matrix eigenvalue problem on a computer. Although this is a good way of finding the energy dispersion relation and even to find individual Bloch wavefunctions there is no way of ensuring that the Fourier components of the Bloch wavefunction vary continuously across the band. We will now describe a method proposed by Slater [17] and Risken [18] based on the method of continued fractions which has the advantage that it automatically ensures the Bloch states vary continuously with quasi-momentum.

The first step is to write the stationary Schrödinger equation in the momentum representation

\[
\left[ \frac{p^2}{2} + \kappa - E_n(p) \right] v_n(p) - \frac{\kappa}{2} [v_n(p + \hat{k}) + v_n(p - \hat{k})] = 0. \quad (3.28)
\]

This equation can be thought of as a matrix eigenvalue problem or as Slater observed it can be thought of as a tridiagonal recurrence relation with the two boundary conditions \( v_n(p) \to 0, \ p \to \pm \infty \). If we know the energy \( E_n(p) \) then we can reconstruct \( v_n(p) \) as follows. First define the quotient variables \( G_m^\pm(E_n) \)

\[
G_m^-(E_n) = \frac{v_n(p + (m - 1)\hat{k})}{v_n(p + m\hat{k})}, \quad (3.29)
\]

\[
G_m^+(E_n) = \frac{v_n(p + (m + 1)\hat{k})}{v_n(p + m\hat{k})}, \quad (3.30)
\]

where \( p \) is in the first Brillouin zone. Using Eq. (3.28) these variables can be expressed as continued fractions via the recursion relations

\[
G_m^+(E_n) = \left[ \frac{2}{\kappa} \left( \frac{(p + (m + 1)\hat{k})^2}{2} - E_n(p) \right) - \frac{\kappa}{2} G_{m+1}^+(E_n) \right]^{-1}, \quad (3.31)
\]

\[
G_m^-(E_n) = \left[ \frac{2}{\kappa} \left( \frac{(p + (m - 1)\hat{k})^2}{2} - E_n(p) \right) - \frac{\kappa}{2} G_{m-1}^+(E_n) \right]^{-1}, \quad (3.32)
\]
with the asymptotic behavior

\[
G^+_m(E_n) \to 0, \quad m \to +\infty,
\]
\[
G^-_m(E_n) \to 0, \quad m \to -\infty.
\] (3.33)

To approximate this continued fraction choose \(G^\pm_{\pm M}(E_n) = 0\) for a large positive integer \(M\). Since \(E_n(p)\) is assumed known equations (3.31, 3.32) can be iterated to yield all of the \(G^\pm_m\), which determines the function \(v_n(p)\) up to a constant that can be found from the normalization condition Eq. (3.25). In order to find \(E_n(p)\) we use the property that for the correct choice of \(E = E_n(p)\), \(S(E) = 0\). Here the function \(S(E)\) is given by

\[
S(E) = G^+_0(E) + G^-_0(E) - \frac{2}{\kappa} \left[ \frac{p^2}{2} + \kappa - E \right].
\] (3.34)

For any value of \(E\), \(S(E)\) can be calculated using the method just described and its zeros found by a simple root finding routine. If the sign of \(v_n(p)\) in the region \([0, \pi]\) is chosen positive then the Bloch states turn out always to be continuous in the quasi-momentum. The dispersion relation for the first fifteen bands has been plotted in Fig. 3.5 for the parameters \(\kappa = 1.2\) and \(\k\ell = 0.24\). For values well below the optical potential height the energy is approximately constant. In Fig. 3.6 the corresponding Wannier states in the momentum representation are shown. For bands corresponding to classically bound states the Wannier wavefunctions vary smoothly with momentum much like harmonic oscillator wavefunctions. For energies where the classical motion is unbounded the Wannier states approach discontinuous functions.

The Wannier states are useful in describing the quantum dynamics of an atom bound about the minimum of the optical potential, but as was mentioned before Wannier states are not stationary states and so will change with time. This means that the nearest neighbour amplitudes \(\langle W_n, m + m' | H_a | W_n, m \rangle\) for \(m' \neq 0\) do not vanish in general. To get an idea of the effect of this, assume that the off-diagonal amplitudes decay rapidly enough that only the nearest-neighbour amplitudes are significant. Suppose the atom is initially in a Wannier state centered on the node \(q = 0\). Let \(a_m(t)\) be the amplitude that it is at the node \(q = 2\pi m\) at some later time \(t\), then \(a_m(t)\) is determined by the Schrödinger equation

\[
i\hbar \frac{da_m}{dt} = \bar{E}_n a_m + \frac{k\Delta_n}{2} a_{m+1} + \frac{k\Delta_n}{2} a_{m-1},
\] (3.35)

and the initial condition \(a_m(0) = \delta_{m,0}\). Here \(\bar{E}_n\) is the average energy of a Wannier state and \(k\Delta_n/2\) is the nearest-neighbour hopping amplitude for the \(n\)th band. The eigenstates and eigenvalues of this system constitute a tight-binding model for the atom [16]. Solving this model subject to the
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Fig. 3.5. Dispersion relation for a ground state two-level atom in a stationary standing wave, $\kappa = 1.2$. For values well below the optical potential height, the energy is approximately constant.

Fig. 3.6. Wannier state wavefunctions in the momentum representation.
above initial condition we find that the probability of finding the atom at the site \( q = 2\pi m \) is

\[ P_m(t) = |a_m(t)|^2 = J_m(\Delta_n t)^2. \]  

Here \( J_m(x) \) is the ordinary Bessel function of the first kind of order \( m \). Since the Bessel function decays rapidly in \( m \) for \( |m| > |x| \), at time \( t \) the atom will be confined to nodes \( |m| < \Delta_n t \). The frequency \( \Delta_n \) is related to the energy through the tightbinding dispersion relation

\[ E_n(p) = \bar{E}_n + \hbar \Delta_n \cos(2\pi p/\kappa). \]  

Therefore the width of the \( n \)th band is equal to \( 2\hbar \Delta_n \), and the average energy is equal to \( E_n(\hbar/4) \). Intuitively this is what we expect. If the width of the energy band is sufficiently small the Wannier state can be considered stationary over a sufficiently small time. By sufficiently small we mean that the following condition is satisfied:

\[ \Delta_n t \ll 1. \]  

If the atom is cooled below the maximum energy of the optical potential then for dynamics occurring over a time small compared to \( 1/\Delta_n \), the Wannier states can be regarded as stationary states with energy \( \bar{E}_n \), the average energy of the \( n \)th band.

How is this quantum mechanical description of the atom related to the previous classical discussion? We can see how the classical phase space emerges from quantum mechanics by calculating the \( Q \) function of the Wannier states. For a quantum state \( |\psi(t)\rangle \) the \( Q \) function is defined by

\[ Q(q, p, t) = \frac{1}{2\pi\hbar} |\langle q, p |\psi(t) \rangle|^2. \]  

The states \( |q, p\rangle \) are coherent states for a simple harmonic oscillator with frequency chosen as \( \sqrt{\kappa} \), i.e. the frequency of linear motion around the stable fixed point of the nonlinear pendulum. The \( Q \) function is often used to give a phase space representation to a quantum state. The \( Q \) function for the Wannier state \( |W_7, 0\rangle \) is plotted in Fig. 3.7, \( \kappa = 1.2 \), and \( \hbar = 0.24 \). The phase space representation of the Wannier state is concentrated about the classical trajectory with the same energy.

### 3.2.2 WKB approximation

We now turn to the question of how the center-of-mass spectrum of the atom is related to the classical definition of nonlinearity introduced in the previous chapter. In the previous subsection we were able to use the
Fig. 3.7. The $Q$ function of a bound Wannier state with $n = 7$, $\tilde{E}_n = 1.406$, solid line, $Q$ function half height contour; dashed line, classical separatrix; dot-dashed line, trajectory $H_a = \tilde{E}_n$. 
3.2 Regular quantum motion

tight-binding approximation to find the dispersion relation in terms of the two free parameters $E_n$ and $\Delta_n$. I will now review the estimation of these parameters using the WKB approximation [13]. Importantly we will also make explicit the connection between the quantum mechanical spectrum and the classical frequency of motion, by which we will define what is meant by a quantum mechanical nonlinearity.

Let the energy of the Bloch state $|E_n, p\rangle$ lie below the height of the optical potential barrier, $E_n(p) < V_{\text{max}}$. Classically the atom with energy $E_n(p)$ will be confined to the region $b - 2\pi \leq q \leq a$, where $V(a,t) = V(b,t) = E_n(p)$, but quantum mechanically it can penetrate into the classically forbidden region $a \leq q \leq b$. In the classically accessible region, away from the turning points $q = b - 2\pi$ and $q = a$ the Bloch wave function $u_n(q)$ is approximately equal to

$$u_n(q) \approx \frac{2A}{\sqrt{k(q)}} \cos \left( \int_q^a k(q) \, dq - \frac{\pi}{4} \right) + \frac{B}{\sqrt{k(q)}} \sin \left( \int_q^a k(q) \, dq - \frac{\pi}{4} \right),$$

where for the moment $A$ and $B$ are constants which have to be determined and $k(q) = \sqrt{2 \left(E_n(p) - 2\kappa \sin^2(q/2)/\hbar \right)}/\kappa$. We now use connection formulae which relate the WKB approximation of the wavefunction in the classically allowed region of phase space to the wavefunction in the classically forbidden region to find the approximation in the region $b \leq q \leq a + 2\pi$ [13]

$$u_n(q) \approx \frac{A}{\sqrt{k(q)}} \exp \left( - \int_b^q \tilde{k}(q) \, dq \right) - \frac{B}{\sqrt{k(q)}} \exp \left( \int_b^q \tilde{k}(q) \, dq \right).$$

where $\tilde{k}(q) = \sqrt{2 \left(2\kappa \sin^2(q/2) - E_n(p)\right)/\hbar}$. The connection formulae can be used again to extend the approximation in the forbidden region to the classically allowed region $b \leq q \leq a + 2\pi$. According to the translational properties of the Bloch states the wave function in this new region is related to the original wavefunction by $u_n(q + 2\pi) = \exp(2\pi i p/\hbar) u_n(q)$. Using this property we find that the constants $A$ and $B$ must satisfy the eigenvalue equation

$$\begin{pmatrix} -e^\chi \sin \zeta & -e^\chi \cos \zeta \\ e^\chi \cos \zeta & -2e^\chi \sin \zeta \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \exp(2\pi i p/\hbar) \begin{pmatrix} A \\ B \end{pmatrix},$$

where

$$\chi = \int_a^b \tilde{k}(q) \, dq,$$

$$\zeta = \int_{b-2\pi}^a k(q) \, dq - \frac{\pi}{2}.$$
The eigenvalues in Eq. (3.42) are unimodular. This constrains $\chi$ and $\zeta$ which together must satisfy the inequality
\[
\left( \frac{e^{-\chi}}{2} + 2e^{\chi} \right)^2 \sin^2 \zeta \leq 4. 
\] (3.45)

This identity places a restriction on the allowed values of energy, and the fact that it is an inequality reflects the existence of energy bands. If this inequality is satisfied then $E_n(p)$ is given in terms of the quasi-momentum $p$ by the implicit equation,
\[
\cos(2\pi p/\kappa) = -\frac{1}{2} \left( \frac{e^{-\chi}}{2} + 2e^{\chi} \right) \sin(\zeta). 
\] (3.46)

From Eq. (3.37) the average energy of the $n$th band is given by setting $p$ to $\kappa/4$. The variable $\zeta$ can be written in terms of the classical action using Eq. (3.11). This implies that the average energy of the $n$th band satisfies the Bohr-Sommerfeld quantization condition
\[
J(\bar{E}_n) = \kappa \left( n + \frac{1}{2} \right). 
\] (3.47)

In passing note that equation (3.47) reveals an important limitation of the WKB approximation: it is restricted to integrable models, where it is possible to map to action-angle variables. Using this Eq. (3.47) we can estimate the local energy spacing at the $n$th band $\Delta \bar{E}_n = \bar{E}_n - \bar{E}_{n-1}$.

We find that it is simply related to the classical frequency by
\[
\Delta \bar{E}_n \approx \kappa \omega_{cl}(\bar{E}_n). 
\] (3.48)

We will use this expression as the basis of our definition of quantum nonlinear motion. It is well known that the frequency of the harmonic oscillator is constant and that the quantum harmonic oscillator has fixed energy spacings. On the other hand if motion of the atom is classically nonlinear then according to Eq. (3.48), in the semiclassical limit the energy spacing will change with the band number. We illustrate this connection between classical frequency and quantum energy spacings in Fig. 3.8 where $\Delta E_n/\kappa$ and $\omega_{cl}(\bar{E}_n)$ have been plotted for the nonlinear pendulum, with $\kappa = 1.2$, $\kappa = 0.05$. Both the classical and quantum mechanical definitions of nonlinearity are quite general and in the sense of these definitions most physical systems are nonlinear. The harmonic oscillator is useful in illustrating the transition from classical to quantum mechanics, but it is mainly interesting from the point of view of static properties such as eigenstates and eigenfunctions. But to investigate the effect of quantization on dynamics we must study nonlinear systems.
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Fig. 3.8. In a nonlinear quantum mechanical system the energy spacing changes with the principle quantum number. The energy difference is plotted as a function of the average band energy and marked by crosses. The energy difference follows the classical frequency.

3.2.3 fractional revivals

So far we have seen how the $Q$ function of the Wannier states is related to the classical phase space trajectories and how the Raman spectrum is used to relate classical and quantum nonlinearities. How is quantum nonlinear dynamics the same as or different from classical dynamics? To answer this question we need to know the role that eigenstates and energies play in quantum dynamics.

The standard criteria for deciding whether a quantum mechanical system will behave classically is the size of the principal quantum number $n$. If $n$ is large in some sense then it is often said that the system is semi-classical. What is meant by this statement is that if $n$ is large then the change in the spacing between energy levels must be small compared to $\hbar \omega_{cl}$, and for sufficiently short times the fact that energy is quantized can be ignored. If we are interested in comparing the dynamics of a classical particle with a well defined position and momentum, then one usually adds the condition that in order to have the quantum state localized in an interval $\Delta q$ small compared to the distance between the classical turning points $L$, the wave packet should be made up of $\Delta n$ states where $\Delta n \sim L/\Delta q$ [19]. What do we mean by the term 'sufficiently short time'? In order to observe genuine quantum nonlinear behavior we have to wait for a time that is much larger than the classical period. This time has
to be long enough so that we can resolve the change in the energy spacing. The time scale for quantum nonlinear dynamics $T_{\text{rev}}$ is given by the expression [20, 21]

$$T_{\text{rev}} = T_{\text{cl}} \left( \frac{\kappa}{2} \left| \frac{\partial \omega_{\text{cl}}}{\partial \bar{E}} \right| \right)^{-1}, \quad (3.49)$$

where $T_{\text{cl}} = 2\pi/\omega_{\text{cl}}$. To understand this expression compare it with the estimation for the collapse time $T_{\text{col}}$ given by Eq. (3.19). Thus $T_{\text{rev}}$ is the time it takes adjacent energy phasors to become $4\pi$ out of phase. As our initial state we choose the wave packet given by Eq. (2.40) with means $\langle \hat{p} \rangle = p_0 = 0.0$, $\langle \hat{q} \rangle = q_0 = -1.5$, and a momentum variance $V(p) = \delta = 0.2$. The initial $Q$ function is then a bivariate gaussian (see Eq. (3.17)) centered on $(q_0, p_0)$ with position variance $\sigma_q = \bar{\kappa}/2\sqrt{\kappa} + \kappa^2/4\delta = 0.18$, and $\sigma_p = \bar{\kappa}\sqrt{\kappa}/2 + \delta = 0.33$. The $Q$ function of this state is precisely the classical distribution used in our discussion of classical nonlinear dynamics in Sec. (3.1.3). In Fig. (3.9) we have plotted the mean and variance of the momentum as a function of the strobe number for $\kappa = 1.2$ and $\bar{\kappa} = 0.24$. This figure should be compared with the classical distribution shown on Fig. 3.4. Note that the quantum mean initially follows the classical mean, but at times $s \approx 20, 50$ exhibits partial revivals of the initial values. Between these times the momentum variance shows rapid oscillations. Similar behaviour was demonstrated for a Kerr oscillator in reference [?].

Averbukh and Perelman[19] have shown that when a classical system performs regular periodic motion with a nonlinear frequency, localized wave packets in the semiclassical regime exhibit what they refer to as ‘fractional revivals’ on the characteristic time scale $T_{\text{rev}}$. At times $t = 0.5T_{\text{rev}}$ and $t = T_{\text{rev}}$ the quantum state approximates the initial wave packet evolved to time $t$ according to the linearized dynamics. However, at times $t = M\frac{1}{2}T_{\text{rev}}$ with $M, N$ coprime, the quantum state approximates a superposition of $L$ copies of the initial state, where

$$L = \begin{cases} N, & N \text{ odd} \\ N/2, & N \text{ even}. \end{cases} \quad (3.50)$$

This expression is derived by assuming that the atom is bound around the node $q = 0$. Since the atom is bound, its state can be written in terms of the Wannier states

$$|\psi(t)\rangle = \sum_n a_n \exp \left( -i E_n t/\bar{\kappa} \right) |W_n, 0\rangle. \quad (3.51)$$

One then assumes that the energy varies slow enough with $n$ to allow the following semiclassical estimate about the mean quantum number $\bar{n}$

$$E_n \approx E_{\bar{n}} + \kappa \omega_{\text{cl}}(E_{\bar{n}})(n - \bar{n}) + \kappa^2 \frac{\partial \omega_{\text{cl}}}{\partial J}(E)(n - \bar{n})^2. \quad (3.52)$$
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From equations (3.19) and (3.49) we see that the term quadratic in $n$ is responsible for both the collapse of the momentum mean and for the recombination of the energy phasors at fractional revival times. The energy for a Kerr oscillator is exactly quadratic in the principal quantum number and thus the fractional revivals observed in Ref. [?] were perfect.

For the atom in a standing wave there are higher order corrections to the energy which become important for large enough times [19]. As a result the fractional revivals are not perfect, and will degrade with time.

To illustrate fractional revivals in the atomic wavepacket used in Fig. 3.9 we show in Fig (3.10) the contours of the $Q$ function at times commensurate with the oscillations in the quantum mean and variance. Clearly the state is a superposition of a discrete number of wave packets. For the state $|\psi\rangle$ with $q_0 = -1.5$, $p_0 = 0.0$, $\delta = 0.2$, and $\kappa = 1.2$, $h = 0.24$ we find $T_{rev} = 329$. This is equivalent to a strobe number $s \approx 52$. So Fig (3.10) corresponds to fractional revivals at times $t = \frac{1}{4}T_{rev}$, $\frac{1}{2}T_{rev}$, $\frac{3}{4}T_{rev}$ and $T_{rev}$.

The revivals of the nonlinear pendulum demonstrated above can be realized experimentally by observing the scattering of atoms from an optical standing wave. As an example we propose using Ytterbium atoms [7] with mass $m = 2.9 \times 10^{-25}$ kg prepared in a two-state system with frequency $\omega_0/2\pi = 5.4 \times 10^{14}$ Hz, and an atom/field system with a Rabi frequency $\Omega/2\pi = 1.0 \times 10^8$ Hz, detuning $\Delta/2\pi = 2.9 \times 10^9$ Hz, wave-

Fig. 3.9. Mean momentum and momentum variance for the quantum motion of an atom in a stationary standing wave as a function of strobe number. The mean momentum exhibits large deviations from zero at times $s \approx 20, 50$. At times $s \approx 10$ and $s \approx 55$ the momentum variance rapidly oscillates.
Fig. 3.10. $Q$ function for a two-level atom in a stationary standing wave at four times: (a) $s = 13$; (b) $s = 26$; (c) $t = 39$; (d) $s = 52$. Figures (a) and (c) show the $Q$ function when there are rapid oscillations in the momentum variance. Figures (b) and (d) show the $Q$ function at the times when the magnitude of the mean momentum becomes large.
3.2 Regular quantum motion

length $\lambda = 5.56 \times 10^{-7}$ m and a wave number $k = 1.13 \times 10^7$ m$^{-1}$. For a characteristic frequency of $\omega/2\pi = 1.2 \times 10^5$ Hz we have the dimensionless quantities $\kappa = 1.2$ and $\tilde{\kappa} = 0.24$. A wave packet initially localized at $x = -0.1\lambda$, $\Delta x = 0.02\lambda$, $p_x = 0.0\hbar k$, $\Delta p_x = 3.6\hbar k$ will have a corresponding revival time of $T_{rev} = 4.36 \times 10^{-4}$ s. Collimation of the transverse motion of the atom to the degree stated above will be difficult. We require the width of the atomic beam to be 0.01$\mu$m whereas current experiments have collimated beams to only 10$\mu$m. To observe the revival at $t = \frac{1}{4}T_{rev}$ when the standing wave has dimension 10 mm in the direction of atomic beam propagation the longitudinal velocity of the Ytterbium atoms must be 92 ms$^{-1}$. While this is slow it is within reach of current experimental techniques of atomic optics and laser cooling. The standing wave can be produced by retroreflecting a laser beam using a mirror located within the vacuum chamber. The position of the atomic beam relative to the standing wave anti-nodes can then be set by adjusting the position of the mirror with the aid of a piezo-electric crystal. The Rabi frequency quoted above corresponds to a laser intensity of 84 Wcm$^{-2}$. Intensities of this order are already used in atomic cooling experiments.
4

Quasi-integrable motion

This material is adapted from the PhD thesis of Dr Sigurd Dyrt ing.

In this chapter we consider how the non integrable motion of a two level atom in an optical dipole field. One way to make the motion non-integrable is to make the optical potential time-dependent. When the standing wave intensity is periodically modulated and the dynamics is treated classically, the total energy is no longer a constant of the motion, and the atom is not confined to a single one-dimensional curve in phase space. It is true that if the amplitude of the modulation is too great then the motion of the atom will be globally chaotic, but if it is kept to a moderate value classical phase space becomes complicated, and shows a mixture of regular and chaotic motion. In this regime the motion is said to be near-integrable or quasi-integrable.

It is very useful to study the dynamics of periodically driven systems using the Floquet transformation. This transformation evolves the state of the system forward by one cycle of the driving. For the classical approximation its action is equivalent to a phase space mapping and it is often called a stroboscopic map. When the system is treated fully quantum mechanically it takes the form of a unitary operator on the center-of-mass Hilbert space. The interaction of the atom with the periodically modulated optical potential can be studied using perturbation theory. One decomposes the driven system into the sum of a time-independent part and a modulating part which is in some sense small and which is treated as a perturbation. When this perturbation is resonant with the 'free' motion of the atom there is a drastic change in the phase space trajectories of the classical Floquet map or in the eigenstates of the quantum Floquet operator.

The concept of a resonance is central to an understanding of the dynamics of driven Hamiltonian systems. In the study of classical chaos
the complicated topology of trajectories can be explained in terms of the formation and interaction of resonances at successively finer scales. In particular a resonance can lead to the emergence of a locally stable region of phase space which may persist even after surrounding trajectories have become chaotic and a distribution of points contained within such a region will remain localized. The idea of a resonance is well understood in quantum mechanics, but it is usually discussed in the context of the spectrum of a system were it is not clear how it is related to its classical counterpart. The connection between classical and quantum mechanical resonances becomes clearer with the help of the $Q$ function which gives a phase space representation to quantum mechanical states. We show that resonances in second-order classical perturbation theory imply near resonant denominators at second-order in time-dependent quantum perturbation theory. The perturbed eigenstates of the Floquet operator rapidly develop support on near-resonant free states and, as a result of the interference between these states, there is a change in topography of the $Q$ function.

How does the formation of resonances effect the motion of atomic wave packets initially confined near such regions? A lot of theoretical and numerical work has been done by Berman et al [23, 24, 25] and Lin and Reichl [26] on quantum systems containing many energy levels resonant with a periodic driving force. Under certain conditions these free energy levels will be trapped. That is if the initial state of the perturbed system is an energy eigenstate of the free system, with energy in the resonance zone, the dynamics will not mix in free energy states beyond the resonance zone. This is analogous to the trapping of classical trajectories by KAM surfaces. We will study the dynamic localization of a wave packet initially situated on a classical second-order resonance. The atom-standing wave system is essentially different from those used to study tunnelling because the free dynamics has only one stable fixed point. Bistability arises as a consequence of the modulation and the parity symmetry of the Hamiltonian.

In our system a freely evolving wave packet will quickly become delocalized because of the nonlinear frequency of the pendulum. As the amplitude of the frequency modulation increases from zero both the classical phase space distribution and the quantum mechanical wave packet become localized about the classical second-order resonance. The dynamic phase space localization of a classical distribution can be explained by the increase in width of the classical resonance. Dynamic phase space localization in the quantized motion can be explained by showing that as the perturbation is increased the initial atomic state is made up of two resonant quantum states. Once the classical distribution has become localized a further increase in the perturbation strength causes the classical
region of stable motion to shrink and the distribution to become delocalized. In the corresponding quantum mechanical evolution the wave packet begins to tunnel between resonances. This behavior can be interpreted in terms of the presence of a parity symmetry and the gradual detuning of the dominant quasi-energies.

Tunnelling occurs on a longer time scale than the fractional revivals described in the previous Chapter and therefore it will be more sensitive to decoherence due to spontaneous emission. It is difficult to theoretically estimate the effect of decoherence on tunnelling because it occurs in a non-perturbative regime where a WKB approximation of the Bloch states is no longer valid. Even so, an estimate of the spontaneous emission rate required to destroy tunnelling based upon the case of regular motion is still in reasonable agreement with Monte Carlo simulations.

4.1 Phase space

In the previous Chapter we considered the center-of-mass dynamics of a two-level atom interacting with a far off resonance laser and found that the nonlinear coupling between the position and momentum lead to a shearing of the atomic wavepacket over short times and fractional revivals on a much longer time scale. Although the system was nonlinear, in the classical approximation the dynamics was integrable. Integrability meant that there was a map to action-angle variables and the quantum stationary states and spectrum could be approximated using WKB theory. It is now generally realized that most systems are not integrable, and that the structure of nonlinear dynamics is more rich than examination of integrable models would suggest. The one-dimensional model of the dynamics in a stationary standing wave was integrable because the total energy of the atom was a constant of the motion. If the optical potential is time-dependent then in general the total energy would no longer be conserved.

A simple way to make the optical potential time-dependent is to add a perturbation to the stationary standing wave. To study quasi-integrable motion the amplitude of the standing wave can be made time-dependent by modulating the Rabi frequency as follows

\[ \Omega(t) = \Omega \sqrt{1 - 2\epsilon \cos t}. \] (4.1)

In the limit of large detuning the optical potential is

\[ V(\hat{q}, t) = 2\kappa (1 - 2\epsilon \cos t) \sin^2(\hat{q}/2). \]

This describes a modulation of the potential with a relative amplitude \(2\epsilon\). The dynamics of the atom is now non-autonomous. In order to describe its motion we must know its position and momentum and the phase of the driving. When considering the quantum mechanical motion of the atom
we cannot make use of the eigenstates and eigenvalues of the Hamiltonian operator because these will depend on time. There is a way that autonomous mechanics can be brought over to the case of periodically driven Hamiltonian systems. This is done through the use of an extended Hilbert space for quantum mechanics and an extended phase space for classical mechanics. While this fact will be used in the mathematical treatment of the dynamics, it is not very intuitive to visualize motion in this four dimension extended space. A projection of the dynamics onto two dimensions can be done by using a Poincaré section. For the special case of a one dimensional periodically driven system this technique is equivalent to replacing the Hamiltonian dynamics, changing continuously with time, by a mapping called the Floquet transformation.

4.1.1 classical phase space

If we make the classical approximation and replace the position and momentum operators by c-number variables $q$ and $p$ then the dynamics of the atom is given by Hamilton’s equations and the real potential. This potential is graphed in Fig. 4.1. It is still a periodic function of position with a minimum at the standing wave nodes and a maximum at the anti-node but the height of the potential is time-dependent and equal to $V_{\text{max}}(t) = 2\kappa(1 - 2\epsilon \cos t)$. If terms corresponding to a shift in the zero point of the total energy are dropped then the Hamiltonian for classical motion becomes

$$H(t) = \frac{p^2}{2} - \kappa(1 - 2\epsilon \cos t) \cos q . \quad (4.2)$$

When $\epsilon = 0$, Eq. (4.2) reduces to the Hamiltonian for a stationary standing wave. The frequency of the motion linearized about the fixed point $(q, p) = (0, 0)$ is equal to $\sqrt{\kappa(1 - 2\epsilon \cos t)}$ and so (4.2) also describes a nonlinear pendulum with a modulated linearized frequency. When in the stationary standing wave the atom was confined to trajectory with the topology of a torus. For non-zero $\epsilon$ the coupling of the driving term with the integrable motion of the free nonlinear pendulum leads to a modification of the invariant action and in the case of a classical resonance a change in the topology of phase space orbits. The overlap of resonances leads to the formation of a layer of stochastic motion about the classical separatrix. The resonances that do not overlap persist as stable regions of phase space.

Even though the Hamiltonian is time-dependent it is still possible to retain the theoretical framework of autonomous Hamiltonian mechanics by making use of the notion of the extendent phase space. In this larger phase space $t$ plays the role of a new co-ordinate with its own conjugate
momentum $h$. The dynamics of the new momentum is related to the elementary result that the rate of change of $H(t)$ is given by

$$ \frac{dH}{dt} = \frac{\partial H}{\partial t} . $$

(4.3)

Now introduce the time-like variable $\tau$ related to $t$ by

$$ \frac{dt}{d\tau} = 1 . $$

(4.4)

Equations (4.3), (4.4) are then equivalent to Hamilton’s equations on the extended phase space $(q, p, t, h)$ with the new Hamiltonian $K = h + H(t)$ and the new time variable $\tau$. Notice that $K$ does not depend on $\tau$ and is therefore a constant of the motion. The extended phase space has two degrees of freedom, therefore if there is another constant of the motion, say $I(q, p, t, h)$, then the motion of $(q, p, t, h)$ will be integrable. How does integrability in extended phase space show itself in our usual $(q, p)$ phase space? If $I$ is a constant of the motion then there would be numbers $c_1$ and $c_2$ which constrain the dynamics so that

$$ c_1 = h + H(q, p, t) , $$

(4.5)

$$ c_2 = I(q, p, t, h) . $$

(4.6)

Equations (4.5) and (4.6) imply that at the stroboscopic times $t = t_0 \mod 2\pi$ the position and momentum of the atom must lie on the curve

$$ c_2 - I(q, p, t_0, c_1 - H(q, p, t_0)) = 0 . $$

(4.7)
4.1 Phase space

Therefore integrability in extended phase space reveals itself in the phase space stroboscopic dynamics as motion constrained to a one-dimensional curve. From now on set $t_0$ to zero. The classical stroboscopic dynamics of the variables $q$ and $p$ are determined by the recursive formula

$$ (q', p') = F((q, p)) = (\tilde{q}(q, p, 2\pi), \tilde{p}(q, p, 2\pi)), \quad (4.8) $$

where the functions $\tilde{q}(q, p, t)$ and $\tilde{p}(q, p, t)$ are determined by Hamilton’s equations and the initial conditions $\tilde{q}(q, p, 0) = q$ and $\tilde{p}(q, p, 0) = p$. The map $F$ is called the Floquet or stroboscopic mapping and for the modulated standing wave it possesses the two important symmetries

$$ F \circ P = P \circ F, \quad (4.9) $$

$$ F \circ T = T \circ F^{-1}. \quad (4.10) $$

Here $P : (q, p) \mapsto (-q, -p)$ denotes the parity transformation and $T : (q, p) \mapsto (q, -p)$ denotes the time reversal reflection about the $q$-axis. This is called a time reversal symmetry because under the transformations $T$ and $t \mapsto -t$ Hamilton’s equations are invariant. Henceforth we fix $\kappa = 1.2$ and study the stroboscopic dynamics as $\epsilon$ is increased. In Figure 4.2 we show the classical stroboscopic phase portraits for $\epsilon = 0.0, 0.1, 0.2$ and $0.3$. These pictures were generated by taking points lying along the momentum axis and applying the map $F$ 500 times.

As a consequence of the symmetries $P$ and $T$, the stroboscopic portraits remain unchanged by reflections about either axis. In the absence of an intensity modulation, Fig. 4.2(a), the stroboscopic phase portrait reflects the phase space trajectories of the stationary standing. We stress again that because the motion is integrable in this case, the stroboscopic phase portraits are restricted to one dimensional curves. When $\epsilon = 0.1$ the trajectories near the separatrix are no longer constrained to a curve and fill out a two dimensional area called a resonance layer. These trajectories appear stochastic because of their sensitive dependence on their initial conditions. Away from the separatrix the motion still appears regular.

Notice also the appearance of elliptic fixed points of the Floquet map at $(q, p) \approx (0, 0), (q, p) \approx (0, \pm 1.2)$ and $(q, p) \approx (0, \pm 2.2)$. As the modulation amplitude is increased to $\epsilon = 0.2$ both the resonance layer and the stable regions centered on the two new elliptic fixed points increase in size. We also see the appearance of a resonance layer joining the fixed points $(q, p) \approx (1.2) \text{ and } (q, p) \approx (0, -1.2)$. Note that the stable regions centered on $(q, p) \approx (0, \pm 1.2)$ increase in area as $\epsilon$ increases from 0.0 to 0.2 and begin to decrease when $\epsilon$ is increased to 0.3.

Although the appearance of resonance layers about the separatrix and the bound state elliptic fixed points imply that the motion is no longer
integrable, still in some regions of phase space the motion appears to be confined to one-dimensional curves. The dual behavior of quasi-integrable systems is a consequence of the very important KAM theorem. Stated simply the KAM theorem shows that for smooth perturbations that are sufficiently small there will exist some trajectories far from a resonance that are confined to one dimensional curves. Away from a separatrix these KAM curves bound the stochastic motion to very thin layers so that on the global scale the dynamics in this region appears regular. Close to a separatrix trajectory KAM curves cannot form so that stochastic motion occupies a much larger region of phase space.

4.1.2 quantum phase space

When the mean height of the cosine potential \( \kappa \) is of the same order as the quantum energy spacing at the bottom of the cosine well \( \hbar \sqrt{\kappa} \),
then the quantum mechanical nature of the motion of the atom becomes significant. The motion of the atom is generated by the Hamiltonian

$$\hat{H}_a(t) = \frac{\hat{p}^2}{2} + 2\kappa (1 - \kappa \cos t) \sin^2(\hat{q}/2).$$

(4.11)

This Hamiltonian is time-dependent and so its eigenstates will also depend on time. Therefore it is not fruitful to analyse the dynamics of the atom in terms of stationary states. Let $\hat{U}_a(t_1, t_0)$ be the unitary operator that evolves the atom from time $t_0$ to $t_1$. From the group property of unitary evolution and the periodicity of the ground state Hamiltonian with respect to time, the evolution $\hat{U}_a(t_0 + 2\pi s, t_0)$ is equal to $\hat{U}_a(t_0 + 2\pi, t_0)^s$. Therefore the stroboscopic dynamics of the atom is generated by the single unitary operator $\hat{U}_a(t_0 + 2\pi, t_0)$ which is the solution of the operator differential equation

$$i\kappa \frac{d\hat{U}_a(t, t_0)}{dt} = \hat{H}_a(t)\hat{U}_a(t, t_0),$$

(4.12)

evaluated at $t = t_0 + 2\pi$ subject to the initial condition $\hat{U}_a(t_0, t_0) = \hat{I}$. As for the case of the classical approximation set $t_0 = 0$, and denote the corresponding unitary operator by $\hat{F}$. Because $\hat{F}$ generates the quantum stroboscopic evolution of the atom, it can be thought of as the quantization of the classical mapping $F$ and it is called the Floquet operator. If $|\psi\rangle$ is the initial center-of-mass state of the atom then the stroboscopically evolved state $|\psi_s\rangle$ is given by

$$|\psi_s\rangle = \hat{F}^s|\psi\rangle.$$

(4.13)

The Floquet operator has symmetries which are related to the invariance of $\hat{H}_a$ under translation, parity, and time reversal transformations. The translational symmetry (2.14) of the Hamiltonian is also a property of $\hat{F}$:

$$[\hat{F}, \hat{S}_{2\pi}] = 0.$$

The analogues of the classical symmetries Eq. (4.9) and Eq. (4.10) are

$$\hat{F}\hat{P} = \hat{P}\hat{F},$$

(4.14)

$$\hat{F}\hat{T} = \hat{T}\hat{F}^{-1},$$

(4.15)

where $\hat{P}$ is the linear parity operator with the following action on momentum eigenstates $\hat{P}|p\rangle = |-p\rangle$ and $\hat{T}$ is the anti-linear time-reversal operator with the same action as $\hat{P}$ on the momentum eigenstates.

It is worth dwelling for a while on the subject of anti-linear operators and time-reversal symmetries. These concepts are quite important when
studying quantum signatures of classical chaos [22]. Momentum and parity conservation laws are the result of the periodic and symmetric nature of the physical system. They arise from these geometrical symmetries and the invariance of quantum theory under multiplication of wavefunctions by a global phase. The Schrödinger equation is also invariant under a transformation that is not related to geometry: the operation of complex conjugation of the wavefunction. Complex conjugation is a well defined operation provided it is done with respect to a particular representation of the wavefunction. Furthermore it is an anti-linear operation rather than a linear one. In the position representation Schrödinger’s equation,

\[ i\hbar \frac{d\psi}{dt} = \frac{\hbar^2}{2} \frac{\partial^2 \psi}{\partial q^2} + 2\kappa(1 - 2\epsilon \cos t) \sin^2(q/2)\psi, \]  

is invariant under the combined transformations \( \hat{T} : \psi \mapsto \psi^* \) and \( t \mapsto -t \). Therefore taking the complex conjugate in the position representation is equivalent to time reversal invariance of Schrödinger’s equation. Although the position statistics don’t change under \( \hat{T} \) the momentum is reversed so that \( \hat{T}|p\rangle = |-p\rangle \). It is easy to work out the commutation relations between \( \hat{S}_{2\pi}, \hat{P}, \) and \( \hat{T} \):

\[ [\hat{S}_{2\pi}, \hat{T}] = 0, \]  

\[ [\hat{P}, \hat{T}] = 0, \]  

\[ \hat{S}_{2\pi} \hat{P} = \hat{P} \hat{S}_{-2\pi}. \]  

The Floquet operator is invariant under translations by \( 2\pi \) so its eigenstates \( |e_n, p\rangle \) are labeled by a band number \( n \) and a quasi-momentum variable \( p \in [-\hbar/2, \hbar/2) \). They satisfy the unitary eigenvalue problems

\[ \hat{F}|e_n, p\rangle = \exp \left(-2\pi i e_n(p)/\hbar\right) |e_n, p\rangle, \]  

\[ \hat{S}_{2\pi}|e_n, p\rangle = \exp \left(2\pi i p/\hbar\right) |e_n, p\rangle. \]  

\( e_n(p) \) is called the quasi-energy we see that it is only defined modulo \( \hbar \). These states provide a convenient basis for studying the stroboscopic evolution of the atom because an arbitrary state \( |\psi\rangle \) evolves to

\[ \hat{F}^s|\psi\rangle = \sum_n \int_{-\hbar/2}^{\hbar/2} \exp \left(-2\pi i s e_n(p)/\hbar\right) |e_n, p\rangle \langle e_n, p|\psi\rangle dp, \]  

after \( s \) cycles of the driving term. As for the stationary standing wave case the atomic states \( |e_n, p\rangle \) and \( |e_n, -p\rangle \) have the same quasi-energy. To
4.1 Phase space

see this, restrict $p$ to the interval $[-\hbar/2, 0]$, and define the quasi-stationary states on the other half of the first Brillouin zone by $|e_n, p\rangle = \hat{P}|e_n, -p\rangle$ for $p \in (0, \hbar/2)$. Using the relation (4.19) it can be verified that this new state is an eigenstate of $\hat{S}_2\pi$ with eigenvalue $\exp(2\pi ip/\hbar)$. From the commutation relation (4.14) it follows that $e_n(-p) = e_n(p)$.

The symmetry properties are very useful when numerically diagonalizing the Floquet operator. The quasi-momenta $p = -\hbar/2$ and $p = 0$ are special because the corresponding quasi-stationary states are eigenstates of both $\hat{S}_2\pi$ and $\hat{P}$. For $p \in (-\hbar/2, 0)$ the new quasi-stationary states

$$|e_n, p\rangle_\pm = \frac{1}{\sqrt{2}} (|e_n, p\rangle \pm |e_n, -p\rangle) ,$$

are even (+) and odd (−) parity under $\hat{P}$. Expanding $|e_n, p\rangle_\pm$ in terms of momentum eigenstates,

$$|e_n, p\rangle_\pm = \sum_{m=-\infty}^{\infty} \frac{a_m}{\sqrt{2}} (| - p + m\hbar\rangle \pm |p - m\hbar\rangle) ,$$

it follows from Eqs. (4.14) and the anti-linearity of $\hat{T}$ that

$$\hat{F}\hat{T}|e_n, p\rangle_\pm = \exp(-2\pi ie_n(p)/\hbar)\hat{T}|e_n, p\rangle_\pm .$$

Thus $|e_n, p\rangle_\pm$ and $\hat{T}|e_n, p\rangle_\pm$ are degenerate. We may now form a new basis of quasi-stationary states by symmetric and anti-symmetric combinations of degenerate pairs. In that case the parity condition implies $a_m = \pm a_n^*$, so that the expansion of the new quasi-stationary states in the momentum basis may be chosen real. Using a similar argument one can show that this results also holds for the quasi-momenta $p = -\hbar$ and $p = 0$. The operator $\hat{F}$ may be numerically diagonalized for the quasi-momentum $p = 0$. Using the parity and time-reversal symmetries it is possible to reduce the problem of diagonalizing a complex unitary operator to an equivalent problem of diagonalizing a real symmetric operator. Then one might use Householder’s method and the QL algorithm in the NAG library to ensure that the numerical quasi-stationary states were real in the momentum basis and strictly orthogonal.

In figures 4.3, 4.4, 4.5 and 4.6 the $Q$ function has been used to give a phase space representation to some of the eigenstates of the quantum Floquet operator. The eigenstates are all restricted to the quasi-momentum $p = 0$, and the dimensionless Planck constant $\hbar = 0.05$. Figure 4.3 shows four states corresponding to the four kinds of classical trajectories: stable fixed point, libration, separatrix, and rotation. The separatrix is strongly peaked at the classical unstable fixed point. Figure 4.4 shows some eigenstates for $\epsilon = 0.1$. The stable fixed point state and the libration states are
still found but the separatrix states are now more complicated and quantum states corresponding to the elliptic fixed points at \((q, p) \approx (0, \pm 1.2)\) have formed. When \(\epsilon = 0.2\) (see Fig. 4.5) states concentrated about the fixed points \((q, p) \approx (0, \pm 2.2)\) begin to form and have developed further by the time that \(\epsilon = 0.3\).

### 4.2 Perturbation theory

#### 4.2.1 classical perturbation theory

A discussion of classical perturbation theory was already given in the first part of this subject. Here we present a summary of as much of the formalism as will be required in subsequent sections. Denote the nonlinear pendulum (4.2) in the limit \(\epsilon = 0\) by \(H_0\). There is a canonical transformation from \((q, p)\) to new conjugate variables \((J, \Theta)\) such that \(H_0\)
Fig. 4.4. Some $Q$ functions of Floquet operator eigenstates when $\epsilon = 0.1$. 
Fig. 4.5. Some \( Q \) functions of Floquet operator eigenstates when \( \epsilon = 0.2 \).
Fig. 4.6. Some $Q$ functions of Floquet operator eigenstates when $\epsilon = 0.3$. 
Quasi-integrable motion is a function of $J$ only and the classical frequency of oscillation $\omega_{cl}(J)$ is given by elliptic integrals, with the energy $E$ considered as a function of action. Consider the perturbation of the Hamiltonian, Eq. (4.2) as a power series in $\epsilon$: $H(J, \Theta, t) = H_0(J) + \epsilon H_1(J, \Theta, t)$, where $H_1 = 2\kappa \cos t \cos \theta$. To determine if first-order resonances occur we Fourier analyse the first-order (in $\epsilon$) term i.e. $\epsilon H_1(J, \Theta, t)$:

$$H_1 = \sum_{m=0, \pm1, \pm2,...} H_{1,2m}(\exp(i(t + 2m\Theta) + c.c.). \tag{4.26}$$

Then first-order resonance solutions occur for $J$ given by

$$2m \omega_{cl}(J) - 1 = 0, \quad m = 0, \pm1, \pm2, ... \tag{4.27}$$

To determine if second-order resonances occur we must first find approximate action-angle variables $(\bar{J}, \bar{\Theta})$ for $H(J, \Theta, t)$ up to and including the order $\epsilon$ terms. Provided $J$ is not close to a first-order resonance, we can do this through a canonical transformation so that the new Hamiltonian is

$$\bar{H}(\bar{J}, \bar{\Theta}, t) = H_0(\bar{J}) + \epsilon^2 H_2(\bar{J}, \bar{\Theta}, t) + ... \tag{4.28}$$

There are two things to note here: Firstly there is no order $\epsilon$ term. This is because $H_1$ is purely oscillatory. Up to order $\epsilon$ then the only qualitative changes introduced by the perturbation are due to the first-order resonances. Secondly the canonical transformation has introduced an $\epsilon^2$ term into the new Hamiltonian; $\epsilon^2 H_2$. It is the Fourier analysis of this term that shows the second-order resonance solutions. Here

$$H_2 = \sum_{m=0, \pm1, \pm2} H_{2,2m}(\exp(i(2t + 2m\Theta) + c.c)$$

$$+ \text{time independent terms}. \tag{4.29}$$

So second-order resonances occur for $\bar{J}$ given by

$$m \omega_{cl}(\bar{J}) - 1 = 0, \quad m = 0, \pm1, \pm2, ... \tag{4.30}$$

If $J$ (or $\bar{J}$) satisfies a resonance condition it is not an approximate invariant as in an integrable system. In fact it can be shown that a chain of stable and unstable orbits lie in its place. Furthermore there is a region around the stable periodic orbits in which solutions lie on tori, or invariant curves for the stroboscopic map. We can calculate the width $\Delta J$, perpendicular to the invariant $J$ of this region as an estimate of the size of the resonance. For first order resonances the width is of order $\sqrt{\epsilon}$ and for second-order of order $\epsilon$. So for $\epsilon$ small first-order resonances are typically more important. However for the system we have here all the
first-order resonances are clustered near the separatrix. For $\epsilon = 0.1$ they have overlapped to form a chaotic band as seen in Fig. 4.2 (b). But there is one second-order resonance $\omega_{cl}(\bar{J}) = \pm 1$ at a significantly smaller value of $\bar{J}$ which is important. The two stable periodic points that replace the invariant appear in Fig. 4.2 (b) as fixed points of the stroboscopic map at $(q,p) \approx (0.0 \pm 1.2)$ and the width of the resonance is surprisingly large $\Delta \bar{J} \approx 0.44$.

4.2.2 quantum perturbation theory

In the previous section we saw how classical perturbation theory could describe the structure of phase space for systems perturbed slightly away from the integrable Hamiltonian $H_0$. In this section we aim to develop the formalism of quantum perturbation theory as a means of describing quantum phase space for the quantized atomic motion. The perturbation theory of periodically driven quantum system was first formulated by Sambe [?]. In our presentation of that work we will try to emphasize its connection with the classical Poincaré-Von Ziepel perturbation theory of subsection 4.2.1. We begin with the observation that in the limit of $\epsilon = 0$ the quantum stroboscopic map $\hat{F}$ is simply

$$\hat{F} = \exp \left( -\frac{2\pi i H_0}{\hbar} \right),$$  \hspace{1cm} (4.31)

where $\hat{H}_0 = \hat{p}^2/2 - \kappa \cos \hat{q}$. Denote the stationary states of $\hat{H}_0$ with energy $E_n(p)$ by $|E_n,p\rangle$, then $|E_n,p\rangle$ is a quasi-stationary state for $\hat{F}$ with quasi-energy $e_n(p) = E_n(p)$. In analogy with time-independent quantum perturbation theory we assume that for small $\epsilon$ the perturbed quasi-stationary states $|e_n,p\rangle$ and quasifrequency $e_n(p)$ are close to $|E_n,p\rangle$ and $E_n(p)$ respectively, and then attempt to find corresponding asymptotic expansions.

Let $|e_n,p,t\rangle$ denote the state evolving from the initial quasi-stationary state $|e_n,p\rangle$ under the time-dependent dynamics (4.12) generated by the Hamiltonian

$$\hat{H}(t) = \hat{H}_0 + \epsilon \hat{H}_1(t).$$  \hspace{1cm} (4.32)

For the moment consider the general case where $\hat{H}_1(t)$ is any Hermitian operator periodic in time with the symmetries (4.14) and (4.15). Then $|e_n,p,t\rangle$ satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt}|e_n,p,t\rangle = \hat{H}(t)|e_n,p,t\rangle$$  \hspace{1cm} (4.33)

subject to the condition $|e_n,p,2\pi\rangle = \exp(-2\pi i e_n(p)/\hbar)|e_n,p,0\rangle$. We introduce states $|v_n,p\rangle = \exp(i e_n(p)t/\hbar)|e_n,p,t\rangle$ which are periodic in $t$. 
The state $|v_n, p\rangle$ satisfies the equation

$$e_n(p)|v_n, p\rangle = -i\hbar \frac{d}{dt}|v_n, p\rangle + \hat{H}(t)|v_n, p\rangle .$$  (4.34)

In order to use the methods of time-independent perturbation theory we introduce the notion of an extended Hilbert space as follows. Since $|v_n, p\rangle$ is periodic in $t$ it has a Fourier expansion in terms of the momentum eigenstates $|p + m\hbar, l\rangle$ and time:

$$|v_n, p\rangle = \sum_{l,m=\pm\infty}^{\infty} \exp(ilt)v_{nlm}|p + m\hbar, l\rangle.$$  (4.35)

We can think of the function $\exp(ilt)$ as an eigenstate of the momentum-like operator $\hat{h} = -i\hbar \frac{d}{dt}$ in the Hilbert space $L_2(0, T)$. Denote this state by $|l\rangle$. Eq. (4.35) is now thought of as an expansion of $|v_n, p\rangle$ in terms of the states $|p + m\hbar, l\rangle = |p + m\hbar\rangle \otimes |l\rangle$ and Eq. (4.34) becomes an eigenvalue problem

$$e_n(p)|v_n, p\rangle = \hat{K}|v_n, p\rangle ,$$  (4.36)

where $\hat{K}$ is the Hermitian operator $\hat{K} = \hat{h} + \hat{H}(\hat{t})$ acting on the extended Hilbert space $\mathcal{K} = \mathcal{H} \otimes L_2(0, T)$. Notice that $\hat{K}$ is precisely equal to the quantization of the classical Hamiltonian on the extended phase space introduced in subsection (4.1.1). Once the eigenvalue problem Eq. (4.36) has been solved we can recover the quasistationary state $|e_n, p\rangle$ by the projection $|e_n, p\rangle = \langle t = 0|v_n, p\rangle$, where

$$|t\rangle = \sum_{l=-\infty}^{\infty} |l\rangle \exp(ilt).$$  (4.37)

To solve the eigenvalue problem perturbatively we diagonalize the 'free' operator $\hat{K}_0 = \hat{h} + \hat{H}_0$. The eigenstates of $\hat{K}_0$ are just $|E_n, p, l\rangle = |E_n, p\rangle \otimes |l\rangle$ and it is not difficult to verify that

$$\hat{K}_0|E_n, p, l\rangle = (E_n(p) + l\hbar)|E_n, p, l\rangle ,$$  (4.38)

so that $|E_n, p, l\rangle$ has eigenvalue $E_n(p) + l\hbar$. Without loss of generality we look for eigenstates of $\hat{K}$ that reduce to $|E_n, p, 0\rangle$ in the limit as $\epsilon$ vanishes. We assume that the energy level $E_n(p)$ of $\hat{K}$ is nondegenerate and that $|v_n, p\rangle$ and $e_n(p)$ have the following asymptotic expansions

$$e_n(p) = E_n(p) + \epsilon e_n^{(1)}(p) + \epsilon^2 e_n^{(2)}(p) + O(\epsilon^3) ,$$  (4.39)

$$|v_n, p\rangle = |E_n, p, 0\rangle + \epsilon |v_n^{(1)}, p\rangle + \epsilon^2 |v_n^{(2)}, p\rangle + O(\epsilon^3) .$$  (4.40)
The new quasi-energy and quasistationary state are then calculated using standard Rayleigh-Schrödinger perturbation theory \[13\]. Up to second-order the corrections to the quasi-energies are

\[
e^{(1)}_n(p) = \langle E_n, p | \hat{H}_1 | E_n, p \rangle,
\]

\[
e^{(2)}_n(p) = \langle E_n, p | \sum_l \hat{H}_{1l}^\dagger E_n(p) - H_0 - \mathbb{R} \rangle (1 - \delta_0 \hat{P}_n(p)) \hat{H}_{1l} | E_n, p \rangle,
\]

and setting all arbitrary constants to zero before projecting onto \(\mathcal{H}\) the corrections to the quasistationary state are

\[
|e^{(1)}_n(p)\rangle = \hat{A}^{(1)}_n |E_n, p\rangle,
\]

\[
|e^{(2)}_n(p)\rangle = \hat{A}^{(2)}_n |E_n, p\rangle,
\]

where

\[
\hat{A}^{(1)}_n = \sum_l \frac{1}{E_n(p) - H_0 - \mathbb{R}} \left[ 1 - \delta_0 \hat{P}_n(p) \right] \hat{H}_{1l},
\]

\[
\hat{A}^{(2)}_n = -\sum_k \frac{1}{E_n - H_0 - \mathbb{R}} \left[ 1 - \delta_k \hat{P}_n(p) \right] \\
\times \left( e^{(1)}_n(p) \frac{1}{E_n(p) - H_0 - \mathbb{R}} \left[ 1 - \delta_k \hat{P}_n(p) \right] \hat{H}_{1k} \\
- \sum_l \hat{H}_{1l}^\dagger E_n(p) - H_0 - \mathbb{R} \left[ 1 - \delta_l \hat{P}_n(p) \right] \hat{H}_{1k-l} \right).
\]

In the above equations \(\hat{P}_n(p) = |E_n, p\rangle \langle E_n, p|\) denotes the projection onto \(|E_n, p\rangle\) and \(\hat{H}_{1l}\) is the Fourier component of \(\hat{H}_1\) rotating at frequency \(l\). Equations (4.41) to (4.46) are the natural generalization of time-independent perturbation theory to the case of perturbations periodic in time. By setting \(\hat{H}_l = 0\) for all \(l \neq 0\) we recover the expressions of normal time-independent perturbation theory \[13\]. Note that the time-dependent components of \(\hat{H}_1(t)\) only begin to contribute to the shift in quasi-energy at second-order. This is analogous to the result that to first-order in \(\epsilon\) the classical Hamiltonian \(\bar{H}(\bar{I})\) only depends on the cycle-averaged part of \(\hat{H}(t)\).

The matrix elements \(\langle E_n', p |\hat{A}^{(1)}_n |E_n, p\rangle\) and \(\langle E_n', p |\hat{A}^{(2)}_n |E_n, p\rangle\) become singular when the free energy levels satisfy the resonance condition \(E_n(p) - E_{n'}(p) = \mathbb{R}\) where \(l\) is an integer. We will call them first or second-order resonances depending at which order the singularity occurs. In the language of time-independent perturbation theory and extended Hilbert
space a quantum resonance indicates that the Hamiltonian $\hat{K}_0$ has degenerate energy levels. In this case we must use degenerate perturbation theory to find the new quasi-stationary states. There is an important difference between the classical and quantum mechanical perturbation theories outlined above: Exact quantum resonances between bands with $E_n < V_{\text{max}} = 2\kappa$ are less likely than classical resonances because the quantum frequency bands are discrete and their width is small compared to their separation, whilst classical frequencies form a continuum. If the system is semi-classical, by which we mean that the principal of quantized action gives a good approximation to the quantum energy levels of the free Hamiltonian $\hat{H}_0$, then for nearby energy levels the local classical frequency is related to the energy difference by the equation

$$E_n - E_{n-\Delta n} \approx \Delta n \kappa \omega_{cl}(J_n),$$

(4.47)

where $J_n$ is the semi-classical action. For each classical resonance $\Delta n \omega_{cl}(J) - l = 0$ there will be energy bands with $E_n(p)$ and $E_{n-\Delta n}(p)$ satisfying the near-resonance condition $E_n(p) - E_{n-\Delta n}(p) \approx \Delta n \kappa$. The perturbed quasi-stationary state $|e_n, p\rangle$ will rapidly develop a significant component along $|e_{n-\Delta n}, p\rangle$ as $\epsilon$ is increased. In the work by Berman et al [23, 24, 25], and in our following analysis it is assumed that the average free energy spacing is well approximated by a low order expansion in the principal quantum number $n$. When this is not the case we would expect there to be quantum resonances that are not present in the classical model.

Now consider the special case (4.2) where $\hat{H}_1(t) = 2\kappa \cos t \cos \hat{q}$. For the classical second-order resonance where $\Delta n = l = \pm 2$ there will be energy levels satisfying

$$E_n - E_{n\pm 2} \approx \pm 2\kappa.$$  

(4.48)

We see from Eq. (4.46) that these states give rise to near resonant denominators in second-order expansions of quantum perturbation theory. In Figure 4.7 we have expanded the odd parity state $|e_{-}, 0\rangle$ represented in Fig. 4.5(b) in terms of the unperturbed stationary states $|E_n, 0\rangle$. We find that it is a superposition of a dominant state $|E_{11}, 0\rangle$, the $Q$ function of which is shown in Fig. 4.3(b), and two other states $|E_9, 0\rangle$ and $|E_{13}, 0\rangle$ satisfying the near-resonant conditions: $E_{11}(0) - E_9(0) = 0.103 \approx 2\kappa$, and $E_{11}(0) - E_{13}(0) = -0.101 \approx -2\kappa$. Evidently the interference between near resonant states has caused the $Q$ function in Figure 4.5(b) to become concentrated about the stable regions of the classical second-order resonance.
4.3 Dynamics on a resonance

The appearance of stable regions in the classical stroboscopic phase portrait and the changes in topography of the quantum mechanical $Q$ functions both result from nonlinear resonances. The interaction between the driving frequency and the natural nonlinear frequency causes the topology of phase space to change. We will now see how this change in phase space is reflected in the dynamics of the atom.

It is expected that the dynamics of a distribution of atoms initially localized far from a resonance will deviate little from the regular motion described in the previous chapter. Conversely it will be shown that the gradual formation of resonance islands in phase space gives rise to a drastic change in the qualitative dynamics, and even in the classical approximation atoms on a second order resonance will not undergo shearing but will remain localized in phase space. It is worth emphasizing that this is a dynamic stability that only occurs when the intensity of the standing wave is modulated. When the atom is treated fully quantum mechanically we see that as well as localization it is now possible for the atomic wavepacket to tunnel from one resonance island to another through a classically inaccessible region of phase space.

4.3.1 classical dynamics

We studied the change in the classical evolution of an ensemble of 1000 points as the perturbation $\epsilon$ is increased from 0.0 to 0.3. The points are initially distributed with the Gaussian density given in the previous chap-
The parameters \((q_0, p_0) = (0, 1.0), \sigma_q = 0.084\) and \(\sigma_p = 0.036\) were chosen to ensure that points was centered on the second-order resonance \((q, p) \approx (0.0, 1.2)\). In Figure 4.8 we have plotted the momentum mean \(\langle p \rangle\) and variance \(V(p)\) as a function of the strobe number \(s\) after the points were evolved by the classical dynamics.

When \(\epsilon = 0.0\) we see that the mean momentum quickly drops to zero and the momentum variance rises as the classical distribution is smeared out over the trajectories of constant energy. This behaviour was described in the previous chapter on regular motion and is due to the nonlinear dependence of the free Hamiltonian on the action. As the perturbation parameter \(\epsilon\) is increased from 0.0 to 0.2 the growth in momentum variance is suppressed and the mean momentum remains near its initial value indicating that the classical distribution is being localized about the stable fixed point. We interpret this as follows. The width of the stable region is increasing linearly with \(\epsilon\) until the classical distribution is contained within the region of the elliptic fixed point. As noted in the previous section when \(\epsilon\) is increased to 0.3 the stable region of phase space begins to shrink because of the destruction of KAM tori. As a result we see in Figure 4.8 (d) that the classical distribution becomes delocalized again.

### 4.3.2 Quantum dynamics

In our simulations of the quantum dynamics of Eq. (4.13) we have taken \(\hbar = 0.05\). From the discussion of regular motion we assume that to a good approximation the band structure of the driven Hamiltonian can be neglected and have therefore restricted our simulations to states with the quasi-momentum \(p = 0\). The Floquet operator \(\hat{F}\) was found by numerically integrating the operator differential equation (4.12) in the momentum representation. Since \(\hat{P}\) and \(\hat{T}\) are symmetries of the quantum evolution and the quasistationary states are real in the momentum basis the problem of finding eigenstates of \(\hat{F}\) reduces to the diagonalization of a real symmetric matrix. The stationary states \(|E_n, p\rangle\) and the energies \(E_n(p)\) were found by diagonalizing the Hamiltonian \(\hat{H}_0\) in the momentum representation and are labelled in order of increasing energy from the ground state \(n = 0\).

We have graphed the quantum mean \(\langle \hat{p} \rangle\) and variance \(V(\hat{p})\) of momentum as a function of the strobe number \(s\) in Figure 4.9. The initial state \(|\psi\rangle\) was chosen to be a minimum-uncertainty state with \(\langle \hat{q} \rangle = 0.0, \langle \hat{p} \rangle = 1.0, \text{ and } \langle \Delta \hat{p}^2 \rangle = 0.01\) so that its \(Q\) function was equal to the classical probability distribution used in the classical approximation. Once the Floquet operator had been diagonalized we use Eq. (4.22) to calculate the quantum stroboscopic evolution. When \(\epsilon = 0.0\) we see that initially
Fig. 4.8. Plot of classical momentum statistics versus strobe number $s$. (a) $\epsilon = 0.0$, (b) $\epsilon = 0.1$, (c) $\epsilon = 0.2$, (d) $\epsilon = 0.3$. Solid line, $\langle p \rangle$; dashed line, $V(p)$. 
Fig. 4.9. Plot of quantum momentum statistics versus strobe number $s$. (a) $\epsilon = 0.0$, (b) $\epsilon = 0.1$, (c) $\epsilon = 0.2$, (d) $\epsilon = 0.3$. Solid line, $\langle \hat{p} \rangle$; dashed line, $V(\hat{p})$. 
4.3 Dynamics on a resonance

Fig. 4.10. Quasistationary state distribution of a minimum uncertainty state. (a) $\epsilon = 0.0$, (b) $\epsilon = 0.2$.

the mean momentum quickly drops to zero and the momentum variance rises as the quantum wave packet becomes delocalized. This is due to the nonlinear dependence of $E_n(p)$ on the quantum number $n$. The decrease in momentum variance when $s$ is a multiple of 150 indicates a revival of the initial wave packet due to the quadratic dependence of $E_n(p)$ on $n$.

Like the classical dynamics of the atom we find that as $\epsilon$ increases from 0.0 to 0.2 the growth in the quantum momentum variance is suppressed and the mean becomes fixed about its initial value indicating that the atom is being localized. In Figure 4.10 we have represented the probability distribution of the state $|\psi\rangle$ in the $\epsilon = 0.0$ and $\epsilon = 0.2$ bases of quasi-stationary states using the method introduced by Sanders and Milburn [?]. The length of each phasor $\chi_m$ equals the overlap probability $|\langle e_n, p |\psi\rangle|^2$ and its angle equals the eigenphase $-2\pi e_n(p)/\hbar$. Comparing the two distributions we see that as the perturbation parameter is increased the support on the quasistationary states has decreased to two states with almost identical quasifrequencies. We have verified that these states have opposite parity and for the purpose of this discussion $|e_+, 0\rangle$ and $|e_-, 0\rangle$ will denote the even and odd states respectively. The state $|e_-, 0\rangle$, represented in Fig. 4.5(b) and discussed in subsection 4.2.2, is strongly peaked about the stable fixed points and is an example of a second order quantum nonlinear resonance. The state $|e_+, 0\rangle$ also arises from a second order quantum resonance and has a $Q$ function peaked at the classical resonances $(q, p) \approx (0, \pm 1.2)$. Now we see the role of the quantum resonance in the dynamic localization of quantum wave packets. It has caused the resonant quasistationary states to become strongly peaked about the stable fixed points such that the initial minimum uncertainty
state is approximated by a sum of two states with opposite parity. Since these two states have almost identical quasifrequencies the minimum uncertainty is approximately stationary.

When $\epsilon$ is increased to 0.3 we would expect the quantum motion to reflect the delocalization of the classical atomic distribution shown in Figure 4.8 (d). Since the minimum uncertainty state is the sum of two quasistationary states with opposite parity we would expect to find that it is now possible for the atom to coherently tunnel between the resonances $(q, p) \approx (0.0, 1.2)$ and its reflected partner $(q, p) \approx (0.0, -1.2)$. This is precisely what we see in Figure 4.9(d) and is due to the detuning of the two dominant quasi-energies.

Even though it has been stressed that localization occurs because of a second-order resonance in quantum perturbation theory it would be expected from the results of Sec. 4.2 that localization and tunnelling will occur at first-order resonances as well. Indeed, since the small denominators occur at lower order in $\epsilon$ the localization should develop faster than for second-order resonances.
Dynamical localisation.

5.1 The Kicked rotor

We consider a system composed of a free rotor subject to impulsive torques:

\[ H(t) = \frac{L^2}{2} + k \cos \theta \sum_n \delta(t - n) \]  

(we measure time in units of the kick period). The stroboscopic map is then defined by

\[ \theta_{n+1} = \theta_n + L_{n+1} \]  
\[ L_{n+1} = L_n + k \sin \theta_n \]

where \( \theta_n, \ L_n \) are the values of the phase space variables immediately after the n’th kick. For small values of \( k \), the phase space is dominated by mostly regular motion. For \( k = k_c = 0.9716 \ldots \) the last of the invariant torus is destroyed and globally chaotic motion is evident. At this point the angle variable is changing rapidly and seemingly at random from kick to kick while the angular momentum appears to slowly diffuse. This can be seen as follows. As soon as \( |L_n| \) is of the order of \( 2\pi \) or larger, successive \( \theta \) are uncorrelated due to the modular nature of the angle variable (that is to say mod \( 2\pi \)). In that case the sign of \( \sin \theta_n \) is essentially a random variable and thus successive increments of \( L_n \) are random and the angular momentum begins to look like a random walk.

If we begin with an initial distribution of points in phase space, the apparently random, yet deterministic motion will cause the points to move apart rapidly in angle and more slowly in angular momentum. Let the initial distribution be given by \( P(L, \theta; 0) \). We will assume that this distribution factorises so that

\[ P(L, \theta; 0) = \frac{1}{2\pi} P_0(L) \]
which is uniformly distributed in angle. The contours of the distribution are bands in the cylindrical phase space of the rotor. We will assume that the distribution is very sharply peaked at \( L = L_0 \), that is \( P_0(L) = \delta(L - L_0) \). Under deterministic dynamics the phase space distribution at \( n \) kicks is

\[
P(L, \theta; n) = \int_{-\infty}^{\infty} dL' \int_{0}^{2\pi} d\theta' \delta(L - L_n(L', \theta')) \delta(\theta - \theta_n(L', \theta')) P(L', \theta'; 0)
\]

\[
= \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \delta(L - L_n(L_0, \theta')) \delta(\theta - \theta_n(L_0, \theta'))
\]

We now change variables by defining the \( L = L_0 + \Delta L \). The marginal probability for the change in momentum to be \( \Delta L \) after \( n \) kicks is obtained by integrating over \( \theta \),

\[
P(\Delta L; n) = \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \delta(\Delta L - L_n(L_0, \theta') + L_0)
\]

Using the Fourier transform representation of the delta function this may be written as

\[
P(\Delta L; n) = \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix(\Delta L - L_n + L_0)}
\]

\[
= \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix\Delta L} \prod_{p=0}^{n-1} e^{-ix(L_{p+1} - L_p)}
\]

\[
= \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix\Delta L} \prod_{p=0}^{n-1} e^{-ixk \sin \theta_p}
\]

where we must keep in mind that \( L_n = L_n(L_0, \theta') \) and thus \( \theta_k = \theta_k(L_0, \theta') \).

We now assume that for large \( p \) the values of \( \theta_p \) are uncorrelated, independent random variables with the same distribution as the original uniform distribution. The integral over \( \theta' \) can be performed using

\[
\int_{0}^{2\pi} \frac{d\theta'}{2\pi} e^{-ixk \sin \theta} = J_0(xk)
\]

where \( J_0(y) \) is a Bessel function. Thus

\[
P(\Delta L; n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{ix\Delta L} [J_0(kx)]^n
\]

Now the \( N \)th power of the Bessel function is a rapidly oscillating function of \( x \), so the integral will be dominated by terms near \( x = 0 \). For large
5.2 Quantum kicked rotor

values of $n$ and small $x$ we can use the approximation

$$[J_0(kx)]^n = e^{n \ln J_0(kx)} = \exp\left[-\frac{n}{4}(kx)^2 + \ldots\right]$$

(5.10)

In the limit $n \to \infty$ the unwritten terms in this equation can be neglected. Finally we need only perform a Fourier transform of a Gaussian in Eq.(5.9),

$$P(\Delta L; n) = \frac{1}{k\sqrt{\pi n}} \exp\left[-\frac{(\Delta L)^2}{k^2 n}\right]$$

(5.11)

Thus the variance of the increment $\Delta L$ is

$$\langle (\Delta L)^2 \rangle = \frac{k^2}{2n}$$

(5.12)

We see that the change in momentum increases linearly in discrete time and is thus a diffusion process with a diffusion constant

$$D = \frac{k^2}{2}$$

(5.13)

A better approximation for the integral over the Bessel function can be obtained to give departures from this quadratic dependence.

5.2 Quantum kicked rotor

The Floquet operator for kicked systems is easy to obtain (which is why kicked systems are so popular among theoreticians). Given a periodic Hamiltonian of the form

$$H(t) = H_0 + V_0 \sum_n \delta(t - n\tau)$$

(5.14)

where $\tau$ is the period and $V_0$ is some potential function. Now replace the delta a function by a pulse of width $\Delta \tau$ and height $(\Delta \tau)^{-1}$, where we will eventually take the limit of $\Delta \tau \to 0$. The we can write

$$H(t) = \begin{cases} -\frac{H_0}{\Delta \tau}V_0 & n\tau < t < (n+1)\tau - \Delta \tau \\ H_0 + \frac{1}{\Delta \tau}V_0 & (n+1)\tau - \Delta \tau < t < (n+1)\tau \end{cases}$$

(5.15)

The Hamiltonian is piecewise constant in time so we can integrate to get the time evolution operator directly, which gives

$$F = \exp\left[\frac{-i}{\hbar} \left(H_0 + \frac{1}{\Delta \tau}V_0\right) \Delta \tau\right] \exp\left(\frac{-i}{\hbar}H_0(\tau - \Delta \tau)\right).$$

(5.16)
Then in the limit $\Delta \tau \to 0$, we get

$$ F = \exp \left( -\frac{i}{\hbar} V_0 \right) \exp \left( -\frac{i}{\hbar} H_0 \tau \right) \quad (5.17) $$

The Floquet operator for the kicked rotor is

$$ F = \exp \left( -\frac{i}{\hbar} k \cos \theta \right) \exp \left( -\frac{i}{\hbar} \tau \hat{L}^2 \right) \quad (5.18) $$

where we have included an explicit dependence on the kick period $\tau$. In the basis which diagonalises $\theta$ the angular momentum operator is a generator of displacement, thus

$$ \hat{L} = \frac{i}{\hbar} \frac{\partial}{\partial \theta} \quad (5.19) $$

The eigenstates of $\hat{L}$ are simply

$$ |n\rangle = \frac{1}{\sqrt{2\pi}} e^{in\theta} \quad n = 0, \pm 1, \pm 2, \ldots \quad (5.20) $$

The matrix elements of $F$ in this basis are easily determined;

$$ F_{nm} = \langle n | F | m \rangle $$

$$ = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta} \exp \left( -\frac{i}{\hbar} k \cos \theta \right) \exp \left( -\frac{i}{\hbar} \tau \hat{L}^2 \right) e^{im\theta} $$

$$ = \exp \left( -\frac{i}{\hbar} \frac{m^2 \tau}{2} \right) \frac{1}{2\pi} \int_0^{2\pi} \exp \left( -\frac{i}{\hbar} k \cos \theta \right) e^{-i(m-n)\theta} d\theta $$

$$ = \exp \left( -\frac{i}{\hbar} \frac{m^2 \tau}{2} \right) i^{m-n} J_{k-l}(k/\hbar) . \quad (5.21) $$

In this representation the Floquet matrix elements fall off rapidly as we move away from the diagonal. This gives a banded structure to the matrix.

We can now consider what happens for an initial state $|\psi_0\rangle$. We can expand such states in the diagonal representation of $\theta$,

$$ |\psi_0\rangle = \int_0^{2\pi} a(\theta) |\theta\rangle \quad (5.22) $$

In the basis which diagonalises the angular momentum operator $\hat{L}$ this state may be written

$$ |\psi_0\rangle = \sum_{n=-\infty}^{\infty} a_n |n\rangle \quad (5.23) $$
where the transformation of the coefficients between the two bases is

\[ a_n = \frac{1}{2\pi} \int_0^{2\pi} a(\theta)e^{-in\theta} d\theta \]  

(5.24)

The variance in \( \hat{L}^2 \) after \( n \) kicks is

\[ \langle (\Delta \hat{L})^2 \rangle_n = \langle \psi_0 | (F^n)^\dagger (\Delta \hat{L})^2 F^n | \psi_0 \rangle \]  

(5.25)

where \( \Delta \hat{L} = \hat{L} - \langle \hat{L} \rangle \).

In the eigenbasis of \( \hat{L} \) this may be written

\[ \langle (\Delta \hat{L})^2 \rangle_n = \hbar^2 \left( \sum_{l,k,k'} l^2 (F^n)_{lk}(F^n)_{lk'} a_k a_{k'}^* \right) \]  

(5.26)

where we have assumed that the initial state is chosen so that \( \langle \hat{L} \rangle_n = 0 \).

We need to choose an initial state which corresponds to the classical case of a distribution that is uniform in angle, but well localised on a particular angular momentum, \( L_0 \), which we take to be zero. The simplest example of such a state is the angular momentum eigenstate \( |0\rangle \). (See Eq. (5.24)).

For such a state it is easy to prove that the average angular momentum remains zero for all time.

In figure 5.1(a) we plot the variance \( \langle (\Delta \hat{L})^2 \rangle_n \) versus \( n \) for kick strength \( k = 5 \). Also shown is the variance for the classical case with an equivalent initial distribution in phase space. The classical case undergoes diffusive growth as expected. However the quantum case diffuses for a short time (up to around 50 kicks), and then saturates at an almost constant value after about 1000 kicks. The diffusion is suppressed for the quantum case and the state remains localised: this is dynamical localisation. In figure 5.1(b) we present the log of the distribution function \( P(L; 1000) \), for both the classical and quantum description \( P(L = \hbar l; 1000) = |\langle l | \psi \rangle_{1000}|^2 = P_s(l) \) at kick 1000. The classical case is quadratic indicating an approach to a Gaussian distribution as expected. However the quantum case is very nearly linear. The quantum distribution at saturation can be fitted to

\[ P_s(l) = \frac{1}{l_s} \exp \left( -\frac{2|l|}{l_s} \right) \]  

(5.27)

where \( l_s \) is called the localisation length.

The fact that the quantum case saturates is entirely due to the discrete nature of the eigenvalue spectrum of the Floquet operator and its banded structure (ie in the angular momentum basis the off diagonal elements fall off rapidly). If we diagonalise the Floquet operator by means of a unitary transformation \( U \),

\[ F_{ln} = \sum_k e^{-i\phi_k} U_{lk}^* U_{kn} \]  

(5.28)
where $\phi_k$ are the quasienergies, then for the initial state chosen above

$$\langle \hat{L}^2 \rangle = \hbar^2 \sum_{l,k,k'} l^2 e^{i(k-k')\phi_k} U_{kl}^* U_{k0} U_{k'0} U_{k'l}^*$$  \hspace{1cm} (5.29)$$

As the Floquet matrix is banded, so are the unitaries that diagonalise it. Thus the sums in this expression are essentially truncated when the indices $k,k'$ exceed some maximum value $l_s$. The Floquet phases associated are almost uniformly distributed on the unit circle with a mean density of $l_s/2\pi$. The smallest phase difference occurring in the sum is thus of the order of $2\pi/l_s$. For kick numbers $n \leq l_s$ the system does not see the discreteness of the distribution. For $n >> l_s$ however the phase factors oscillate rapidly and all terms except $k = k'$ average to zero, and

$$\langle \hat{L}^2 \rangle = \hbar^2 \sum_{l,k} l^2 |U_{kl}|^2 |U_{k0}|^2$$  \hspace{1cm} (5.30)$$

which is independent of the kick number, $n$. The crossover between the two regions occurs around the kick number $n \sim l_s$; it is also easy to see that when localisation occurs, $\langle \hat{L}^2 \rangle \sim l_s^2$. If we substitute this in the distribution, Eq.(5.27) we find

$$l_s^2 \sim \frac{k^2}{2} l_s = Dl_s$$  \hspace{1cm} (5.31)$$
and thus
\[ l_s = \alpha D \]  \hspace{1cm} (5.32)
which is to say the quantum localisation length is proportional to the classical diffusion constant. Unfortunately the constant of proportionality can only be determined numerically. However for the potential,
\[ V(\theta) = V_0 \arctan(\epsilon - 2k \cos \theta) \]  \hspace{1cm} (5.33)
(the Lloyd model), the proportionality constant is found analytically to be \( \alpha = 1/2 \). The numerical results for the kicked rotor indicate that \( \alpha \) is also close to 1/2.

### 5.3 Experimental demonstration of dynamical localisation.

See handout:

“Atom optics realisation of the quantum \( \delta \) kicked rotor.”

6
Quantum billiards, random matrices and mesoscopic systems.

6.1 Mesoscopic system.
Modern fabrication technology has advanced to the stage where it is possible to fabricate confining potentials for electrons that constitute small cavities for de Broglie waves. Such devices are often called quantum dots as the electron is confined in all three spatial dimensions. In GaAs devices these cavities are made by first confining electrons to a thin layer, called a two dimensional electron gas (2DEG), between a crystal of GaAs and a crystal of AlGaAS. Then a surface gate is used to deplete electrons in the 2DEG in a way that reflects the geometry of the surface gate (see figure 6.1). An alternative way to fabricate a quantum dot is to use a very small metallic grain. In such devices the standard laws of electronics, such as Ohms law, no longer hold. A small conductor shows Ohmic behaviour when its dimensions are much larger than three crucial length scales:

- the de Broglie wavelength as determined by the kinetic energy of the electron,
- the mean free path, the distance an electron travels before its initial momentum is destroyed by scattering,
- the phase relaxation length, the distance an electron travels before the corresponding de Broglie wave suffers a random phase shift.

In typical semiconductor devices at low temperature (below 4K) the mean free path and phase relaxation length are comparable between 10 and 100 microns. The mean free path in polycrystalline metal films can be as small as 50nm. In semiconductors the de Broglie wavelength is between 10 nm and 100nm. In metals the de Broglie wavelength is of the order of the distance between atoms, 0.1nm to 1nm.

In both semiconductors and metals the systems must be held at very low temperature to ensure that the motion of an extra electron injected,
6.1 Mesoscopic system.

Fig. 6.1. Schematic indication of confined two dimensional electronic system using 2DEG heterostructure and surface gates.

with a definite momentum, into the device is \textit{ballistic}. This also requires low bias voltages so that the energy of the injected electron is not too large. This means that the plane wave corresponding to this injected electron propagates without inelastic scattering and this can happen at low temperatures in very pure materials. In reality of course this is not strictly true and the electron will scatter off an impurity or another electron excited above the zero temperature Fermi level. The average distance a ballistic electron travels before scattering is called the phase coherence length $L_\phi$. It can be thought of as the distance the plane wave propagates before its phase undergoes a random shift. At temperatures of around 50mk in GaAs/AlGaAs heterostructures this length is typically 30-40µm. This is usually bigger than the size of the confining region.

A ballistic electron injected into the confining region behaves like a free particle until it bounces elastically off the confining potential. When working at very low temperatures, the Fermi energy is much greater than the thermal excitation energy, $k_BT$. In that case it is no longer appropriate to view the current as due to a slow drift of carriers in a Fermi gas, but rather the current is carried by a few electrons close to the Fermi energy which move much faster. Thus conductance in such \textit{degenerate} conductors is determined by the properties of electrons near the Fermi energy rather than the entire sea of electrons. If the confining region is two dimensional, the system is very much like a Hamiltonian billiard system. This is the case we will consider in some depth. On the other hand, the electron is a very quantum mechanical object and if it is in a state of definite momentum then we should describe it quantum mechanically as a plane wave. We are thus faced with the necessity of finding a quantum description of Hamiltonian billiards if we are to describe such a mesoscopic system. As we shall see, a knowledge of the corresponding classical system provides a path to understanding the quantum scattering of an electron in a mesoscopic system. As much of the future of semiconductor technology will be based on such devices, this is an important problem.

For further information on mesoscopic systems see:

6.2 Prelude to quantum scattering

Consider a one dimensional potential of the form,

\[
V(x) = \begin{cases} 
\infty & x \leq 0 \\
0 & x < a \\
V_0 & a \leq x \leq b \\
0 & x > b
\end{cases}
\]  

(6.1)

Let \(u_\pm(x)\) be the position probability amplitude for particles traveling in the \(\pm x\) direction, in the region \(x > b\), with definite energy \(E < V_0\). These are plane wave states of the form

\[
u_\pm(x) = e^{\pm ikx}
\]

(6.2)

where \(k^2 = \frac{2mE}{\hbar^2}\). By matching the boundary condition it is easy to show that at \(x = b\),

\[
\frac{u_+(b)}{u_-(b)} = -e^{2i\phi(k)}
\]

(6.3)

where

\[
\tan \phi(k) = \frac{k}{\alpha} \left[ f(k)e^{\alpha(b-a)} + e^{-\alpha(b-a)} \right] \\
\frac{f(k)e^{\alpha(b-a)} - e^{-\alpha(b-a)}}{
\frac{\alpha \tan ka + k}{\alpha \tan ka - k}}
\]

(6.4)

where

\[
\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}
\]

(6.5)

\[
f(k) = \frac{\alpha \tan ka + k}{\alpha \tan ka - k}
\]

(6.6)

There is only a phase shift between left-going and right-going states.

We can calculate the (relative) probability \(P(k)\) to find the particle in \(0 \leq x \leq a\), relative to the probability to find a particle at \(x > b\) with negative momentum,

\[
P(k) = 4 \left\{ \sin \phi(k) \cosh(\alpha(b-a)) - \frac{k}{\alpha} \cos \phi(k) \sinh(\alpha(b-a)) \right\}^2
\]

(6.7)

We now define the dimensionless parameters, the scaled energy \(x\), the scaled barrier strength \(w\) and the scaled barrier length \(l\),

\[
x = ka
\]

(6.8)

\[
w^2 = \frac{2mV_0}{\hbar^2}(b-a)
\]

(6.9)

\[
l^2 = \frac{b}{a} - 1
\]

(6.10)
In figure 6.2 we plot the function $P(k)$ and $\cos \phi(k)$ versus the scaled input energy, $x$. This is a kind of spectrum of excitation for the quasi-bound state in the well. Note the resonance at a particular value of input energy. Why does this maximum occur?

In a classical description of this system, if the energy of the particle is $E < V_0$ it cannot penetrate the barrier and there are two regions of motion one bounded, inside the well and the other unbounded outside the well. The bounded motion is periodic with period $T$ given by the time taken to traverse the well from $x = 0$ to $x = a$ and back again. At the boundaries the collisions are elastic so energy is conserved. The period is easily seen to be given by

$$T(E) = a \sqrt{\frac{2m}{E}} \quad (6.11)$$

As the period (and frequency) depend on energy this is a nonlinear oscillator. It is obviously non harmonic. The nonlinear frequency can also be obtained by computing the action $J(E)$ on a periodic orbit. The action of an orbit is defined as the phase space area bounded by the orbit divided by $2\pi$. Thus

$$J(E) = \frac{a}{\pi} \sqrt{2mE} \quad (6.12)$$

from which the nonlinear frequency is given by $\omega(E) = (dJ/dE)^{-1}$ which gives the same result for the period as Eq.(6.11).

We can now use the semiclassical quantisation rules to estimate the allowed energy levels for the equivalent problem. Recall that the rule says we are only allowed those orbits for which the phase space area divided by $\hbar$, and adjusted for the Maslov index, is an integer multiple of $2\pi$. For billiard problems the Maslov index correction is not the same as the case of a soft potential. In fact each reflection leads to a phase
change of $\pi$ rather than $\pi/4$. There are two turning points in this case. The semiclassical quantisation condition then becomes

$$2L\sqrt{2mE} - 2\pi = 2\pi n \quad n = 0, 1, 2, \ldots$$

(6.13)

from which we find the allowed energies are

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \quad n = 1, 2, \ldots$$

(6.14)

This is the spectrum of energies for the states of the infinite square well.

If we now return to the excitation spectrum in Eq.(6.7) it is easy to show that in the limit of $E << V_0$ the peak of the spectrum corresponds to the allowed energies of the bound state of the infinite square well. We can now draw together some lessons. The infinite square well is a very simple kind of one dimensional billiard. The allowed energies of which can be found by finding the classical periodic orbits and then applying the semiclassical quantisation rules, which is this case work exactly. If we now weaken one boundary so that we can probe the allowed energies by scattering particles of fixed energy we can excite the allowed bound states in the well which correspond to a rapid phase change of the scattered quantum probability amplitude. However the very act of weakening the potential in order to probe necessarily shifts the resonances slightly from the infinite square well result. However we can try and make this disturbance as small as possible.

This example serves to illustrate our approach to the problem of two dimensional billiard systems. As for this one dimensional billiard, we will approach the physics of the system as a kind of scattering problem. The classical dynamics of the corresponding closed system will determine, to a good approximation, what we see in the quantum scattering problem. However we need to keep in mind that to probe a billiard spectroscopically we need to weaken the classical perfect billiard system to some extent. We need to keep the disturbance due to this measurement to a minimum. Given this, we seek to understand the quantum scattering problem by determining the classical billiard problem first. The key question however is how well the semiclassical intuition can work for a chaotic billiard problem.

6.3 Quantum billiards and microwave cavities.

In a two dimensional billiard system a particle of mass $m$ moves freely in the plane until it encounters a wall, at which point it undergoes a perfectly elastic collision. The quantum description of this problem is in
terms of the Schrödinger equation in the coordinate representation

\[ i\hbar \frac{\partial \psi(x, y, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, t) \]  
(6.15)

subject to the Dirichlet boundary condition

\[ \psi(x, y, t)|_S = 0 \]  
(6.16)

where \( S \) denotes the curve that defines the boundary of the billiard. The energy eigenstates \( \psi_n(x, y) \) and allowed energies, \( E_n = \hbar \omega_n \), are obtained by separating the time dependence as

\[ \psi_n(x, y, t) = \psi_n(x, y)e^{-i\omega_nt} \]  
(6.17)

and solving the time independent equation

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi_n(x, y) = E_n \psi_n(x, y) \]  
(6.18)

\[ \nabla^2 \psi_n(x, y) + k_n^2 \psi(x, y) = 0 \]  
(6.19)

with the dispersion relation

\[ \omega_n = \frac{\hbar}{2m} k_n^2 , \]  
(6.20)

subject to the same boundary condition Eq.(6.16).

There is a very similar system of equations for the case of an electromagnetic wave sustained inside a conducting boundary; a resonant cavity. The equation for the electric and magnetic field amplitudes are

\[ (\nabla^2 + k^2)E = 0 \]  
(6.21)

\[ (\nabla^2 + k^2)B = 0 \]  
(6.22)

with the dispersion relation \( \omega = ck \) and the boundary conditions

\[ \vec{n} \times \vec{E} = 0 \]  
(6.23)

\[ \vec{n} \cdot \vec{B} = 0 \]  
(6.24)

where \( \vec{n} \) is a unit normal to the surface of the boundary. To make this look like a quantum billiard problem we consider resonators with cylindrical symmetry, but varying cross sections. Taking the \( z \) axis parallel to the axis of cylindrical symmetry the boundary conditions are

\[ E_z|_S = 0 \]  
(6.25)

\[ \nabla \cdot B_z|_S = 0 , \]  
(6.26)
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Fig. 6.3. From 2.12 in Stockman. The spectra at two different temperatures are recorded. At room temperature there is a significant amount of thermally excited background radiation that masks the cavity spectrum. At low temperature with the walls are superconducting, and the spectra reflects more closely the billiard spectrum.

where $\vec{\nabla}_\bot$ denotes the normal derivative. These can be satisfied for transverse magnetic modes (TM)

$$E_z(x, y, z) = E(x, y) \cos(n\pi z/d)$$  \hspace{1cm} (6.27)

$$B_z(x, y, z) = 0$$  \hspace{1cm} (6.28)

where

$$\left[ \nabla^2 + k^2 - \left(\frac{n\pi}{d}\right)^2 \right] E = 0$$  \hspace{1cm} (6.29)

with Dirichelet boundary condition $E(x, y)|_S = 0$ on the surface. For frequencies $\nu < c/2d$ ($k < \pi/d$) only TM modes with $n = 0$ are possible. Thus the electric field in the $x, y$ plane must satisfy $(\nabla^2 + k^2)E = 0$ with Dirichelet boundary conditions. The dispersion relation for electromagnetic waves however is different ($\omega = ck$). The equivalence to the quantum billiard problem is apparent. For this reason many early experiments on quantum billiards were in fact microwave cavity experiments. However it is worth stressing the crucial difference between the quantum and microwave case. In the microwave case we are concerned with a true field amplitude in the cavity. In the quantum case the analogous object is a probability amplitude. This means the kinds of measurements that we could consider in the two cases are very different. It is possible to measure a field amplitude, while generally we cannot measure a quantum probability amplitude directly (for that matter we cannot measure a probability directly either!). Rather we measure some other quantity, such as position of an electron, the statistics of which measurements are determined by the quantum probability amplitude.

In the microwave cavity experiments we need to find a way to measure the field inside the cavity. This requires that we open the cavity up in some way, so the cavity walls are no longer perfectly reflecting. This is usually done by introducing a small antenna into the resonator through a small hole, and measuring the amount of power reflected back when the antenna is used to excite the cavity. An example is shown in figure 6.3. The reflected power is monitored as a function of the frequency of the injected signal to give a spectrum. Each minimum in the reflected power corresponds to a resonant eigenfrequency of the cavity.
The spectrum in Figure 6.3 looks very complex, which we will see reflects the corresponding complex chaotic trajectories of the corresponding billiard problem. Many decades ago similar complex spectra turned up in nuclear physics. An approach to analysis was adopted based on eigenvalue spacing distributions. The sequence of successive eigenvalue differences $s_n = E_n - E_{n-1}$ is computed and the relative frequency of values of $s_n$ plotted to construct a distribution $P(s)$ of eigenvalue spacings. The variable $s_n$ is scaled so that the average spacing is unity. It was found that these distributions could be classified into a few general classes that reflected fundamental dynamical properties of the system. In particular it was found that eigenvalues either tended to bunch so that $P(s)$ was peaked at zero or they seemed to repel each other so that $P(s)$ is peaked away from zero. In the case of the stadium billiard the spacing distribution is well fitted by the Wigner distribution

$$P(s) = \frac{\pi}{2} s \exp[-\frac{\pi}{4} s^2]$$ (6.30)

It is no coincidence that this distribution is associated with a billiard problem that is chaotic. Indeed if we measure the spectrum of a rectangular cavity, for which the corresponding billiard problem is integrable, we find that

$$P(s) = e^{-s}$$ (6.31)

a Poisson distribution which exhibits level bunching.

In the case of nuclear spectra the conjecture was made that the spacing distributions could be understood if the corresponding Hamiltonians were drawn from an ensemble of random matrices. This work was largely pioneered by Wigner, Dyson and Mehta. In 1984 however Bohigas, Giannoni and Schmidt conjectured that random matrix theory could be used to describe the statistical level spacing of quantum systems which were classically chaotic. The BGS conjecture says that:

“statistical properties of long sequences of energy levels of generic quantum systems whose classical counterparts are chaotic have their pattern in long sequences of eigenvalues of large random Hermitian matrices with independent, identically distributed entries.”

This has subsequently been vindicated in countless real and numerical experiments. Yet curiously a rigorous proof is elusive.

### 6.4 Random matrices.

A hamiltonian for a complex system may exhibit certain symmetries, for example it may be invariant under rotations. In quantum mechanics this
meets that the Hamiltonian is invariant under a unitary transformation representing an element of the symmetry group. The generator of the transformation will then commute with the Hamiltonian which implies that it is a constant of the motion. Thus if the system starts in an eigenstate of the generator it remains in an eigenstate of the generator. Another consequence of the commutation of the generator and the Hamiltonian is that both operators may be simultaneously diagonalised. Consider the case of the hydrogen atom. The central Coulomb potential is invariant under arbitrary rotations which are represented by a unitary operator of the form \( U(\vec{n}, \theta) = \exp(-i\theta \vec{L} \cdot \vec{n}) \) where \( \vec{n} \) is a unit vector while \( \theta \) represents the angle of rotation around the direction \( \vec{n} \). The operator valued vector \( \vec{L} = \hat{L}_x \vec{x} + \hat{L}_y \vec{y} + \hat{L}_z \vec{z} \) is the operator for angular momentum. The eigenvalues of total angular momentum squared, \( \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \) are \( \hbar^2 l(l+1) \), \( l = 0, 1, 2, \ldots \). The Hamiltonian may then be represented in block diagonal form where each block corresponds to a fixed value of \( l \). In the case of the hydrogen atom there are extra symmetries which permit us to completely diagonalise the Hamiltonian in terms of three quantum numbers \( n, l, m \) corresponding to conservation of total energy, total angular momentum and one component of angular momentum. As the number of constants of the motion is equal to the number of degrees of freedom the system is totally integrable.

However this is the exception rather than the rule and in general we will only be able to block diagonalise the Hamiltonian with each block corresponding to some reduced set of conserved quantities for subspaces that remain invariant under the corresponding symmetry transformation. This is precisely the situation for nuclear physics where the only symmetries are angular momentum and parity. However for nuclei with many nucleons the number of degrees of freedom is very large and the systems are non-integrable. When we make a statistical analysis of the spectrum of a Hamiltonian we must first block diagonalise the matrix and compare eigenvalues only within a block corresponding to one of the eigenvalues of the conserved quantity: this is called subspectra. Determining the symmetries of a complex Hamiltonian is the first step.

The next step requires that we rescale the energies so that the average density of states is unity. Then various statistics may be calculated, for example the nearest neighbour spacing distribution \( p(s) \). Bohigas and co-workers have compiled a large number of energy levels for complex nuclei known as the nuclear data ensemble. In figure 6.4 is shown the spacing distribution for combining the results of 30 different subspectra.

In figure 6.4 the Poisson distribution is also shown. This corresponds to the spectra of fully integrable systems. In such systems the Hamiltonian is completely diagonalised and each eigenvalue makes up a symmetry class.
6.4 Random matrices.

Fig. 6.4. The nearest neighbour spacing distribution for the nuclear data ensemble. It contains 1726 energy levels of 36 sequences of 32 nuclei. The distribution peaked away from $s = 0$ is the Wigner distribution also known as the gaussian orthogonal ensemble (from Stöckman fig 3.1).

Fig. 6.5. Level spacing distribution for the first 100,000 eigenvalues of a rectangular billiard (figure 3.3 Stöckman).

of its own. It is thus reasonable to assume the eigenvalues are completely uncorrelated. Let the probability to find an eigenvalue between $E$ and $E + dE$ be a constant which we take as unity after rescaling the average energy eigenvalue spacing. Let us now calculate the probability, $p(s)$, that from a given eigenvalue, we will find only one other a distance $s$ away, with no other eigenvalues between. If we divide up the interval of length $s$ into $N$ equally spaced intervals, the probability is easily calculated as

$$p(s) ds = N \lim_{N \to \infty} \left(1 - \frac{s}{N}\right)^N ds$$

(6.32)

In the limit this is $p(s) = e^{-s}$.

In figure 6.5 is shown the eigenvalue distribution for a rectangular billiard with side length $a, b$, with $a/b = \sqrt{\pi/3}$, irrational. The eigenvalues are easily given by

$$E_n = \frac{\hbar^2}{2m} \left[ \left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2 \right], \quad n, m = 0, 1, 2...$$

(6.33)

To define a random matrix, $H$, we simply imagine that in an arbitrary basis the matrix elements are random numbers with some form of distribution, for example gaussian. However we must ensure that the matrix is indeed a valid hamiltonian, which is to say it is Hermitian $H^\dagger = H$. In the eigenbasis every Hamiltonian is real. However we are at liberty to use any basis which is a unitary transformation of the eigenbasis. In general this will result in a complex hermitian matrix. We can classify hermitian matrices into classes according to how they transform under different classes of unitary transformations.

If the Hamiltonian is not time reversal invariant (eg it contains a magnetic field), then the most we can require is that the hermiticity property
is preserved. The ensemble of such random matrices is then called the random unitary ensemble.

If the Hamiltonian is invariant under time reversal and does not contain spin half interactions, it can always be chosen as real (see Stöckmann, chapter 3, for a full discussion). This property is preserved under orthogonal transformations.

\[ H' = OHO^T \quad OO^T = 1 \] (6.34)

In that case we must restrict the class of unitary transformations to be simply orthogonal matrices, and we will refer to the ensemble of random matrices with this property as an orthogonal ensemble.

Consider systems with time reversal invariance and with spin interactions. A typical example is the spin-orbit interaction

\[ H = g \vec{L} \cdot \vec{S} \] (6.35)

where

\[ \vec{L} = -i\hbar \vec{r} \times \vec{p} \] (6.36)

is orbital angular momentum and \( \vec{S} = \frac{\hbar}{2} \vec{\sigma} \) is the spin of the particle and \( \vec{\sigma} = \sigma_x \vec{x} + \sigma_y \vec{y} + \sigma_z \vec{z} \) and \( \sigma_\alpha \) are the Pauli matrices.

It turns out that all such Hamiltonians are even dimensional and transform into each other under the symplectic transformation:

\[ H' = SHS^R \] (6.37)

where \( S \) is a sympletic matrix which means it must satisfy

\[ SS^R = 1 \quad \text{with} \quad S^R = ZS^T Z^{-1} \] (6.38)

where

\[ Z_{nm} = i\delta_{nm}\sigma_y \] (6.39)

We will only consider in detail the case of the orthogonal ensemble with gaussian distributions. We are thus led to the gaussian orthogonal ensemble or GOE. The other two symmetry classes with gaussian statistics are called the gaussian unitary ensemble (GUE) and the gaussian symplectic ensemble (GSE).

A real symmetric matrix in \( N \) dimensions requires \( N(N + 1)/2 \) real numbers to specify the matrix elements. The joint probability distribution \( p(H_{11}, H_{12}, \ldots, H_{NN}) \) is then invariant under orthogonal transformations \( p(H_{11}, H_{12}, \ldots, H_{NN}) = p(H'_{11}, H'_{12}, \ldots, H'_{NN}) \). Now the trace of any matrix is invariant under orthogonal transformation \( \text{tr}(OAO^T) = \text{tr}(A) \). This means that the joint distribution must be a function of the trace of powers of the Hamiltonian:

\[ p(H_{11}, H_{12}, \ldots, H_{NN}) = f[\text{tr}H, \text{tr}(H^2), \ldots] \] (6.40)
If we now require the matrix elements to be uncorrelated
\[ p(H_{11}, H_{12}, \ldots, H_{NN}) = p(H_{11})p(H_{12}) \ldots p(H_{NN}) \]  
(6.41)
the only way to satisfy both Eqs.(6.40,6.41) is if
\[ p(H_{11}, H_{12}, \ldots, H_{NN}) = C \exp \left[ -B \text{tr}(H) - A \text{tr}(H^2) \right] \]  
(6.42)
As this is Gaussian in form, we can shift the average to ensure that \( B = 0 \). The normalisation fixes the factor \( C \),
\[ \int p(H_{11}, H_{12}, \ldots, H_{NN}) dH_{11} \ldots dH_{NN} = 1 \]  
(6.43)
We are thus led to the distribution
\[ p(H_{11}, H_{12}, \ldots, H_{NN}) = \left( \frac{A}{\pi} \right)^{N/2} \left( \frac{2A}{\pi} \right)^{N(N-1)/2} \exp \left( -A \sum_{n,m} H_{nm}^2 \right) \]  
(6.44)
We now turn to the eigenvalue distribution. The Hamiltonian may be diagonalised by an orthogonal transformation \( H_{nm} = \sum_k O_{nk} E_k O_{mk} \). It would appear that we need to know the actual \( N(N-1)/2 \) matrix elements, \( p_\alpha \), which diagonalises the Hamiltonian. However if we use the fact that the trace is the same in any basis,
\[ \sum_{n,m} H_{nm}^2 = \sum_k E_k^2 \]  
(6.45)
we can write the new probability distribution in terms of the new variables \( E_k \) as
\[ p(H_{11}, H_{12}, \ldots, H_{NN}) dH_{nm} \sim \exp \left( -A \sum_k E_k^2 \right) |J| dE_k dp_\alpha \]  
(6.46)
where \( J \) is the Jacobian of the transformation
\[ |J| = \left| \frac{\partial(H_{NM})}{\partial(E_k, p_\alpha)} \right| \]  
(6.47)
It can be show that the determinant of \( J \) can be written as
\[ |J| = g(p_\alpha) \prod_{i>j} (E_i - E_j) \]  
(6.48)
where \( g(p_\alpha) \) is a function of the diagonalising matrix alone. After integrating over the variables \( p_\alpha \) we find
\[ P(E_1, E_2, \ldots, E_N) \sim \prod_{n>m} (E_n - E_m) \exp \left( -A \sum_n E_n^2 \right) \]  
(6.49)
As an example we consider the case of real symmetric $2 \times 2$ matrices

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$  \hspace{1cm} (6.50)

The eigenvalues are given by

$$E_{\pm} = \frac{1}{2} (H_{11} + H_{22}) \pm \frac{1}{2} \left[ (H_{11} - H_{22})^2 + 4H_{12}^2 \right]^{1/2}$$  \hspace{1cm} (6.51)

The orthogonal transformation that achieves this diagonalisation depends on a single parameter $\theta$ so that

$$H_{11} = E_+ \cos^2 \theta + E_- \sin^2 \theta$$
$$H_{22} = E_+ \sin^2 \theta + E_- \cos^2 \theta$$
$$H_{12} = (E_+ - E_-) \cos \theta \sin \theta$$

The Jacobian is then

$$J = \det \frac{\partial (H_{11}, H_{22}, H_{12})}{\partial (E_+, E_-, \theta)} = E_+ - E_-$$  \hspace{1cm} (6.52)

Thus $P(E_+, E_-) = C |E_+ - E_-| e^{-A(E_+^2 + E_-^2)}$.

**Exercise:**

Find the eigenvalue distribution for random $2 \times 2$ Hermitian matrices with complex entries.

An important function of the spectrum of a quantum system is the density of states defined as

$$\rho(E) = \sum_n \delta(E - E_n)$$  \hspace{1cm} (6.53)

This is a standard way to capture the spectrum of a quantum mechanical system. In many cases it has been found that we can write the density of states as the sum of a smooth part, called the average density of states and a quasiperiodic oscillating part,

$$\rho(E) = \overline{\rho(E)} + \rho_{osc}(E)$$  \hspace{1cm} (6.54)

The average here is a spectral average taken over the energy eigenvalues. However it can be shown that this can often be replaced to a good approximation by an average over some ensemble of random matrices provided that the number of levels is very large. This is a kind of ergodic theorem for energy eigenvalues and underpins the BGS conjecture. A great deal of mathematical effort has gone into characterising the oscillatory part
of the density of states. Gutzwiller demonstrated a semiclassical method to calculate $\rho_{osc}(E)$ based on an understanding of the periodic orbits of the corresponding classical system. We will return to this later. For now we concentrate on the average density of states for the random matrix ensemble.

What is the average density of states, averaged over the complete ensemble of random matrices? Before doing this however we describe a way to represent the density of states as a trace formula. We begin by representing the delta function as the limit if a Lorentzian curve of zero width

$$\delta(E) = \lim_{\epsilon \to 0} \frac{\epsilon}{\pi} \frac{1}{\epsilon^2 + E^2}$$

(6.55)

**Exercise 6.1** Show that this is indeed a representation of the delta function, that is, show that

$$\lim_{\epsilon \to 0} \int dE f(E - E_0) \frac{\epsilon}{\pi} \frac{1}{\epsilon^2 + E^2} = f(E_0)$$

(6.56)

Thus

$$\rho(E) = \lim_{\epsilon \to 0} \frac{\epsilon}{\pi} \sum_n \frac{1}{\epsilon^2 + (E - E_n)^2}$$

(6.57)

$$= -\lim_{\epsilon \to 0} \frac{1}{\pi} \text{Im} \sum_n \frac{1}{E - E_n + i\epsilon}$$

(6.58)

Now we can use

$$\sum_n \frac{1}{E - E_n} = \text{tr} \left( \frac{1}{E - H} \right)$$

(6.59)

so that

$$\rho(E) = -\frac{1}{\pi} \text{Im} \left( \text{tr} \left( \frac{1}{E - H} \right) \right)$$

(6.60)

where the $i\epsilon$ term is not written explicitly to simplify notation but must be inserted. The average density of states may thus be calculated by

$$\mathcal{E}(\rho(E)) = -\frac{1}{\pi} \text{Im} S$$

(6.61)

where

$$S = \mathcal{E} \left( \text{tr} \left( \frac{1}{E - H} \right) \right)$$

(6.62)

$$= \sum_{n=0}^{\infty} \frac{1}{E_{n+1}} \mathcal{E}(\text{tr} H^n)$$

(6.63)
where the series converges if \( E \) exceeds all the eigenvalues of \( H \) in magnitude.

The explicit calculation of the average over the gaussian distributions is tedious. Let us take the dimension of \( \hat{H} \) is \( N \). The result is

\[
\mathcal{E}(\rho(E)) = \begin{cases} 
\frac{A}{\pi} \sqrt{\frac{2N}{A} - E^2} & |E| < \frac{\sqrt{2N}}{A} \\
0 & |E| > \frac{\sqrt{2N}}{A}
\end{cases} 
\]  

(6.64)

It is usual to write to choose

\[
A = \frac{\pi^2}{2N}
\]  

(6.65)

we get the Wigner semicircle law,

\[
\mathcal{E}(\rho(E)) = \begin{cases} 
\sqrt{1 - (\frac{2N}{\pi E})^2} & |E| < \frac{2N}{\pi} \\
0 & |E| > \frac{2N}{\pi}
\end{cases} 
\]  

(6.66)

For energies \( |E| \ll N \) the density of states is constant. we will now only consider this limit. As the Hamiltonians of real chaotic systems have infinite dimension this is a reasonable thing to do.

There is another way to write the density of states as a trace formula. Using the Fourier representation of a delta function we can write

\[
\rho(E) = \sum_n \int_{-\infty}^{\infty} dt e^{it(E - E_n)}
\]  

(6.67)

\[
= \int_{-\infty}^{\infty} dt \mathcal{P}(t) e^{iEt}
\]  

(6.68)

where

\[
\mathcal{P}(t) = \sum_n e^{-iE_n t}
\]  

(6.69)

\[
= \text{tr}(U(t))
\]  

(6.70)

In other words the density of states is the Fourier transform of the trace of the unitary evolution operator for the dynamical system.

The nearest neighbour spacing distribution is now easily calculated. We will only consider the \( 2 \times 2 \) case as the results are independent of the dimension.

\[
p(s) = \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 P(E_1, E_2) \delta(s - |E_1 - E_2|)
\]  

(6.71)

\[
= C \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 |E_1 - E_2| \exp \left( -A \sum_n E_n^2 \right)
\times \delta(s - |E_1 - E_2|)
\]  

(6.72)

(6.73)
the two constants are fixed by

\[ \int_0^\infty p(s)ds = 1 \quad (6.74) \]

\[ \int_0^\infty sp(s)ds = 1 \quad (6.75) \]

Thus

\[ p(s) = \frac{\pi}{2s} \exp\left(-\frac{\pi}{4}s^2\right) \quad (6.76) \]

For completeness we give the eigenvalue spacing distributions for the GUE and the GSE as well as the GOE.

\[ p(s) = \begin{cases} \frac{\pi}{2s} \exp\left(-\frac{\pi}{4}s^2\right) & \text{(GOE)} \\ \frac{\pi^2}{24}s^2 \exp\left(-\frac{4}{\pi}s^2\right) & \text{(GUE)} \\ \frac{21s}{2\sqrt{\pi}}s^4 \exp\left(-\frac{2}{\pi}s^2\right) & \text{(GSE)} \end{cases} \quad (6.77) \]

Note the dependence at small spacing. The GOE is linear, the GUE is quadratic and the GSE is quartic. In the case of Floquet operators we need to consider Gaussian circular ensembles as all eigenvalues lie on the unit circle. There is an equivalent breakdown in terms of orthogonal, unitary and sympletic transformations.

### 6.5 Mesoscopic electronics

We now consider the scattering of electrons from mesoscopic billiard systems as described in the introduction. The mesoscopic cavity is connected to leads which act as waveguides for the de Broglie waves of electrons. The leads are connected to reservoirs maintained at local equilibrium by an external voltage. The measured quantity is the conductance \( G \) of the total device. The objective is to understand the conductance through the elastic scattering of an electron in the mesoscopic cavity. The multiple scattering of the electron wave reflected from the cavity walls that gives rise to complex interference effects and ensures the conductance has a strong dependence on the energy of the injected electrons (which is essentially the Fermi energy \( \epsilon_f \) of the reservoir connected to this lead) as well as the geometry of the cavity. If an external magnetic field is present additional interference effects can arise due to the Aharonov-Bohm effect in which electron paths that enclose magnetic flux can acquire additional phase shifts. The changing interference causes the conductance to change. The sensitive dependence of \( G \) on small changes in the parameters of the system is known as conductance fluctuations. In what follows we will assume that there is no magnetic field and that spin can be ignored (that is there is no spin-orbit coupling).
Fig. 6.6. A 2d mesoscopic cavity connected to $L$ one dimensional leads or waveguides. The arrows indicate ingoing, $a_n^{(l)}$, or outgoing waves, $b_n^{(l)}$. In waveguide $l$ there can be $N_l$ such modes. (from Mello and Baranger, Waves Random Media, 9, 105 (1999)).

A schematic of the model is shown in figure 6.6. The cavity is connected to $L$ leads or electron waveguides. The $l$th lead can support $N_l$ modes. How many modes there are in each lead is determined by the geometry of the lead. We will assume that the walls of the lead and the cavity are impenetrable, that is they present a potential barrier much greater than any electron kinetic energy. In each lead, $l$ we have a system of coordinates such that $x_l$ axis runs along the lead and $y_l$ runs transverse to the lead. Each lead is of fixed width $W_l$. In the $l$th lead we then have the plane waves

$$\exp[\pm ik_n^{(l)} x_l] \chi_n(y_l)$$

where the positive sign means and ingoing wave and a negative sign means an outgoing wave. The functions $\chi_N(y_l)$ are the familiar square well energy eigenstate probability amplitudes;

$$\chi_n(y_l) = \sqrt{\frac{2}{W_l}} \sin K_n^{(l)} y_l, \quad K_n^{(l)} = \frac{n\pi}{W_l}, \quad n = 1, 2, \ldots \quad (6.78)$$

where $K_n^{(l)}$ is the transverse wave number. The transverse quantisation condition means only particular solutions, labeled by $n$ can propagate in the lead. Each allowed solution is called a mode or channel. Thus there are $L$ leads in each of which there are some maximum number $N_l$ of modes. Far away from the scattering region the most general form of the probability amplitude in each lead is a superposition of ingoing and outgoing amplitudes,

$$\sum_{n=1}^{N_l} \left( a_n^{(l)} \frac{1}{\sqrt{v_n^{(l)}}} e^{-ik_n^{(l)} x_l} + b_n^{(l)} \frac{1}{\sqrt{v_n^{(l)}}} e^{ik_n^{(l)} x_l} \right) \quad (6.79)$$

where

$$v_n^{(l)} = \frac{\hbar k_n^{(l)}}{m} \quad (6.80)$$

is the ballistic velocity of the $n$th mode of the $l$th lead. We have divided out by the square root of the velocity so that the amplitude squared of the wave function in each channel will have units of flux.
We now define an \( \mathbf{N_l} \) dimensional vector

\[
\mathbf{\vec{a}}(l) = (a_{1}^{(l)}, a_{2}^{(l)}, \ldots, a_{N_l}^{(l)})
\]  

(6.81)

that contains the \( N_l \) incoming amplitudes in the \( l \)th lead. We can then combine all these amplitudes for each lead into a single vector,

\[
\mathbf{\vec{a}} = (\mathbf{\vec{a}}^{(1)}, \mathbf{\vec{a}}^{(2)}, \ldots, \mathbf{\vec{a}}^{(L)})^T
\]  

(6.82)

We can define a similar vector for the outgoing modes. The incoming and outgoing modes are then related by a \textit{scattering matrix}

\[
\mathbf{\vec{b}} = S \mathbf{\vec{a}}
\]  

(6.83)

As an example consider the case of just two leads, \( L = 2 \), each with \( N \) modes. Then the scattering matrix is a \( 2N \times 2N \) matrix and takes the form

\[
s = \begin{bmatrix}
    r & t' \\
    t & r'
\end{bmatrix}
\]  

(6.84)

where \( r \) is a \( N \times N \) matrix containing the reflection amplitudes for the modes of the first lead to be reflected back into the same lead, \( r' \) is for reflection from the second lead back into the second lead, \( t \) gives the transmission amplitude from modes in lead 2 to modes in lead 1, while \( t' \) gives the transmission amplitudes for modes in lead 1 into lead 2.

We now need to make a connection with the conductance. At first sight it seems strange to talk about the conductance of a system with only elastic, hamiltonian, processes. The traditional view of resistance for normal metals treats it as due to many inelastic collisions of electrons in the Fermi sea with the ionic cores. However in mesoscopic system there are elastic collisions between the electrons and the walls of the cavity. The puzzle was solved long ago by Landauer and Buttiker. They showed that for perfectly elastic and ballistic electron transport a resistance (or conductance) could be defined in terms of the \textit{transmission probability} for an electron to pass through the device. For example, consider a single lead so narrow that it can only support one transverse mode. Unless the reservoir connected to this lead can supply an electron with an energy that exactly matches the allowed energy of the mode in the channel, the electron will not enter the channel but will always be reflected. In that case the conductance would be zero corresponding to the zero transmission probability for the channel. As we increase the width of the channel we decrease the lowest allowed energy in the lead until it eventually falls below the Fermi energy in the reservoir. Then the transmission probability rises to unity and the conductance makes a jump from zero to a non zero value. A plot of conductance versus the width of the channel would
show a series of steps as new modes open up for the reservoir to match energy. In each case the transmission probability goes from zero to unity. These conductance steps have now been observed in many experiments. The size of each conductance step is called the quantum of conductance and is given by

$$\frac{2e^2}{h}$$

a remarkable result linking fundamental constants to conductance. In the theory of Landauer and Buttiker the actual conductance of a channel of transmission probability $T$ is

$$G = \frac{2e^2}{h} T$$

where $T = |t_{ab}|^2$ and $t_{ab}$ is the relevant S matrix amplitude for scattering from a single mode of lead $a$ to a single mode of lead $b$. In the case of multiple leads and multiple modes per channel we need to sum over initial and final modes. For the two lead case the conductance formula then becomes

$$G = \frac{2e^2}{h} \text{tr}(tt^\dagger)$$

We can simplify this by finding the eigenvalues, $\tau_\alpha$, of the hermitian matrix $tt^\dagger$

$$G = \frac{2e^2}{h} \text{tr} \sum_\alpha \tau_\alpha$$

The conductance is determined by the eigenvalues of a hermitian matrix.

To find the scattering matrix is no easy task. As we saw for the simple square well scattering problem it is ultimately determined by the allowed energy levels of the cavity responsible for the scattering. The scattering matrix is itself a unitary matrix, however it is determined by the eigenvalues and eigenvectors of the hamiltonian for the cavity. For a classically chaotic cavity these eigenvalues, or spectra, display an apparent randomness. It is at this point that we make a connection with random matrix theory. A random hamiltonian for the cavity will determine a random unitary scattering matrix. We can probe the apparently random spectra of the cavity by measuring the conductance peaks as a function of the energy of the electrons injected into the leads from a Reservoir.

There is one final complication we need to consider. Electrons are not neutral billiard balls but carry a charge. A typical mesoscopic cavity is very small and thus has a very small capacitance, $C$. The energy required to put a single electron into the cavity is

$$E_c = \frac{e^2}{2C}$$
and it is likely that this will be larger than a typical spacing $\Delta E = E_n - E_{n-1}$, for the allowed energies of a neutral particle in a billiard cavity. The effect is to introduce gaps of energy $E_c$ into the spectrum and a plot of conductance versus energy (equivalently the bias voltage) will show peaks spaced equally by the charging energy. This is called a *Coulomb blockade*. However the height of each peak will be determined by the scattering matrix. If there is no magnetic field we can then use the GOE random matrix theory to describe the allowed energies in the cavity which leads to an equivalent random matrix for the unitary scattering matrix $S$. We can then begin to model statistically the conductance peak heights using random matrix theory.

In order to find the scattering matrix we would need to find the *eigenfunctions* as well as the eigenvalues of the quasi bound states inside the dot. The reason for this is that the transmission amplitudes $t_{ab}$ depend on the overlap of the wave function in the lead and the wave function in the dot in the vicinity of the lead. A study of the eigenfunctions of random matrix ensembles takes us beyond the scope of this subject so we will simply state the results.

In figure 6.8 are shown the results of a model presented by Jalabert, Stone and Alhassid (Phys. Rev. Letts. 68, 3468, (1992).) They used a GOE of random matrices to model the mesoscopic conductance of a stadium with two leads as a function of the energy of the an electron injected into one lead, but ignoring Coulomb blockade. The stadium was desymmetrised by replacing one quarter circle by a cosine curve (insert in figure 6.7). The conductance peak heights, $g_n$ are quite variable, apparently random.

A more detailed analysis based on random matrix theory (Alhassd and Lewenkopf, Phys. Rev. B 55, 7749 (1997)), shows that the distribution of peak heights for a symmetric double lead chaotic mesoscopic cavity is

$$P(g) = \sqrt{\frac{1}{\pi s_0 g}} e^{-g/s_0}$$  \hspace{1cm} (6.89)

where $s_0$ determines the average conductance peak height

$$\mathcal{E}(g) = \frac{s_0}{2}$$  \hspace{1cm} (6.90)
Fig. 6.8. (a) A series of Coulomb blockade conductance peaks as a function of gate voltage at zero magnetic field. (b) Distribution of the normalised conductance peak height distributions $\hat{G} = g/\bar{G}$. The solid line is the prediction of Random Matrix Theory of Jalabert et al. (from The Statistical theory of Quantum Dots, Y. Alhassid, Rev. Mod. Phys. 72, 895 (2000)).

This theory is found to be in very good agreement with experiment. In figure ?? are shown results for a different mesoscopic cavity of the experiment of Folk et al. Phys. Rev. Lett. 76, 1699 (1996). Again the experiment was done for almost closed dots with two leads and no magnetic field.
7

Trace formulae.

7.1 Return to semiclassical quantum mechanics

7.2 Gutzwiller trace formula

7.3 Selberg trace formula

7.4 Zeros of the Riemann zeta function
References


