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Contents

1

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, $P(q_1, q_2, \dots, q_n, p_1, p_2, \dots, p_n)$ is positive, real valued, integrable function (with norm one in L^1) on an even dimensional symplectic manifold, the phase space.

The normalisation is

$$\int_{-\infty}^{\infty} dq^n dp^n P(q_i, p_i) = 1 \quad (1.1)$$

Technical note: States are elements of the positive cone, V^+ of the Banach space L^1 , where

$$V^+ = \{x \in L^1 : x \text{ is a positive function}\} \quad (1.2)$$

A symplectic manifold is a manifold endowed with a particular differential two-form,

$$\gamma = \mathbf{dp}_i \wedge \mathbf{dq}^i \quad (1.3)$$

(there is a sum over the repeated index). Here $\mathbf{dq}$, $\mathbf{dp}$ are differential one forms Let f, g be two real valued functions on phase space. Real valued

functions define flow vectors by

$$\mathbf{v}_f(q, p) = \left(-\frac{\partial F}{\partial q^i}, \frac{\partial F}{\partial p_i} \right) \quad (1.4)$$

The canonical two form is then defined by its action on these vectors,

$$\gamma[\mathbf{v}_f, \mathbf{v}_g] = -\{f, g\} \quad (1.5)$$

where $\{f, g\}$ is the Poisson bracket

$$\{f, g\} = \left(\frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q^i} \frac{\partial f}{\partial p_i} \right) \quad (1.6)$$

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

$$P(q, p | q_0, p_0) = \delta^{(2n)}(q - q_0, p - p_0) \quad (1.7)$$

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 symplectic 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^∞ , the dual to the space L^1 of states. The Banach space L^∞ 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^∞ 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:

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

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

we use to determine the state, the *observed* state is $P_{obs}(q, p)$. 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 posteori* state given a particular outcome? The answer is a straightforward application of Baye's theorem:

$$P'(q, p|\bar{q}, \bar{p}) = \frac{P(\bar{q}, \bar{p}|q, p)P(q, p)}{P_{obs}(\bar{q}, \bar{p})} \quad (1.12)$$

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

Exercise 1.2 *Gaussian states are defined by*

$$P(q, p) = (2\pi|\det\sigma|)^{-1/2} \exp \left[-\frac{1}{2}(q - q_0, p - p_0)\sigma^{-1}(q - q_0, p - p_0)^T \right] \quad (1.13)$$

where

$$\langle (q, p) \rangle_P = (q_0, p_0) \quad (1.14)$$

and σ is the covariance matrix. Likewise a Gaussian instrument is defined by

$$P(q, p|q', p') = (2\pi|\det\Delta|)^{-1/2} \exp \left[-\frac{1}{2}(q - q', p - p')\Delta^{-1}(q - q', p - p')^T \right] \quad (1.15)$$

Show that in this case the operation transforms *a priori* Gaussian states to *a posteori* 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,

$$\frac{dA}{dt} = -\{H, A\} + \frac{\partial A}{\partial t} \quad (1.16)$$

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

$$\frac{dF}{dt} = \frac{dq}{dt} \frac{\partial F}{\partial q} + \frac{dp}{dt} \frac{\partial F}{\partial p} + \frac{\partial F}{\partial t} \quad (1.17)$$

$$= \{F, H\} + \frac{\partial F}{\partial t} \quad (1.18)$$

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 transformations 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

$$\frac{\partial P}{\partial t} = \{H, P\} \quad (1.19)$$

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

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_θ and $P_{\theta+d\theta}$. This is given in terms of the Fisher information, F_θ ,

$$\begin{aligned} ds^2 &= \left\langle \left(\frac{\partial \ln P}{\partial \theta} \right)^2 \right\rangle d\theta^2 \\ &= \int dq dp P_\theta(q, p) \left(\frac{\partial \ln(P_\theta(q, p))}{\partial \theta} \right)^2 \\ &= F_\theta d\theta^2 \end{aligned}$$

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

$$L(P_1, P_2) = \int_{-\infty}^{\infty} P_1(x) \log \left(\frac{P_1(x)}{P_2(x)} \right) dx \quad (1.20)$$

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 symplectic 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 *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.

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.

Definition.

The *state* of a physical system is specified by a positive trace class operator, ρ , of trace one acting on Hilbert space L^2 . The operator ρ is called the *density* operator.

Definition.

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

Definition.

The *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, $\langle A \rangle = \text{tr}(A\rho)$.

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

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

for operators with a discrete spectrum and

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

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

$$\begin{aligned} \langle A \rangle &= \text{tr}(A\rho) \\ &= \text{tr}\left(\sum a |a\rangle\langle a| \rho\right) \\ &= \sum a \text{tr}(|a\rangle\langle a| \rho) \\ &= \sum a P(a) \end{aligned}$$

where

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

As ρ 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

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

where $\hat{\Pi}$ is a projection operator on the Hilbert space, $\pi = 0, 1$ are the eigenvalues of the projection operator, and ρ 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

$$P(a) = \text{tr}(F(a)\rho) \quad (1.26)$$

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 Wiseman, *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

$$P(a) = |\langle a|\psi\rangle|^2 \quad (1.27)$$

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,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (1.28)$$

Thus

$$P(a) = \sum_i P_i(a) \quad (1.29)$$

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, ie 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 every thing 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

$$|\psi(0)\rangle = \sum_E c_E |E\rangle \quad (1.30)$$

Thus at a later time

$$|\psi(t)\rangle = \sum_E c_E e^{-iEt/\hbar} |E\rangle \quad (1.31)$$

In differential form,

$$\frac{d|\psi(t)\rangle}{dt} = -\frac{i}{\hbar} \hat{H} |\psi(t)\rangle \quad (1.32)$$

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad (1.33)$$

In the case of probability amplitude for position measurements we find

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t) \quad (1.34)$$

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

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [\hat{H}, \rho] \quad (1.35)$$

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].

$$d(\rho_1, \rho_2) = \arccos F(\rho_1, \rho_2) \quad (1.36)$$

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

$$F(\rho_1, \rho_2) = \text{tr} \left(\sqrt{\rho_1^{1/2} \rho_2 \rho_1^{1/2}} \right) \quad (1.37)$$

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 results 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

$$\int_{-\infty}^{\infty} dq |q\rangle \langle q| = \hat{1}. \quad (1.38)$$

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

$$\langle q|q'\rangle = \delta(q - q'). \quad (1.39)$$

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

$$\psi(q) = \langle q|\psi\rangle, \quad (1.40)$$

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:

$$|\psi\rangle = \int dq |q\rangle \langle q|\psi\rangle = \int dq \psi(q) |q\rangle. \quad (1.41)$$

Here we are using the convention that the limits of integration are $-\infty$ to ∞ 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

$$\langle q|p\rangle = (2\pi)^{-1/2} e^{ipq} \quad (1.42)$$

Here the normalization factor is chosen so that

$$\int dp |p\rangle \langle p| = \hat{1}, \quad \langle p|p'\rangle = \delta(p - p'). \quad (1.43)$$

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:

$$\psi(p) = \langle p|\psi\rangle = (2\pi)^{-1/2} \int dq e^{-ipq} \psi(q) \quad (1.44)$$

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 other wise 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,

$$\langle q|\hat{P}|\psi\rangle = \int dp \int dq' \langle q|p\rangle p \langle p|q'\rangle \langle q'|\psi\rangle \quad (1.45)$$

$$= (2\pi)^{-1} \int dp \int dq' p e^{ip(q-q')} \psi(q'). \quad (1.46)$$

Now $p e^{ip(q-q')} = i \frac{\partial}{\partial q'} e^{ip(q-q')}$, 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

$$\langle q|\hat{P}|\psi\rangle = -i(2\pi)^{-1} \int dp \int dq' e^{ip(q-q')} \frac{\partial}{\partial q'} \psi(q') \quad (1.47)$$

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

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

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

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 ∞ must be finite. Although the space $L^{(2)}(\mathbb{R})$ is infinite, is actually countably infinite. That is, the number of basis states for the Hilbert space $\mathfrak{H} = L^{(2)}(\mathbb{R})$ 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 $\mathfrak{H}$.

1.2.2 Minimum Uncertainty States

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

$$\langle (\Delta P)^2 \rangle \langle (\Delta Q)^2 \rangle \geq 1/4 \quad (1.51)$$

(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 σ .

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 $\wp(q) = |\psi(q)|^2$.

The Fourier transform of a Gaussian is also Gaussian, so in the momentum representation

$$\psi(p) = (\pi/\sigma^2)^{-1/4} \exp[-iq_0p - (p - p_0)^2\sigma^2/2]. \quad (1.55)$$

From this it is easy to show that

$$\langle \hat{P} \rangle = p_0 \quad (1.56)$$

$$\langle (\Delta \hat{P})^2 \rangle = 1/2\sigma^2 \quad (1.57)$$

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

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2 \hat{Q}^2}{2}. \quad (1.58)$$

Here m is the mass of the particle, and ω 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

$$\sigma = \sqrt{\hbar/m\omega} \quad (1.59)$$

where we have temporarily restored $\hbar$ to make its role apparent. If we define

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\frac{\hat{Q}}{\sigma} + i \frac{\sigma \hat{P}}{\hbar} \right) \quad (1.60)$$

then we can rewrite the Hamiltonian as

$$H = \hbar\omega(\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger)/2 = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}). \quad (1.61)$$

Now from the commutation relations of $\hat{Q}$ and $\hat{P}$ we can show that

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (1.62)$$

Also, we can show that the state $|\psi_0\rangle$ with wavefunction

$$\psi_0(q) = \langle q|\psi_0\rangle \propto \exp(-q^2/2\sigma^2) \quad (1.63)$$

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 σ 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)

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

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

$$\begin{aligned} (\hat{a}^\dagger\hat{a})|\psi_n\rangle &= (\hat{a}^\dagger\hat{a})(\hat{a}^\dagger)^n|\psi_0\rangle = \left[n(\hat{a}^\dagger)^n + (\hat{a}^\dagger)^n(\hat{a}^\dagger\hat{a})\right]|\psi_0\rangle \\ &= n(\hat{a}^\dagger)^n|\psi_0\rangle = n|\psi_n\rangle. \end{aligned} \quad (1.65)$$

which establishes the result and identifies the eigenstates.

Thus we have derived the eigenvalues of the harmonic oscillator as $\hbar\omega(n + \frac{1}{2})$. 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

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

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

$$\langle n|m\rangle = \delta_{nm}. \quad (1.67)$$

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

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle = n. \quad (1.68)$$

However we also have

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

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

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

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

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

Similarly it can be shown that

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

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

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \quad (1.73)$$

where α 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

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

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

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

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

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

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

$$|\alpha\rangle = \exp(-|\alpha|^2/2) \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (1.77)$$

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

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

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

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

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

$$\left\langle (\hat{a}^\dagger\hat{a})^2 \right\rangle - \left\langle \hat{a}^\dagger\hat{a} \right\rangle^2 = |\alpha|^2 \quad (1.80)$$

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

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

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

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

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

$$\langle\alpha|\Delta\hat{Q}\Delta\hat{P} + \Delta\hat{P}\Delta\hat{Q}|\alpha\rangle = 0 \quad (1.85)$$

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

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

If α and α' 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 ω (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

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

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

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

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

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

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

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

which gives

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

where T is the period of the motion. Thus

$$\mathcal{N} = 2 \left(\frac{m}{T} \right)^{1/2} \quad (1.95)$$

The states of definite energy, in the position representation $u(x)$, are given in the quantum theory as solutions of

$$\frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) = 0 \quad (1.96)$$

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

$$u(x) = N \cos \left[\frac{1}{\hbar} \int_x^{q_2} dx p_0 - \alpha \right] \quad (1.97)$$

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

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

which satisfies the equation,

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

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

$$u^{(WKB)}(x) = u^{(cl)}(x) u^{(wave)}(x) \quad (1.100)$$

where

$$u^{(cl)}(x) = \frac{\mathcal{N}}{\sqrt{p(x; E)}} \quad (1.101)$$

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

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

The resulting probability density is

$$W^{(WKB)} = [u^{(cl)}]^2 [u^{(wave)}]^2 \quad (1.103)$$

which begins to look a bit more like the classical distribution, apart for 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;

$$\begin{aligned}\bar{W}^{(WKB)} &= \frac{\mathcal{N}^2}{p(x)} \frac{1}{q_1 - q_0} \int_{q_0}^{q_1} dx \frac{1}{2} \left[1 + \cos \left(2 \int_x^{q_1} dx p(x) - \alpha \right) \right] \\ &\simeq \frac{1}{2} \frac{\mathcal{N}^2}{p(x)} = W^{(cl)}(x)\end{aligned}$$

The range of validity of the WKB amplitude is

$$p^2 \gg \sqrt{p} \left| \left(\frac{1}{\sqrt{p}} \right)'' \right| \hbar^2 \quad (1.104)$$

or

$$\frac{\hbar^2}{2m} \left| \frac{5}{16} \frac{(V'(x))^2}{(E - V(x))^3} + \frac{1}{4} \frac{V''(x)}{(E - V(x))^2} \right| \ll 1 \quad (1.105)$$

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,

$$\psi(x) = \frac{\psi_0}{\sqrt{|p(x)|}} \exp \left(\frac{i}{\hbar} \int_x^{q_1} p(x) dx - i\alpha \right) \quad (1.106)$$

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

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \psi(x) \exp \left(-\frac{i}{\hbar} xp \right) \quad (1.107)$$

$$= \frac{\psi_0}{\sqrt{2\pi\hbar}} \int \frac{dx}{\sqrt{|p(x)|}} \exp \left[\frac{i}{\hbar} \left(\int_{q_1}^x p(x) dx - xp \right) \right] \quad (1.108)$$

Integrals in the form

$$I = \int dx A(x) \exp \left(\frac{i}{\hbar} \Phi(x) \right) \quad (1.109)$$

can be approximated using the method of stationary phase. The basic idea is that as $\hbar \rightarrow 0$ the exponential oscillates rapidly except near those

points, x_s , where the phase $\Phi(x)$ varies least rapidly, $\Phi'(x_s) = 0$, ie is stationary. Expanding around the stationary phase point we have

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

The integral is then approximated by

$$I \simeq A(x_s) \exp \left(\frac{i}{\hbar} \Phi(x_s) \right) \int \exp \left[\frac{i}{\hbar} \frac{(x - x_s)^2}{2} \Phi''(x_s) \right] dx \quad (1.111)$$

We may now use the result (*Fresnel*)

$$\int_{-\infty}^{\infty} e^{iax^2} dx = \sqrt{\frac{\pi}{|a|}} \exp \left[i \frac{\pi}{4} \text{sgn}(a) \right] \quad (1.112)$$

Then

$$I \simeq \sqrt{\frac{2\pi\hbar}{|\Phi''(x_s)|}} A(x_s) \exp \left[\frac{i}{\hbar} \Phi(x_s) + \frac{i\pi}{4} \text{sgn}[\Phi''(x_s)] \right] . \quad (1.113)$$

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

$$I \simeq \sqrt{\frac{2\pi i \hbar}{\Phi''(x_s)}} A(x_s) \exp \left[\frac{i}{\hbar} \Phi(x_s) \right] \quad (1.114)$$

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

$$I \simeq \frac{(2\pi i \hbar)^{d/2}}{\sqrt{|\partial^2 \Phi / \partial x_n \partial x_m|}} A(x_s) \exp \left[\frac{i}{\hbar} \Phi(X_s) \right] \quad (1.115)$$

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

$$\tilde{\psi}(p) = \frac{\psi_0}{\sqrt{|p(x_s)p'(x_s)|}} \exp \left\{ \frac{i}{\hbar} \left[\int_{q_1}^{x_s} p(x) dx - p x_s \right] + \frac{i\pi}{4} \text{sgn}[p'(x_s)] \right\} \quad (1.116)$$

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

$$\psi(x) = \frac{\psi_0}{\sqrt{|p(x)|}} \exp \left[\frac{i}{\hbar} \int_{q_1}^x p(x) dx \right] \quad (1.117)$$

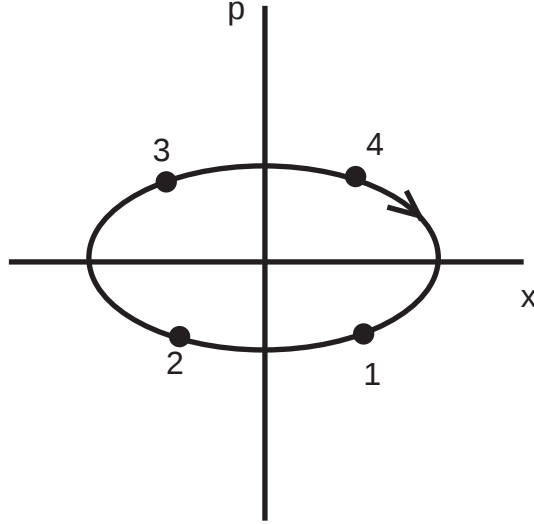


figure 1_2

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

At point 2 we transform to the momentum representation

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

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.

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

We now use the method of stationary phase;

$$\begin{aligned} \Phi(p) &= \frac{1}{\hbar} \left[\int_{q_1}^{x(p)} p(x) dx - px(p) + px \right] \\ \Phi'(p) &= x - x(p) \\ \Phi''(p) &= x'(p) \end{aligned}$$

Repeating the same steps as above we find the position probability amplitude is

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

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

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

where the action on the orbit is

$$S = \oint p(x) dx \quad (1.121)$$

and ν is called the *Maslov index*. If the amplitude is not to be multivalued on a complete orbit we need

$$S - \frac{\nu\pi}{2} = 2\pi n \quad n = 1, 2, \dots \quad (1.122)$$

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,

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

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

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

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

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V(x) = 0 \quad (1.125)$$

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 ρ is

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

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

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

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

The average of a quantum operator is given by

$$\text{tr}(\hat{A}\rho) = \int_{-\infty}^{\infty} dx dp W(x, p) A(x, p) \quad (1.129)$$

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

$$A(x, p) = \int dy \langle x - \frac{y}{2} | \hat{A} | x + \frac{y}{2} \rangle e^{ipy/\hbar} \quad (1.130)$$

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*,

$$W(x, p) = \frac{1}{(2\pi\hbar)^2} \int dy \int dk e^{i(py - kx)/\hbar} \text{tr}(\rho e^{i(k\hat{x} - \hat{p}y)/\hbar}) \quad (1.131)$$

where the Wigner characteristic function is

$$\chi^w(y, k) = \text{tr}(\rho e^{i(k\hat{x} - \hat{p}y)/\hbar}) \quad (1.132)$$

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

$$\text{tr}(\rho(\hat{x}^n \hat{p}^m)_s) = \frac{\partial^{n+m}}{\partial k^n \partial y^m} \chi^w(y, k)|_{y=k=0} \quad (1.133)$$

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

$$\text{tr}(\rho(\hat{x}^n \hat{p}^m)_s) = \int_{-\infty}^{\infty} dx dp W(x, p) x^n p^m \quad (1.134)$$

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

$$\frac{\partial W}{\partial t} = \{H^{(cl)}, W\}_{PB} + \sum_{n \geq 1} \frac{\hbar(-1)^n}{2^{2n}(2n+1)!} \partial_x^{2n+1} V(x) \partial_p^{2n+1} W(x, p) \quad (1.135)$$

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*

$$H = \frac{p^2}{2m} + ax^2 + bx^4 \quad (1.136)$$

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

$$P(q)dq = \text{tr}(\rho|q\rangle\langle q|dq) \quad (1.137)$$

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

$$P(q)dq = \text{tr}(\rho\hat{E}(q)dq) \quad (1.138)$$

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

$$\hat{U} = \exp \left[-i \left(\hat{X} \hat{P}_1 + \hat{P} \hat{P}_2 \right) \right]. \quad (1.139)$$

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

$$\langle x_j | d_j \rangle = (\pi \Delta_j^2)^{-1/4} \exp(-x_j^2 / 2\Delta_j^2) \quad (1.140)$$

where Δ_1 and Δ_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

$$\hat{M}(x_1, x_2) = \langle x_1 | \langle x_2 | \hat{U} | d_2 \rangle | d_1 \rangle \quad (1.141)$$

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

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

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

$$\langle x | (x_1, x_2) \rangle = (\pi)^{-1/4} \exp \left[i x x_2 - \frac{1}{2} (x - x_1)^2 \right] \quad (1.143)$$

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

$$\hat{E}(x_1, x_2) dx_1 dx_2 = \frac{1}{2\pi} |x_1, x_2\rangle \langle x_1, x_2| dx_1 dx_2. \quad (1.144)$$

Exercise 1.22 Show that

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \hat{E}(x_1, x_2) = 1 \quad (1.145)$$

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

$$E[X_1] = \langle \hat{X} \rangle, \quad E[X_1^2] = \langle \hat{X}^2 \rangle + \frac{1}{2}, \quad (1.146)$$

$$E[X_2] = \langle \hat{P} \rangle, \quad E[X_2^2] = \langle \hat{P}^2 \rangle + \frac{1}{2}, \quad (1.147)$$

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, $\wp(x_1, x_2)$. 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, α , 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 $\hat{F}(\alpha) = |\alpha\rangle\langle\alpha|/\pi$ and the resulting probability density $\wp(\alpha)d^2\alpha = \text{Tr}[\hat{F}(\alpha)\rho]d^2\alpha$. 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).

¶ 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.

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