Lecture Notes for Quantum Mechanics

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Niels Bohr (Nobel Prize in Physics 1922).

"If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet."

A visitor to Niels Bohr's country cottage, noticing a horse shoe hanging on the wall, teased Bohr about this ancient superstition. *Can it be true that you, of all people, believe it will bring you luck? Of course not*, replied Bohr, *but I understand it brings you luck whether you believe it or not.*

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Some general remarks:

These notes aim to be self-contained. *Homework questions* are are placed at appropriate positions in the text, i.e. to work them out you will require only the preceeding material. Questions marked by a star are optional. *Asides* give details on derivations we don't have time to go through in the lectures, or present material that goes beyond the core of the course. In some cases this material will be very useful for particular homework problems. *Exercises* are small problems that should be worked out after the lecture they pertain to. They are meant to ensure that you are continuously engaged with the course and not only the days immediately preceeding a tutorial.

This course aims to give an introduction to Quantum Mechanics. Let us start with some general context.

- QM is arguably humanity's greatest achievement. Actually, forget about the "arguably" part...
- Its understanding is the basis of much of our technological progress over the last 80 years.
- QM is intellectually challenging and only a minute fraction of humanity has any idea what it is about.
- We don't have an intuitive understanding of QM. As Richard Feyman famously said "Nobody understands quantum mechanics". An important addendum to this statement is that one naturally can not understand QM on a multitude of different levels, and the ultimate aim of this course is to elevate your ununderstanding to levels beyond your wildest imagination. Your ultimate goal should of course be to reach Feynman's level of ununderstanding...

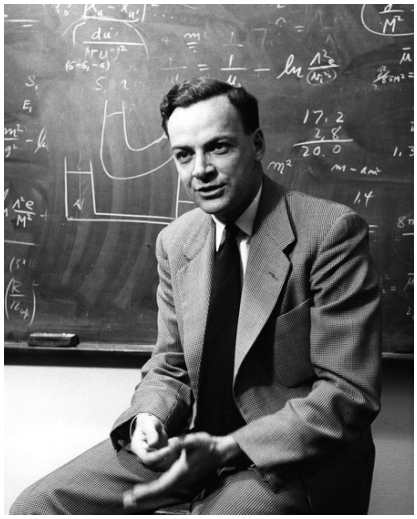


Figure 1: Richard Feynman (Nobel Prize in Physics 1965).

Part I
The Mathematical Structure of Quantum Mechanics

αγεωμετρητως μηδεις εισιτω Inscription on Plato's door.

QM is fundamentally different from Classical Mechanics in several ways:

- It does aim to provide a description of physical reality, but merely to make predictions for measurements. It is by its very design a *theory of measurement*.
- It accounts for the fact that measurements disturb the system; if the latter is small this is a large effect!
- QM is inherently probabilistic in nature: in general it cannot predict the outcome of a particular measurement exactly, but it rather provides a *probability distribution* for a set of possible outcomes.

  Examples of quantities that can be measured are energy, momentum, position, angular momentum. These are called *observables*. Measuring an observable can in general have many possible outcomes. These can be either *discrete* or *continuous*: position measurements will typically result in an outcome that various continuously in some interval $[a, b]$, but measuring energy will often result in a "quantized" set of outcomes E_1, E_2, ... Note that here and in the following we think of measurements in a rather abstract way and are not concerned with questions of experimental inaccuracies.

  The aim of QM is to provide *probability distributions* associated with measurements of observables

$$P(E_1),\ P(E_2), \dots \qquad \sum_j P(E_j) = 1. \tag{1}$$

  These distributions give us a statistical understanding of what happens if we repeat a given experiment many times.

1 Probability Amplitudes and Quantum States

1.1 Probability Amplitudes

A key aspect of QM is that probability enters in an unusual way. To stress this point let's recall that "classical" probabilities fulfil rules like

- If A,B are independent events with probabilities P(A) and P(B), then the probability for A *and* B is P(A and B)= P(A)P(B).
- If A,B are exclusive events with probabilities P(A) and P(B), then the probability for A *or* B is P(A or B)= P(A)+P(B).

QM works differently by construction. To understand why we follow Master Quantum Mechanic Richard Feynman's exquisite discussion (Feynman Lectures on Physics Vol 3) of double-slit thought experiments, which, incidentally, in German is of course a single word "Doppelspaltgedankenexperimente" – don't you just love it!

Feynman first considers the double-slit experiment for classical bullets. These can go through either slit,

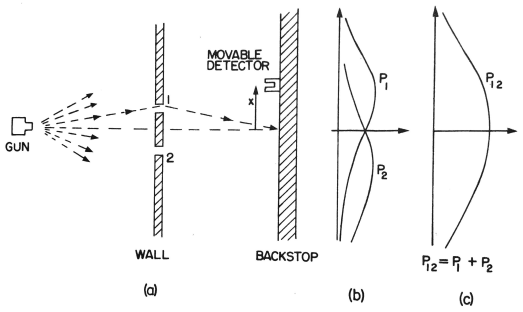


Figure 2: A double-slit experiment with indestructable bullets.

and the probability $P_{12}(x)$ of bullets arriving at position x on the detector screen is simply the sum of the probabilities $P_1(x)$ and $P_2(x)$ obtained by closing holes 2 and 1 respectively, i.e.

$$P_{12} = P_1 + P_2. \tag{2}$$

So for classical bullets we are dealing with classical probabilities.

Quantum mechanics works completely differently, as can be seen by repeating the double-slit experiment for electrons. What one observes is that electrons still reach the detector in "lumps", but now $P_{12}(x) \neq P_1(x) + P_2(x)$. Moreover, the observed probability distribution looks suspiciously like the interference pattern we would observe when conducting the experiment with waves! For waves we understand perfectly that intensities do not add, but instead we have

$$I_1 = |h_1|^2 \ , \quad I_2 = |h_2|^2 \ , \quad I_{12} = |h_1 + h_2|^2 \ , \tag{3}$$

where $h_{1,2}$ are the *amplitudes* of the waves. What the Doppelspaltgedankenexperiment shows is that electrons in some way behave like particles (lumpiness at detector) and in some ways like waves (interference)! This is called *particle-wave duality*.

The way to encode the baffling interference phenomenon into the fabric of QM is to postulate that the fundamental objects in QM are not probabilities, but *probability amplitudes* A.

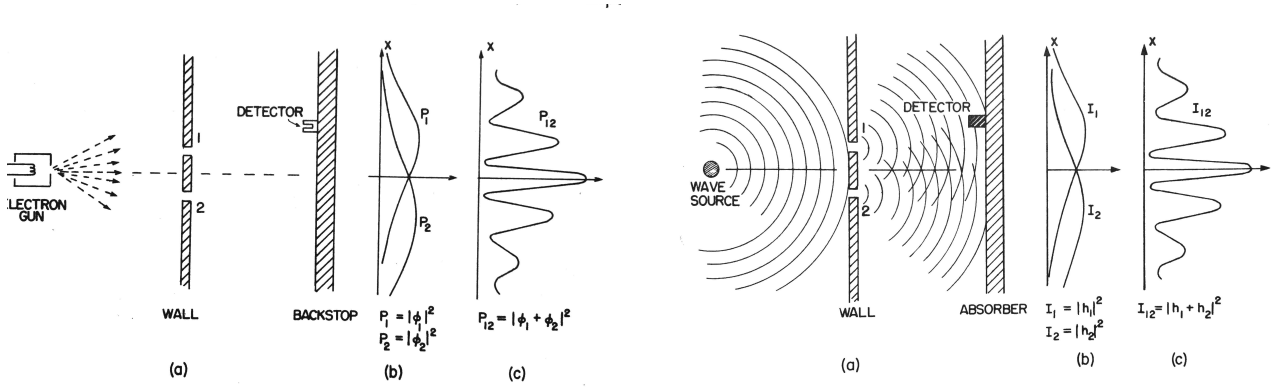


Figure 3: A double-slit experiment with (a) electrons and (b) waves.

Postulate 1: Probabilities from Probability Amplitudes

Probability amplitudes are complex numbers associated with the outcomes of measurements. The corresponding probabilities are obtained as

$$P(A) = |A|^2. \tag{4}$$

If there are several ways of arriving at a particular measurement outcome the associated probability amplitudes add.

This postulate allows us to understand why there is an interference pattern in out double-slit experiment for electrons. By Postulate 1 we have

$$P(x) = |\text{Probability amplitude to go from the electron gun to x}|^2 \ . \tag{5}$$

Clearly there are two paths from the gun G to position x on the screen. The electron could travel via slit 1 or via slit 2. Denoting the associated probability amplitudes by $A(1)$ and $A(2)$ respectively we have by our postulate

$$P(x) = |A(1) + A(2)|^2 \ , \tag{6}$$

because probability amplitudes add. Working this out we have

$$P(x) = |A(1)|^2 + |A(2)|^2 + \underbrace{2\mathrm{Re}\left[A(1)A^*(2)\right]}_{\text{“Interference term”}}. \tag{7}$$

Expressing the complex amplitudes in terms of their magnitudes and phases $A(1) = \sqrt{P(1)}e^{i\phi(1)}$ we can rewrite this as

$$P(x) = P(1) + P(2) + 2\sqrt{P(1)P(2)}\cos\big(\phi(1) - \phi(2)\big). \tag{8}$$

This is clearly very different from the “classical” rule for adding probabilities for exclusive events! For $x \approx 0$ we have $P(1) \approx P(2)$ and therefore

$$P(x) \approx 2P(1)\left[1 + \cos\big(\phi(1) - \phi(2)\big]\right. . \tag{9}$$

The “classical” result would simply be $2P(1)$, while QM predicts a probability distribution that oscillates between 0 and $4P(1)$ as a consequence of “QM interference”. Before we take leave of our double-slit experiments there is one more variation we need to consider. Now we position a light source behind the double slit, which allows us to measure through which slit the individual electrons go. In this experimental setup

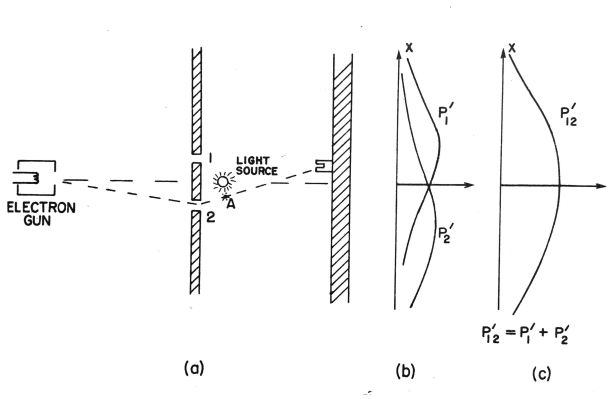


Figure 4: Double-slit experiments with electrons where we measure through which slit the electrons go.

the interference disappears and probabilities add! If this does not give you goosebumps there is something seriously wrong with you! Our framework for QM will have to account for this bizarre interference-killing effect as well.

NB 1

The fundamental idea in QM is to associate probability amplitudes with measurement outcomes of given observables.

- Example 1: Let $E_0, E_1, \ldots$ be the possible outcomes of an energy measurement. With each energy we associate a complex probability amplitude $A(E_j)$ such that the probability for measuring E_j is $P(E_j) = |A(E_j)|^2$ and
$$\sum_j P(E_j) = 1. \tag{10}$$

- Example 2: Consider a position measurement in one dimension (like the one above). The possible outcomes are then real numbers in some interval $x \in [a, b]$. With each position x we associate a complex probability amplitude $\psi(x)$ such that $P(x) = |\psi(x)|^2$ and
$$\int_a^b dx\ P(x) = 1. \tag{11}$$
In this case the set of probability amplitudes can be viewed as a complex valued function.

1.2 Complete sets of amplitudes and quantum states

Knowing all amplitudes $A(E_j)$ provides us with a probabilistic description of repeated energy measurements in the following sense.

- Set up an experiment in a particular way. This fixes a particular set of probability amplitudes $\{A(E_0), A(E_1), \ldots\}$.
- Measure the energy. The result is E_j Write the result down.
- Repeat the experiment many times (we imagine that we can set things up in precisely the same way each time). The ultimate result of our efforts is a *histogram* that gives probabilities $P(E_j)$ for the various observed measurement outcomes E_j. QM asserts that $P(E_j) = |A(E_j)|^2$.
- Changing our experimental setup would result in a different set of amplitudes $\{A'(E_0), A'(E_1), \ldots\}$.

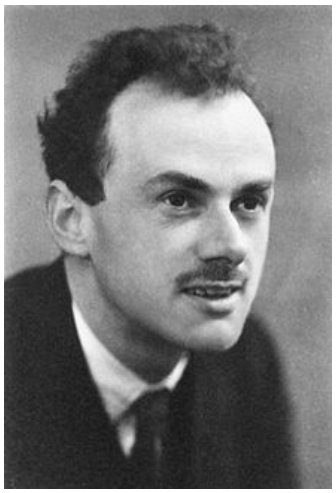
So far so good. The next step is a crucial one.

Definition 1 *A key aspect of QM is that specifying amplitudes for e.g. an energy measurement can provide enough information to obtain probabilistic descriptions of measurement outcomes of* any *other observable. Such sets of amplitudes are called* **complete**.

An efficient way of encoding the information contained in a complete set of amplitudes $\{A(E_0), A(E_1), \dots\}$ is to combine them into a *vector*

$$|\psi\rangle = (A(E_0), A(E_1), \dots). \tag{12}$$

We call this a *state* or *ket-state* using a terminology (and very clever notation) invented by P.A.M. Dirac.



Paul A.M. Dirac (Nobel Prize in Physics 1933).

"If you are receptive and humble, mathematics will lead you by the hand".

1.3 Dirac notation for complex linear vector spaces

It is easy to see that ket states form a complex linear vector space V. Addition of two kets is defined in terms of addition of the associated amplitudes

$$|\psi\rangle + |\phi\rangle = (A(E_0) + A'(E_0), A(E_1) + A'(E_1), \dots) \ , \tag{13}$$

while multiplication by complex numbers is defined as

$$c|\psi\rangle = (cA(E_0), cA(E_1), \dots). \tag{14}$$

The vector space structure makes it clear that there are special states such that all amplitudes are zero except $A(E_j) = 1$. We denote these states by $|E_j\rangle$. By construction they are such that an energy measurement in a system described by the ket $|E_j\rangle$ returns the result E_j with probability 1. In other words they are *states of definite energy*. If $\{A(E_j)\}$ is a complete set of amplitudes these form a *basis* of V: any ket $|\psi\rangle$ can be expressed as a linear combination

$$|\psi\rangle = \sum_j \psi_j |E_j\rangle \ , \quad \psi_j \in \mathbb{C}. \tag{15}$$

1.3.1 Dual ("bra") states

Given a state $|\psi\rangle$ we want a quick way for extracting individual amplitudes. Mathematically speaking we are searching for linear maps

$$\begin{aligned} V &\longrightarrow \mathbb{C} \\ |\psi\rangle &\longrightarrow \psi_j \end{aligned} \tag{16}$$

such that $\alpha|\psi\rangle + \beta|\phi\rangle$ maps to $\alpha\psi_j + \beta\phi_j$. For finite dimensional linear vector spaces such maps form a linear vector space V^*, the *dual space*, of the same dimension as V. Dirac notations provide us with a very neat way of constructing a basis of V^*:

- Start with an orthonormal basis $B = \{|j\rangle\}$ of V.
- Define corresponding "bra" states $\langle j| \in V^*$ by specifying their action on B

$$\langle n|j\rangle = \delta_{n,j} \ , \quad \text{"bra-ket" – Dirac's only joke.} \tag{17}$$

- Extend this to general states $|\psi\rangle = \sum_j \psi_j |j\rangle$ by the rule

$$\langle\psi| = \sum_j \psi_j^* \ \langle j| \ . \tag{18}$$

In this way $\langle\psi|\phi\rangle$ turns into the usual scalar product for complex linear vector spaces

$$\langle\psi|\phi\rangle = \sum_j \psi_j^* \phi_j = (\langle\phi|\psi\rangle)^* \ , \tag{19}$$

and

$$\langle\psi|\psi\rangle = \sum_j |\psi_j|^2 \geq 0 \quad \text{"Length" of } |\psi\rangle. \tag{20}$$

NB 2

he length of state vectors in QM must always be 1, because probabilities must add up to 1.

1.4 ... AND BACK TO MEASUREMENTS

To describe the measurement of an observable A we express the ket $|\psi\rangle$ that describes our system as a linear combination of basis states that correspond to definite outcomes a_j

$$|\psi\rangle = \sum_j \psi_j |a_j\rangle \ , \quad \psi_j = \langle a_j|\psi\rangle \ , \quad \sum_j |\psi_j|^2 = 1. \tag{21}$$

The probability to obtain a_j in our measurement is

$$|\psi_j|^2 = |\langle a_j|\psi\rangle|^2 \qquad \text{"Born's rule."} \tag{22}$$

An important question is what "state" a quantum mechanical system is in just after a particular observable has been measured. As QM deals with very small things measurements can greatly disturb the QM system, i.e. *change its QM state*. What should we expect? To be more precise let's start with a QM system described by the state $|\psi\rangle$, then measure the observable A and obtain the result a_j.

Postulate 2: Projective nature of measurements

We expect that if we measure A again straight away, we will obtain the result a_j with certainty. This is only possible if the first measurement leaves the system in the state $|a_j\rangle$ – meaning that





Figure 5: Max Born (Nobel Prize in Physics 1954) ... and his more famous granddaughter. Born is said to have thought that the Copenhagen interpretation of QM should really be called the Göttingen interpretation. He has a point...

measurements are **projective**:

$$\boxed{|\psi\rangle \longrightarrow \text{measure A, obtain result } a_j \Rightarrow \text{ system left in the state } |a_j\rangle.} \tag{23}$$

1.5 Arbitrariness of the overall phase

Let us now consider the two states $|\psi\rangle$ and $|\psi'\rangle = e^{i\alpha}|\psi\rangle$ where α is an arbitrary phase. According to the rules we have presented, there is no way of telling these two states apart through any quantum mechanical measurement! Indeed we have

$$|\psi'\rangle = e^{i\alpha}|\psi\rangle = \sum_j e^{i\alpha}\langle a_j|\psi\rangle \ |a_j\rangle. \tag{24}$$

Hence the possible measurement outcomes are again given by the set $\{a_j\}$ and the corresponding probabilities are

$$|\langle a_j|\psi'\rangle|^2 = |e^{i\alpha}\langle a_j|\psi\rangle|^2 = |\langle a_j|\psi\rangle|^2. \tag{25}$$

This tells us that $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle$ *describe the same quantum mechanical state.* In the mathematical literature the states $e^{i\alpha}|\psi\rangle$, $\alpha \in \mathbb{R}$ are called a *ray.* In practice we will always fix the overall phase of quantum states in a convenient way.

Summary 1

1. QM systems are described by *quantum "ket" states* $|\psi\rangle$. These correspond to different ways of experimentally "setting up" the system. States that differ only by an overall phase factor describe the same physical situation and are to be identified.
2. Kets form a complex linear vector space V.
3. To each state $|\psi\rangle$ we can associate a complex valued linear map $\langle\psi|$. These "bra-vectors" form

a linear vector space V^* of the same dimension as V.

4. To describe a measurement of an observable A we express the state $|\psi\rangle$ describing our system as a linear superposition of basis states that correspond to definite measurement outcomes a_j for A

$$|\psi\rangle = \sum_j \psi_j |a_j\rangle \ , \quad \psi_j = \langle a_j|\psi\rangle \ , \quad \sum_j |\psi_j|^2 = 1. \tag{26}$$

The probability to obtain a_j in our measurement is

$$|\psi_j|^2 = |\langle a_j|\psi\rangle|^2 \qquad \text{"Born's rule."} \tag{27}$$

5. After the measurement the system is left in the state $|a_j\rangle$ (if the outcome of the measurement was a_j).

Homework 1: Probability amplitudes, probabilities and Dirac notation

1.1 What physical phenomenon requires us to work with probability amplitudes rather than with probabilities?

1.2 Given that $|\psi\rangle = e^{i\pi/5}|a\rangle + e^{i\pi/4}|b\rangle$, express $\langle\psi|$ as a linear combination of $\langle a|$ and $\langle b|$.

1.3 An electron can be in one of two potential wells that are so close that it can 'tunnel' from one to the other. Its state vector can be written

$$|\psi\rangle = a|A\rangle + b|B\rangle, \tag{28}$$

where $|A\rangle$ is the state of being in the first well and $|B\rangle$ is the state of being in the second well and all kets are correctly normalised. What is the probability of finding the particle in the first well given that: (a) $a = i/2$; (b) $b = e^{i\pi}$; (c) $b = \frac{1}{3} + i/\sqrt{2}$?

1.4 An electron can "tunnel" between potential wells that form a linear chain, so its state vector can be written as

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} a_n |n\rangle, \tag{29}$$

where $|n\rangle$ is the state of being in the n^{th} well, where n increases from left to right. Let

$$a_n = \frac{1}{\sqrt{2}} \left(\frac{-i}{3}\right)^{\frac{|n|}{2}} e^{in\pi}. \tag{30}$$

(a) What is the probability of finding the electron in the n^{th} well?
(b) What is the probability of finding the electron in well 0 or anywhere to the right of it?

2 Operators and Observables

In the lab we (i.e. our experimental colleagues) can *manipulate* quantum states, i.e. devise protocols that map states to other states. In our mathematical framework this is described by considering *linear operators* acting on V

$$\begin{aligned} \mathcal{O}: \quad & V \longrightarrow V \\ & |\psi\rangle \longrightarrow \mathcal{O}|\psi\rangle \ , \end{aligned} \tag{31}$$

where $\mathcal{O}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha\mathcal{O}|\psi\rangle + \beta\mathcal{O}|\phi\rangle$. Dirac notation provides us with a very useful way of expressing operators. A general operator can be expressed in terms of basis states $|j\rangle$ and their dual states $\langle j|$ as follows:

- The object $|j\rangle\langle k|$ is a linear operator.

  Proof:
  $$|k\rangle\langle j|\Big(\alpha|\psi\rangle + \beta|\psi\rangle\Big) = |k\rangle\Big(\alpha\langle j|\psi\rangle + \beta\langle j|\psi\rangle\Big) = \underbrace{\alpha\langle j|\psi\rangle}_{\in\mathbb{C}}|k\rangle + \beta\langle j|\psi\rangle|k\rangle \ . \tag{32}$$

- The identity operator is
  $$\mathbf{1} = \sum_j |j\rangle\langle j|. \tag{33}$$

  Proof: Act with $\mathbf{1}$ on a general state $|\psi\rangle = \sum_k \psi_k|k\rangle$:
  $$\Big[\sum_j |j\rangle\langle j|\Big]|\psi\rangle = \sum_k \psi_k \sum_j |j\rangle \underbrace{\langle j|k\rangle}_{\delta_{j,k}} = \sum_k \psi_k|k\rangle = |\psi\rangle. \tag{34}$$

- A general operator A can be written in the form
  $$\boxed{A = \sum_{j,k}\langle j|A|k\rangle\ |j\rangle\langle k| \ .} \tag{35}$$

  the complex numbers $\langle j|A|k\rangle$ are called *matrix elements* of A in the basis $\{|j\rangle\}$.

  Proof:
  $$A = \mathbf{1}A\mathbf{1} = \big(\sum_j |j\rangle\langle j|\big)A\big(\sum_k |k\rangle\langle k|\big) \ . \tag{36}$$

NB 3

For finite dimensional linear vector spaces linear operators correspond to square matrices.

Like for matrices, a very useful way to characterize an operator is through its *eigenvalues* and *eigenvectors* ("eigenstates"). The eigenvalue equation for an operator $\mathcal{O}$ is
$$\boxed{\mathcal{O}|o_j\rangle = o_j|o_j\rangle.} \tag{37}$$
The eigenvalues $\{o_j\}$ form the *spectrum* of the operator $\mathcal{O}$. The most important operator in QM is the *Hamiltonian*, or energy operator. It is defined by
$$\boxed{H = \sum_j E_j|E_j\rangle\langle E_j|,} \tag{38}$$
where $|E_j\rangle$ are the quantum states introduced above that give result E_j with probability one when the energy is measured.The Hamiltonian fulfils by construction
$$H|E_j\rangle = E_j|E_j\rangle. \tag{39}$$
Hence the spectrum of the Hamiltonian is equal to the set of possible outcomes of energy measurements. This generalizes to other observables: with each observable we can associate an operator by
$$A = \sum_j a_j|a_j\rangle\langle a_j| \ , \tag{40}$$
where $\{|a_j\rangle\}$ is a complete set of states that return the result a_j with probability one when the observable under consideration is measured. As the outcomes of the measurements we have in mind (energy, momentum, position etc) are real numbers the operators representing observables must be special.

2.1 Hermitian Operators

In QM observables are represented by *Hermitian* operators

$$\boxed{A \text{ Hermitian} \Leftrightarrow (\langle\phi|A|\psi\rangle)^* = \langle\psi|A|\phi\rangle \ .} \tag{41}$$

Hermitian operators have three crucial properties that we will use constantly in the following:

(H1) Their eigenvalues are real.

(H2) Eigenstates corresponding to different eigenvalues are orthogonal

$$\langle a_j|a_k\rangle = 0 \text{ if } a_j \neq a_k. \tag{42}$$

(H3) One can always construct an orthonormal basis of V from the eigenstates of a Hermitian operator.

Aside 1: Hermitian Operators

You have already seen this in your Linear Algebra course, but in order to be self-contained and to get you fluent in Dirac notations the proofs of these statements are summarized below. Let A be a Hermitian operator with eigenvalue equation

$$A|a_k\rangle = a_k|a_k\rangle. \tag{43}$$

As A is Hermitian we have

$$(\langle a_k|A|a_\ell\rangle)^* = \langle a_\ell|A|a_k\rangle \ . \tag{44}$$

Using the eigenvalue equation this implies $a_\ell^*\langle a_k|a_\ell\rangle^* = a_k\langle a_\ell|a_k\rangle$ and using that $\langle a_k|a_\ell\rangle^* = \langle a_\ell|a_k\rangle$ we have

$$(a_\ell^* - a_k)\langle a_\ell|a_k\rangle = 0 \ . \tag{45}$$

- Setting $k = \ell$ gives

$$(a_\ell^* - a_\ell)\langle a_\ell|a_\ell\rangle = 0, \tag{46}$$

  which implies

$$a_\ell = a_\ell^* \Rightarrow \text{(H1)}. \tag{47}$$

- Taking $a_k \neq a_\ell$ in (45) we have

$$\langle a_\ell|a_k\rangle = 0 \ , \tag{48}$$

  which immediately implies (H2).

- For eigenstates with the same eigenvalue we can carry out a Gram-Schmidt orthogonalization procedure. Together with (H2) this implies (H3).

Definition 2 *The Hermitian conjugate $B^\dagger$ of an operator B is defined by*

$$\langle\phi|B^\dagger|\psi\rangle = (\langle\psi|B|\phi\rangle)^* \ . \tag{49}$$

Hermitian operators fulfil $A = A^\dagger$. The following rules for taking Hermitian conjugates will be useful:

$$(A+B)^\dagger = A^\dagger + B^\dagger \ , \tag{50}$$

$$(cA)^\dagger = c^* A^\dagger \ , \tag{51}$$

$$(AB)^\dagger = B^\dagger A^\dagger \ . \tag{52}$$

Aside 2: Hermitian conjugation

The properties (52) are straightforward to establish and provide an excellent exercise in Dirac notation (so make sure that you are happy with each of the steps!). The first property follows from considering

$$\langle\phi|(A+B)^\dagger|\psi\rangle = (\langle\psi|A+B|\phi\rangle)^* = (\langle\psi|A|\phi\rangle)^* + (\langle\psi|B|\phi\rangle)^* = \langle\phi|A^\dagger|\psi\rangle + \langle\phi|B^\dagger|\psi\rangle. \tag{53}$$

The second property holds because

$$\langle\phi|(cA)^\dagger|\psi\rangle = (\langle\psi|cA|\phi\rangle)^* = (c\langle\psi|A|\phi\rangle)^* = c^*\langle\phi|A^\dagger|\psi\rangle \tag{54}$$

To establish the third property consider

$$\begin{aligned}\langle\psi|(AB)^\dagger|\phi\rangle &= (\langle\phi|AB|\psi\rangle)^* = (\langle\phi|A\underbrace{\sum_k |k\rangle\langle k|}_{\mathbf{1}} B|\psi\rangle)^* = \sum_k (\langle\phi|A|k\rangle)^*(\langle k|B|\psi\rangle)^* \\ &= \sum_k \langle k|A^\dagger|\phi\rangle\langle\psi|B^\dagger|k\rangle = \langle\psi|B^\dagger\sum_k |k\rangle\langle k|A^\dagger|\phi\rangle = \langle\psi|B^\dagger A^\dagger|\phi\rangle. \end{aligned} \tag{55}$$

Homework 2: Operators

1.5 Let Q be the operator of an observable and let $|\psi\rangle$ be the state of our system.
(a) What are the physical interpretations of $\langle\psi|Q|\psi\rangle$ and $|\langle q_n|\psi\rangle|^2$, where $|q_n\rangle$ is the n^{th} eigenket of the observable Q and q_n is the corresponding eigenvalue?
(b) What is the operator $\sum_n |q_n\rangle\langle q_n|$, where the sum is over all eigenkets of Q? What is the operator $\sum_n q_n|q_n\rangle\langle q_n|$?

1.6 Which of the following operators are Hermitian, given that $\hat{A}$ and $\hat{B}$ are Hermitian:
$\hat{A}+\hat{B}$; $c\hat{A}$; $\hat{A}\hat{B}$; $\hat{A}\hat{B}+\hat{B}\hat{A}$.
Show that in one dimension, for functions which tend to zero as $|x|\to\infty$, the operator $\partial/\partial x$ is not Hermitian, but $-\mathrm{i}\hbar\partial/\partial x$ is. Is $\partial^2/\partial x^2$ Hermitian?

1.7 Given that $\hat{A}$ and $\hat{B}$ are Hermitian operators, show that $i[\hat{A},\hat{B}]$ is a Hermitian operator.

1.8 Given that for any two operators $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$, show that

$$(\hat{A}\hat{B}\hat{C}\hat{D})^\dagger = \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger.$$

2.2 Commutators and Compatible Observables

Definition 3 *The commutator of two operators A and B is*

$$[A,B] = AB - BA. \tag{56}$$

In QM commutators play an important role because of the following theorem.

Theorem 1 *Let A and B be two Hermitian operators. If $[A,B]=0$ there exists a complete set of simultaneous eigenstates of the operators A and B, i.e.*

$$A|u_j\rangle = a_j|u_j\rangle\ , \quad B|u_j\rangle = b_j|u_j\rangle, \tag{57}$$

and $\{|u_j\rangle\}$ form a basis of the LVS on which A and B act.

Proof: One direction is simple: if A and B have a complete set of simultaneous eigenstates $|u_j\rangle$ we have

$$\langle u_j|[A,B]|u_k\rangle = (a_k b_k - b_k a_k)\langle u_j|u_k\rangle = 0, \tag{58}$$

which implies that the commutator is zero (because the $|u_j\rangle$ form a basis). Let's now turn to the other direction of the proof, i.e. let's assume $[A, B] = 0$ and show that this implies the existence of a complete set of simultaneous eigenstates. As A is Hermitian we know that is has a complete set of orthogonal eigenstates

$$A|a_j\rangle = a_j|a_j\rangle \ , \quad \langle a_j|a_k\rangle = \delta_{j,k}. \tag{59}$$

Now consider the matrix elements of the commutator in this basis

$$0 = \langle a_j|[A, B]|a_k\rangle = (a_j - a_k)\langle a_j|B|a_k\rangle \tag{60}$$

This tells us that if all eigenvalues a_j are different, we have $\langle a_j|B|a_k\rangle \propto \delta_{j,k}$, i.e. the eigenstates $|a_j\rangle$ of A are simultaneous eigenstates of B. The situation is a bit more complicated if some of the a_j are equal. Let us assume that n of the a_j are equal and let's label the eigenstates of A such they correspond to $a_1 = a_2 = \cdots = a_n = a$. Then

(i) Any linear combination $\sum_{j=1}^{n} \alpha_j|a_j\rangle$ is an eigenstate of A with eigenvalue a.

(ii) On the subspace spanned by $\{|a_1\rangle, \ldots, |a_n\rangle\}$ B is represented by Hermitian matrix $B_{jk} = \langle a_j|B|a_k\rangle$. Hence it can be diagonalized, i.e. we can construct eigenstates $|u_k\rangle$ of B by taking appropriate linear combinations of the $|u_k\rangle = \sum_{j=1}^{n} \beta_j^{(k)}|a_j\rangle$. These are simultaneous eigenstates of A by (i).

This generalizes straightforwardly to the case where we have several "degenerate" eigenvalues.

Even though all this Linear Algebra is of course very interesting in itself, you may be asking yourselves at this point what on earth this has to do with QM. As you may have guessed, it has to do with measurements! Let us consider two Hermitian operators A and B that correspond to two observables in an experiment. We know that the respective eigenstates of A and B can be used to construct an orthonormal basis of our linear vector space of quantum states

$$A|a_i\rangle = a_i|a_i\rangle, \quad B|b_i\rangle = b_i|b_i\rangle \Rightarrow |\psi\rangle = \sum_i \langle a_i|\psi\rangle \ |a_i\rangle = \sum_i \langle b_i|\psi\rangle \ |b_i\rangle. \tag{61}$$

Let us now make the following Gedankenexperiment: we first measure the observable corresponding to A, and then straight away measure the observable corresponding to B (without re-initializing our experiment). We want to compare this to the reverse order of measurements. Here we go:

- Measure A, then B

$$\begin{aligned} |\psi\rangle \quad &\longrightarrow \quad \text{measure A: } a_i \text{ with prob. } |\langle a_i|\psi\rangle|^2, \text{ system in state } |a_i\rangle \\ &\longrightarrow \quad \text{measure B: } b_j \text{ with prob. } |\langle b_j|a_i\rangle|^2 \ . \end{aligned} \tag{62}$$

  So the final outcome is a table of outcomes with associated probabilities

$$\text{outcome } (a_i, b_j) \text{ probability } |\langle a_i|\psi\rangle|^2 \ |\langle b_j|a_i\rangle|^2 \tag{63}$$

- Measure B, then A

$$\begin{aligned} |\psi\rangle \quad &\longrightarrow \quad \text{measure B: } b_j \text{ with prob. } |\langle b_j|\psi\rangle|^2, \text{ system in state } |b_j\rangle \\ &\longrightarrow \quad \text{measure A: } a_i \text{ with prob. } |\langle a_i|b_j\rangle|^2 \ . \end{aligned} \tag{64}$$

  So here the final outcome is a table

$$\text{outcome } (a_i, b_j) \text{ probability } |\langle b_j|\psi\rangle|^2 \ |\langle a_i|b_j\rangle|^2 \tag{65}$$

Clearly, the tables of measurement outcomes we obtain in the two ways will generally be different! That. Is. Deep. If the order of measurement does not matter, the observables corresponding to A and B are called *compatible*. As the order of measurement for two compatible observables does not matter and we always end up in a quantum state where both observables have a definite value, one could in principle set up an experiment that measures both observables *simultaneously*.

Theorem 2 *Two observables are compatible if and only if the commutator between the associated Hermitian operators vanishes*

$$[A, B] = 0. \tag{66}$$

Proof: If $[A, B] = 0$ there exists a basis of simultaneous eigenstates of A and B. Using this basis in the above consideration it is easy to see that the two outcomes are identical. On the other hand, if $[A, B] \neq 0$ there must be at least one eigenstate $|a_j\rangle$ of A that is not an eigenstate of B. As the state $|\psi\rangle$ above is arbitrary we can choose it to be $|a_j\rangle$. By considering the two sets of outcomes we see that they can only be equal if $|a_j\rangle$ is an eigenstate of B, giving a contradiction. This completes the proof.

Homework 3: COMMUTATORS

1.9 Show that if there is a complete set of mutual eigenkets of the Hermitian operators $\hat{A}$ and $\hat{B}$, then $[\hat{A}, \hat{B}] = 0$. Explain the physical significance of this result.

1.10 Does it always follow that if a system is an eigenstate of $\hat{A}$ and $[\hat{A}, \hat{B}] = 0$ then the system will be in a eigenstate of $\hat{B}$? If not, give a counterexample.

1.11 Show that
(a) $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$
(b) $[\hat{A}\hat{B}\hat{C}, \hat{D}] = \hat{A}\hat{B}[\hat{C}, \hat{D}] + \hat{A}[\hat{B}, \hat{D}]\hat{C} + [\hat{A}, \hat{D}]\hat{B}\hat{C}$. Explain the similarity with the rule for differentiating a product.
(c) $[\hat{x}^n, \hat{p}] = \mathrm{i}\hbar n\hat{x}^{n-1}$
(d) $[f(\hat{x}), \hat{p}] = \mathrm{i}\hbar\frac{\mathrm{d}f}{\mathrm{d}x}$ for any function $f(x)$.

1.12 Let A and B be two Hermitian operators. Prove that if $[A, B] = 0$ there exists a complete set of simultaneous eigenstates of the operators A and B, i.e.

$$A|u_j\rangle = a_j|u_j\rangle \ , \quad B|u_j\rangle = b_j|u_j\rangle, \tag{67}$$

and $\{|u_j\rangle\}$ form a basis of the LVS on which A and B act.

1.13 Prove that two observables are compatible if and only if the commutator between the associated Hermitian operators vanishes.

1.14 What does it mean to say that two operators commute? What is the significance of two observables having mutually commuting operators?
Given that the commutator $[P, Q] \neq 0$ for some observables P and Q, does it follow that for all $|\psi\rangle \neq 0$ we have $[P, Q]|\psi\rangle \neq 0$?

2.3 EXPECTATION VALUES

Definition 4 *The* **expectation value** *of an operator $\mathcal{O}$ in a quantum state $|\psi\rangle$ is defined as*

$$\langle\psi|\mathcal{O}|\psi\rangle \ . \tag{68}$$

Expectation values are hugely important in QM. To see why let us consider a Hermitian operator $A = A^\dagger$ associated with some observable. Any state can be written as linear combination of the eigenstates of A (why?)

$$|\psi\rangle = \sum_j \langle a_j|\psi\rangle \ |a_j\rangle. \tag{69}$$

Hence

$$\boxed{\langle\psi|A|\psi\rangle = \sum_j a_j|\langle a_j|\psi\rangle|^2.} \tag{70}$$

This expression has an important physical meaning: a_j are the outcomes of measuring the observable to which A corresponds, and $|\langle a_j|\psi\rangle|^2$ are the associated probabilities.

NB 4

So the expectation value gives the *average* over many measurements of our observable when the system is in the quantum state $|\psi\rangle$.

Let us now consider the expectation values

$$\langle\psi|A^n|\psi\rangle = \sum_j a_j^n |\langle a_j|\psi\rangle|^2. \tag{71}$$

These are nothing but the *moments of the probability distribution* associated with measuring the observable associated with A in the state $|\psi\rangle$! Nice.

3 Position and Momentum Representations

All animals are equal, but some are more equal than others. George Orwell.

The basic objects in QM are quantum states. In order to work with them we usually express them in some particular basis. Which choice is most convenient depends on the particular problem one is interested in. Having said this, some choices of basis are of particular importance.

3.1 Position Representation

This is obtained by working with probability amplitudes $\psi(x)$ for finding a particle at position x (in 1 dimension). In Dirac notation

$$|\psi\rangle = \int dx\ \psi(x)\ |x\rangle, \tag{72}$$

where $|x\rangle$ are quantum states in which a position measurement returns the result x with probability 1.

Definition 5 *The probability amplitude $\psi(x)$ is called a* wave function.

Now recall that we introduced bra-vectors to extract amplitudes from states. Here we want

$$\langle x'|\psi\rangle = \psi(x') = \int dx\ \psi(x)\ \langle x'|x\rangle. \tag{73}$$

This requires

$$\langle x'|x\rangle = \delta(x - x'), \tag{74}$$

where $\delta(x)$ is the *Dirac delta-function*. Indeed, a defining property of the delta-function is that (for all sufficiently well-behaved functions $f(x)$)

$$\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x - x') = f(x'). \tag{75}$$

At this point students usually feel somewhat uncomfortable, because the scalar product of bras and kets involves a delta-function rather than a Kronecker delta. The reason for this is that x is a *continuous variable* and the same situation arises for other observables where the outcome of measurements can vary continuously. The resolution of the identity in terms of the states $|x\rangle$ reads

$$\mathbf{1} = \int dx\ |x\rangle\langle x|. \tag{76}$$

Check:

$$\mathbf{1}|\psi\rangle = \int dx\ |x\rangle\langle x|\psi\rangle = \int dx\ \psi(x)\ |x\rangle. \tag{77}$$

3.1.1 Position operator

Given a basis of states of definite position we can introduce the associated *position operator*

$$\boxed{\hat{x} = \int dx\ x\ |x\rangle\langle x|.} \tag{78}$$

By construction the position operator has eigenstates $|x\rangle$ with eigenvalues x

$$\hat{x}|x'\rangle = \int dx\ x\ |x\rangle\langle x|x'\rangle = \int dx\ x\ |x\rangle\ \delta(x - x') = x'|x'\rangle. \tag{79}$$

It acts on general states as

$$\hat{x}|\psi\rangle = \int dx\ x\ |x\rangle\langle x|\psi = \int dx\ x\psi(x)\ |x\rangle\ , \tag{80}$$

i.e. *it multiplies the wave function by x*. By concatenating (79) we find

$$\hat{x}^n|x'\rangle = (x')^n|x'\rangle, \tag{81}$$

and therefore

$$\boxed{V(\hat{x})|x'\rangle = V(x')|x'\rangle\ ,} \tag{82}$$

where $V(x)$ is a function that is to be understood in terms of its Taylor expansion around $x = 0$. For a QM particle moving in one dimension $V(\hat{x})$ would be the operator describing its *potential energy*. (Why?) We note that

$$\langle\psi|\hat{x}^n|\psi\rangle = \int dx\ |\psi(x)|^2 x^n\ , \tag{83}$$

so $\langle\psi|\hat{x}|\psi\rangle$ is the *average position* and $\langle\psi|\hat{x}^2|\psi\rangle - \langle\psi|\hat{x}|\psi\rangle^2$ the *variance* if we look at the histogram of many position measurements.

3.1.2 Position representation for other operators

An important question is how other operators look like in the position representation. For a general operator A we have

$$A = \mathbf{1}\ A\ \mathbf{1} = \int dx\ dx'\ |x\rangle\langle x'|\ \langle x|A|x'\rangle. \tag{84}$$

As usual in order to define the operator we require its matrix elements $\langle x|A|x'\rangle$. A particular important operator is the *momentum operator*. It is defined (in one dimension) as

$$\hat{p} = \int dp\ p\ |p\rangle\langle p|, \tag{85}$$

where $|p\rangle$ are states such that a momentum measurement returns the value p with certainty. In the position representation (see below for some motivation) one has

$$\boxed{\langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\ \delta(x - x').} \tag{86}$$

This gives

$$\boxed{\langle x|\hat{p}|\psi\rangle = \int dx'\langle x|\hat{p}|x'\rangle\ \psi(x') = -i\hbar\frac{\partial\psi(x)}{\partial x}.} \tag{87}$$

Aside 3: Momentum operator

At this point we have simply asserted that the position representation of the momentum operator is given by eqn (86). The justification will be given in Part III of the lectures, when we will consider translations in QM. The logic that underlies the identification of the momentum operator goes as follows. In classical mechanics momentum can be defined as the generator of translations. One then defines the momentum operator in quantum mechanics as the generator of translations in QM. This leads to (86).

3.2 Heisenberg Uncertainty Relation



Werner Heisenberg (Nobel Prize in Physics 1932).
"What we observe is not nature itself, but nature exposed to our method of questioning."

Heisenberg also gave an excellent definition of experts: *"An expert is someone who knows some of the worst mistakes that can be made in their subject, and how to avoid them."*

Let us consider the commutator $[\hat{x},\hat{p}]$

$$\langle x|[\hat{x},\hat{p}]|\psi\rangle = \langle x|\hat{x}\hat{p}-\hat{p}\hat{x}|\psi\rangle = -i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar\frac{\partial}{\partial x}\big[x\psi(x)\big] = i\hbar\langle x|\psi\rangle. \tag{88}$$

As $|\psi\rangle$ is arbitrary this tells us that

$$\boxed{[\hat{x},\hat{p}] = i\hbar.} \tag{89}$$

So momentum and position are *incompatible observables*! Now consider the variances for position and momentum measurements in the state $|\psi\rangle$

$$\langle\psi|(\hat{x}-x_0)^2|\psi\rangle\ , \quad \langle\psi|(\hat{p}-p_0)^2|\psi\rangle, \tag{90}$$

where $x_0 = \langle\psi|\hat{x}|\psi\rangle$ and $p_0 = \langle\psi|\hat{p}|\psi\rangle$. For general Hermitian operators $A = A^\dagger$ and $B = B^\dagger$ we have

$$2i\ \mathrm{Im}\langle\psi|AB|\psi\rangle = \langle\psi|[A,B]|\psi\rangle. \tag{91}$$

But the imaginary part of a complex number is always smaller than its magnitude and so

$$\mathrm{Im}\langle\psi|AB|\psi\rangle \le |\langle\psi|AB|\psi\rangle|. \tag{92}$$

Next we use the Schwarz inequality, which in Dirac notations reads

$$|\langle\phi|\phi'\rangle| \le \sqrt{\langle\phi|\phi\rangle\ \langle\phi'|\phi'\rangle}. \tag{93}$$

In the usual vector notation and for real vector spaces this reads $|\vec{a}\cdot\vec{b}| \le ||\vec{a}||\ ||\vec{b}||$, which is obviously true because $\vec{a}\cdot\vec{b} = ||\vec{a}||\ ||\vec{b}||\cos\varphi$, where φ is the angle between the two vectors. Applying the Schwarz inequality to the states $B|\psi\rangle$ and $A|\psi\rangle$ on the rhight-hand-side of (92) and then using (91) we obtain

$$\frac{1}{2i}\langle\psi|[A,B]|\psi\rangle \le \sqrt{\langle\psi|A^2|\psi\rangle\ \langle\psi|B^2|\psi\rangle}. \tag{94}$$

Finally we substitute $A = \hat{x} - x_0$, $B = \hat{p} - p_0$ and use $[A, B] = i\hbar$ to arrive at the *Heisenberg uncertainty relation*

$$\boxed{\frac{\hbar}{2} \leq \underbrace{\sqrt{\langle\psi|(\hat{x}-x_0)^2|\psi\rangle}}_{\Delta X}\underbrace{\sqrt{\langle\psi|(\hat{p}-p_0)^2|\psi\rangle}}_{\Delta P}.} \tag{95}$$

The physical content of the Heisenberg uncertainty relation is that the product of the variances of the QM probability distributions for position and momentum measurements must always be larger than $(\hbar/2)^2$. So if the state $|\psi\rangle$ is such that the variance of the position probability distribution is very small, i.e. we can determine the position very precisely, the variance of the probability distribution of momentum must be large enough to satisfy the inequality (95), i.e. very large. So, in a probabilistic sense, we can never know both the position and the momentum of a particle very precisely.

3.3 Momentum Representation

Momentum eigenstates fulfil $\hat{p}|p\rangle = p|p\rangle$. We can work out the corresponding wave functions by considering

$$\langle x|\hat{p}|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle. \tag{96}$$

This is a first order ODE with solution

$$\boxed{\langle x|p\rangle = A\ e^{\frac{i}{\hbar}px}.} \tag{97}$$

So the wave function of momentum eigenstates are *plane waves*! As $|\langle x|p\rangle|^2 = |A|^2$ is position independent a particle in a momentum eigenstates is equally likely to be found anywhere in space when its position is measured. The constant A is fixed by the normalization condition

$$\langle p|p'\rangle = \delta(p - p')\ , \tag{98}$$

which ensures that the resolution of the identity has the form

$$\mathbf{1} = \int dp\ |p\rangle\langle p|. \tag{99}$$

We have

$$\langle p|p'\rangle = \int dx\ \langle p|x\rangle\langle x|p'\rangle = \int dx\ |A|^2 e^{\frac{i}{\hbar}(p'-p)x} = |A|^2\ 2\pi\hbar\ \delta(p - p'), \tag{100}$$

so $A = (2\pi\hbar)^{-1/2}$. The momentum representation is obtained by expressing states and operators in terms of a basis of momentum eigenstates

$$|\psi\rangle = \int_{-\infty}^{\infty} dp\ \langle p|\psi\rangle\ |p\rangle\ , \quad \mathcal{O} = \int dp\ dp'\langle p|\mathcal{O}|p'\rangle\ |p\rangle\langle p'|. \tag{101}$$

Using $|\psi\rangle = \int_{-\infty}^{\infty} dx\ \langle x|\psi\rangle\ |x\rangle = \int_{-\infty}^{\infty} dp\ \langle p|\psi\rangle\ |p\rangle$ we can relate the momentum and position representations

$$\langle p|\psi\rangle = \int_{-\infty}^{\infty} dx\ \psi(x)\ \frac{e^{-\frac{i}{\hbar}px}}{\sqrt{2\pi\hbar}}\ , \qquad \langle x|\psi\rangle = \int_{-\infty}^{\infty} dp\ \langle p|\psi\rangle\ \frac{e^{\frac{i}{\hbar}px}}{\sqrt{2\pi\hbar}}. \tag{102}$$

This is precisely the (inverse) *Fourier transformation* of the wave function!

3.4 Generalization to 3 Dimensions

In three spatial dimensions we use a basis of quantum states $|\vec{x}\rangle$ of definite position $\vec{x} = (x, y, z)$. These states fulfil the normalization condition

$$\langle \vec{x}|\vec{x}'\rangle = \delta^{(3)}(\vec{x} - \vec{x}') = \delta(x - x')\delta(y - y')\delta(z - z'). \tag{103}$$

The resolution of the identity is

$$\mathbf{1} = \int d^3\vec{x}\ |\vec{x}\rangle\langle\vec{x}|. \tag{104}$$

A general state can be written as a linear combination of these basis states

$$\boxed{|\psi\rangle = \int d^3\vec{x}\ \underbrace{\langle\vec{x}|\psi\rangle}_{\psi(\vec{x})}\ |\vec{x}\rangle.} \tag{105}$$

Now we can define operators corresponding to each of the three components of position

$$\begin{aligned} \hat{x} &= \int d^3\vec{x}\ x\ |\vec{x}\rangle\langle\vec{x}|\ , \\ \hat{y} &= \int d^3\vec{x}\ y\ |\vec{x}\rangle\langle\vec{x}|\ , \\ \hat{z} &= \int d^3\vec{x}\ z\ |\vec{x}\rangle\langle\vec{x}|\ . \end{aligned} \tag{106}$$

By the same kind of argument as in the 1D case we have

$$V(\hat{x}, \hat{y}, \hat{z})|\vec{x}\rangle = V(x, y, z)|\vec{x}\rangle, \tag{107}$$

where $V(x, y, z)$ is to be understood in terms of its Taylor expansion around $(0, 0, 0)$. In D=3 we also have three components of momentum and can define the associated quantum states $|\vec{p}\rangle$, which return the result p_α with certainty when the α-component of momentum is measured ($\alpha = x, y, z$). Their normalization is as you may have already guessed

$$\langle\vec{p}|\vec{p}'\rangle = \delta^{(3)}(\vec{p} - \vec{p}') = \delta(p_x - p'_x)\delta(p_y - p'_y)\delta(p_z - p'_z). \tag{108}$$

Following our construction for D=1 we can define three Hermitian operators associated with the three components of momentum by

$$\hat{p}_\alpha|\vec{p}\rangle = p_\alpha|\vec{p}\rangle\ , \qquad \alpha = x, y, z \tag{109}$$

In the position representation we have

$$\langle\vec{x}'|\hat{p}_\alpha|\vec{x}\rangle = -i\hbar\frac{\partial}{\partial x_\alpha}\delta^{(3)}(\vec{x} - \vec{x}')\ , \qquad \alpha = x, y, z. \tag{110}$$

This implies that

$$\boxed{\langle\vec{x}|\hat{p}_\alpha|\psi\rangle = -i\hbar\frac{\partial}{\partial x_\alpha}\psi(\vec{x})\ .} \tag{111}$$

4 Time Evolution in Quantum Mechanics

Newtonian mechanics is about equations of motion for physical quantities. The analogue in QM is time evolution of quantum states.

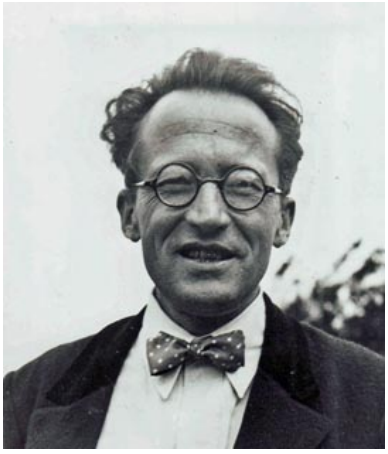
4.1 Time dependent Schrödinger equation and Ehrenfest's theorem

Postulate 3

The time evolution of quantum states is described by the **time-dependent Schrödinger equation**

$$\boxed{i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle,} \tag{112}$$

where H is the Hamiltonian of the system.



Erwin Schrödinger (Nobel Prize in Physics 1933).
"I insist upon the view that all is waves."

"I knew of Heisenberg's theory, of course, but I felt discouraged, not to say repelled, by the methods of transcendental algebra, which appeared difficult to me, and by the lack of visualizability." (Schrödinger in 1926)

The more I think about the physical portion of Schrödinger's theory, the more repulsive I find it. What Schrödinger writes about the visualizability of his theory is probably not quite right, in other words it's crap (in German "Mist")." (Heisenberg, writing to Pauli in 1926).

The associated equation for the bra-state is

$$\boxed{-i\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|H.} \tag{113}$$

The general rules are

$$\boxed{c|\psi\rangle \longrightarrow c^*\langle\psi|\ , \qquad A|\psi\rangle \longrightarrow \langle\psi|A^\dagger\ .} \tag{114}$$

To see what the bra-state corresponding to $A|\psi\rangle$ is we expand both the state and the operator in a basis

$$|\psi\rangle = \sum_j \psi_j|j\rangle\ , \quad A = \sum_{k,l}\langle k|A|l\rangle\ |k\rangle\langle l|\ . \tag{115}$$

Using $\langle l|j\rangle = \delta_{l,j}$ we then have

$$A|\psi\rangle = \sum_{k,l}\langle k|A|l\rangle\ \psi_l\ |k\rangle\ . \tag{116}$$

The associated bra state is

$$\sum_{k,l}(\langle k|A|l\rangle\ \psi_l)^*\ \langle k| = \sum_{k,l}(\langle k|A|l\rangle)^*\ \psi_l^*\ \langle k| = \sum_{k,l}\langle l|A^\dagger|k\rangle\ \psi_l^*\ \langle k| = \sum_l \psi_l^*\langle l|A^\dagger\sum_k|k\rangle\langle k| = \langle\psi|A^\dagger. \tag{117}$$

By combining the TDSEs for $|\psi(t)\rangle$ and $\langle\psi(t)|$ we obtain the evolution equation for the expectation values of (time-independent) operators

$$\boxed{-i\hbar\frac{\partial}{\partial t}\langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \langle\psi(t)|[H,\mathcal{O}]|\psi(t)\rangle\ .} \tag{118}$$

This is called *Ehrenfest's theorem*. As a first application of this equation let us consider a free QM particle with Hamiltonian $H = \hat{p}^2/(2m)$, i.e. only kinetic energy. Then

$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{2m}\langle\psi(t)|[\hat{p}^2,\hat{x}]|\psi(t)\rangle \ . \tag{119}$$

The commutator is worked out using a standard trick

$$[\hat{p}^2,\hat{x}] = \hat{p}^2\hat{x} - \hat{p}\hat{x}\hat{p} + \hat{p}\hat{x}\hat{p} - \hat{x}\hat{p}^2 = \hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p} = -2i\hbar\hat{p}. \tag{120}$$

This tells us that

$$m\frac{\partial}{\partial t}\langle\hat{x}\rangle = \langle\hat{p}\rangle. \tag{121}$$

This is precisely what we would expect classically (and shows that our definition of momentum operator is reasonable).

4.2 Time independent Schrödinger equation

The eigenvalue equation for the Hamiltonian is also known as the *time-independent Schrödinger equation*

$$\boxed{H|E_n\rangle = E_n|E_n\rangle \ .} \tag{122}$$

As H is Hermitian we can obtain an orthonormal basis of energy eigenstates and hence write any state as linear combination

$$|\psi(t)\rangle = \sum_j \psi_j(t)|E_j\rangle \ . \tag{123}$$

Substituting this back into the TDSE we have

$$i\hbar\sum_j \frac{\partial\psi_j(t)}{\partial t}|E_j\rangle = \sum_j \psi_j(t)E_j|E_j\rangle. \tag{124}$$

Extracting the amplitudes for $|E_n\rangle$ by acting with $\langle E_n|$ we have

$$i\hbar\frac{\partial\psi_n(t)}{\partial t} = E_n\psi_n(t) \ . \tag{125}$$

This first order differential equation is easily solved

$$\psi_n(t) = \psi_n(0)e^{-\frac{i}{\hbar}E_n t} \ . \tag{126}$$

In Dirac notations

$$\boxed{|\psi(t)\rangle = \sum_n \langle E_n|\psi(0)\rangle \ e^{-\frac{i}{\hbar}E_n t} \ |E_n\rangle \ .} \tag{127}$$

NB 5

Given the solutions of the time-independent Schrödinger equation we can construct the solutions to the time-dependent Schrödinger equation for a given initial quantum state $|\psi(0)\rangle$ using (127). This is why the study of the TISE is so important!

For energy eigenstates themselves we have

$$\boxed{|E_n, t\rangle = e^{-\frac{i}{\hbar}E_n t}\ |E_n\rangle\ .} \tag{128}$$

So energy eigenstates only acquire a phase under time evolution. As a result the probabilities $|\langle x|E_n, t\rangle|^2$ to find a particle in an energy eigenstate at a given position x are time-independent. This is why energy eigenstates are also known as *stationary states*.

4.3 Schrödinger equation in the position representation

A key point is that we can express the TDSE in the position representation

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi(t)\rangle = \langle x|H|\psi(t)\rangle. \tag{129}$$

This is very useful for Hamiltonians of the form

$$H = \underbrace{\frac{\hat{p}^2}{2m}}_{\text{kinetic energy}} + \underbrace{V(\hat{x})}_{\text{potential energy}}\ . \tag{130}$$

Given that

$$\langle x|\hat{p}|\psi(t)\rangle = -i\hbar\frac{\partial\psi(x,t)}{\partial x} \tag{131}$$

we have

$$\langle x|\hat{p}^2|\psi(t)\rangle = \int dx'\ \langle x|\hat{p}|x'\rangle\langle x'|\hat{p}|\psi(t)\rangle = -\hbar^2\int dx'\ \frac{\partial}{\partial x}\delta(x-x')\frac{\partial\psi(x',t)}{\partial x'} = -\hbar^2\frac{\partial^2\psi(x,t)}{\partial x^2}\ . \tag{132}$$

This gives

$$\langle x|H|\psi(t)\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)\ . \tag{133}$$

Substituting this back into (129) we see that for Hamiltonians of the form (130) the TDSE can be represented as a *partial differential equation for the wave function*

$$\boxed{i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)\ .} \tag{134}$$

Now you are starting to see where Schrödinger's view that "all is waves" comes from! The generalization to 3D is straightforward and we only quote the result

$$\boxed{i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t)\ .} \tag{135}$$

In the position representation the TISE reads

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)\ .} \tag{136}$$

Here $\psi(x)$ are the wave functions of energy eigenstates. Many QM text approach the subject using the position representation on the Schrödinger equation as a starting point.

4.4 Probability Current

The probability density of finding a particle at position $\vec{x}$ at time t is according to Born's rule is

$$\rho(\vec{x},t) = |\psi(\vec{x},t)|^2 = \psi(\vec{x},t)\psi^*(\vec{x},t) \ . \tag{137}$$

Taking the time derivative gives

$$\frac{\partial\rho(\vec{x},t)}{\partial t} = \psi^*(x,t)\frac{\partial\psi(\vec{x},t)}{\partial t} + \psi(x,t)\frac{\partial\psi^*(\vec{x},t)}{\partial t} \ . \tag{138}$$

We now use the TDSE for the wave function (135) and its complex conjugate to rewrite the right-hand side

$$\frac{\partial\rho(\vec{x},t)}{\partial t} = \frac{i\hbar}{2m}\left[\psi^*(x,t)\nabla^2\psi(\vec{x},t) - \psi(x,t)\nabla^2\psi^*(\vec{x},t)\right] . \tag{139}$$

The right-hand side of this equation can be written as a divergence

$$\frac{\partial\rho(\vec{x},t)}{\partial t} = -\vec{\nabla}\cdot\vec{J}(\vec{x},t) \ , \tag{140}$$

where $\vec{J}(\vec{x},t)$ is called *probability current*

$$\vec{J}(\vec{x},t) = \frac{i\hbar}{2m}\left[\psi(x,t)\vec{\nabla}\psi^*(\vec{x},t) - \psi^*(x,t)\vec{\nabla}\psi(\vec{x},t)\right] . \tag{141}$$

Eqn (140) takes the form of a continuity equation that expresses the conservation of probability. Its integral form follows from the divergence theorem

$$\frac{d}{dt}\int_V d^3\vec{x}\ \rho(\vec{x},t) = -\int_V d^3\vec{x}\ \vec{\nabla}\cdot\vec{J}(\vec{x},t) = -\oint_{\partial V} d^2\vec{S}\cdot\vec{J}(\vec{x},t) \ , \tag{142}$$

where ∂V is the boundary of the volume V. So the change in the probability for the particle to be found inside V is minus the integral over the volume's bounding surface of the probability flux out of the volume.

Homework 4: Time dependence and the Schrödinger equation

2.1 Write down the time-independent (TISE) and the time-dependent (TDSE) Schrödinger equations. Is it necessary for the wavefunction of a system to satisfy the TDSE? Under what circumstances does the wavefunction of a system satisfy the TISE?

2.2 Why is the TDSE first-order in time, rather than second-order like Newton's equations of motion?

2.3 A particle is confined in a potential well such that its allowed energies are $E_n = n^2\mathcal{E}$, where $n = 1, 2, \ldots$ is an integer and $\mathcal{E}$ a positive constant. The corresponding energy eigenstates are $|1\rangle$, $|2\rangle$, $\ldots$, $|n\rangle, \ldots$ At $t = 0$ the particle is in the state

$$|\psi(0)\rangle = 0.2|1\rangle + 0.3|2\rangle + 0.4|3\rangle + 0.843|4\rangle.$$

(a) What is the probability, if the energy is measured at $t = 0$, of finding a number smaller than $6\mathcal{E}$?
(b) What is the mean value and what is the rms deviation of the energy of the particle in the state $|\psi(0)\rangle$?

(c) Calculate the state vector $|\psi\rangle$ at time t. Do the results found in (a) and (b) for time t remain valid for arbitrary time t?
(d) When the energy is measured it turns out to be $16\mathcal{E}$. After the measurement, what is the state of the system? What result is obtained if the energy is measured again?

2.4 A particle moves in the potential $V(\boldsymbol{x})$ and is known to have energy E_n. (a) Can it have well-defined momentum for some particular $V(\boldsymbol{x})$? (b) Can the particle simultaneously have well-defined energy and position?
2.5 Let $\psi(x,t)$ be the correctly normalized wave function of a particle of mass m and potential energy $V(x)$. Write down the expressions for the expectation values of (a) $\hat{x}$; (b) $\hat{x}^2$; (c) $\hat{p}_x$; (d) $\hat{p}_x^2$; (e) the energy.
What is the probability that the particle will be found in the interval (x_1, x_2)?

2.6 Consider a quantum mechanical particle with Hamiltonian

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

that is initially prepared in a state $|\psi(0)\rangle$. Using the TDSE show that the expectation value of an operator $\hat{Q}$ fulfils the following evolution equations

$$i\hbar \frac{d}{dt}\langle\psi(t)|\hat{Q}|\psi(t)\rangle = \langle\psi(t)|[\hat{Q}, H]|\psi(t)\rangle.$$

Consider the particular cases of the position and momentum operators and comment on the resulting equations

Part II
Wave Mechanics and Oscillators

Erwin with his psi can do
Calculations quite a few. Erich Hückel, freely translated by Felix Bloch.

5 Wave mechanics

5.1 Free particle in one dimension

Let us start with the case where our QM particle only has kinetic energy. Then the Hamiltonian is

$$H = \frac{\hat{p}^2}{2m} \ . \tag{143}$$

The TISE reads

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \ . \tag{144}$$

The solutions to this differential equation are the momentum eigenstates

$$u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}, \tag{145}$$

where the energy is given by

$$E_p = \frac{p^2}{2m}. \tag{146}$$

In this case the energy eigenvalues are *not* quantized. Given the energy eigenstates we are now is a position to solve the time-dependent Schrödinger equation. We need to adjust our previous result

$$|\psi(t)\rangle = \sum_n \langle E_n|\psi(0)\rangle e^{-\frac{i}{\hbar}E_n t}|E_n\rangle \tag{147}$$

because the energy eigenvalues are continuous rather than discrete here. Using that the energy eigenstates are also momentum eigenstates we have

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} dp\ \langle p|\psi(0)\rangle e^{-\frac{ip^2}{2m\hbar}t}|p\rangle. \tag{148}$$

The corresponding wave function is

$$\langle x|\psi(t)\rangle = \psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \langle p|\psi(0)\rangle e^{-\frac{ip^2}{2m\hbar}t+\frac{i}{\hbar}px}\ . \tag{149}$$

Let us consider a state that at time $t = 0$ corresponds to a Gaussian wave packet

$$\psi(x,0) = \langle x|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma^2}+\frac{i}{\hbar}p_0 x}\ . \tag{150}$$

Going over to the momentum representation we have

$$\langle p|\psi(0)\rangle = \int dx\ \langle p|x\rangle\langle x|\psi(0)\rangle = \left[\frac{2\sigma^2}{\pi\hbar^2}\right]^{\frac{1}{4}} e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}. \tag{151}$$

This describes a superposition of momentum eigenstates with momenta centred around p_0 and probability amplitudes that become very small when $|p - p_0| \gg \frac{\hbar}{\sigma}$. Substituting this back into (149) and carrying out the integral (how?) we obtain

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{2\pi\hbar^2|b(t)|^2}} e^{-\frac{\sigma^2}{2\hbar^2|b(t)|^2}(x-p_0 t/m)^2}\ , \qquad \hbar^2 b^2(t) = \sigma^2 + \frac{i\hbar t}{2m}\ . \tag{152}$$

This describes a Gaussian wave packet moving with velocity p_0/m that *broadens* in time as

$$\sigma^2(t) = \sigma^2 + \left(\frac{\hbar t}{2m\sigma}\right)^2\ . \tag{153}$$

We can understand this by noting that initially there is an uncertainty in momentum (as at time $t = 0$ we are dealing with a superposition of momentum eigenstates), which translates into an increasing uncertainty in position at later times.

5.2 Infinite square well

Let us consider a QM particle moving in a one-dimensional potential well

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{else.} \end{cases} \tag{154}$$

The TISE for the wave function $\psi(x)$ reads

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)\ . \tag{155}$$

As we are interested in finite E solutions the wave function must vanish at $x < 0$ and $x > a$. Continuity at $x = 0, a$ then imposes the boundary conditions

$$\psi(0) = 0 = \psi(a). \tag{156}$$

In the interior of the potential we then have

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \ . \tag{157}$$

The general solution is

$$\psi(x) = A\cos(kx) + B\sin(kx) \ , \quad E = \frac{\hbar^2 k^2}{2m}. \tag{158}$$

Imposing the boundary conditions gives $A = 0$ and the wave number k gets *quantized*

$$k_n = \frac{\pi n}{a} \ , \quad n = 1, 2, 3, \ldots \tag{159}$$

The corresponding quantized energies are

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}. \tag{160}$$

Normalizing the wave functions by imposing

$$\int_0^a dx|\psi(x)|^2 = 1 \ , \tag{161}$$

we arrive at the following result for the energy eigenstates

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x\right). \tag{162}$$

We note that the *overall phase* of the wave functions is arbitrary and we fix it to be equal to one. The lowest energy state is called the *ground state*. The wave functions $\psi_n(x)$ are either symmetric or antisymmetric

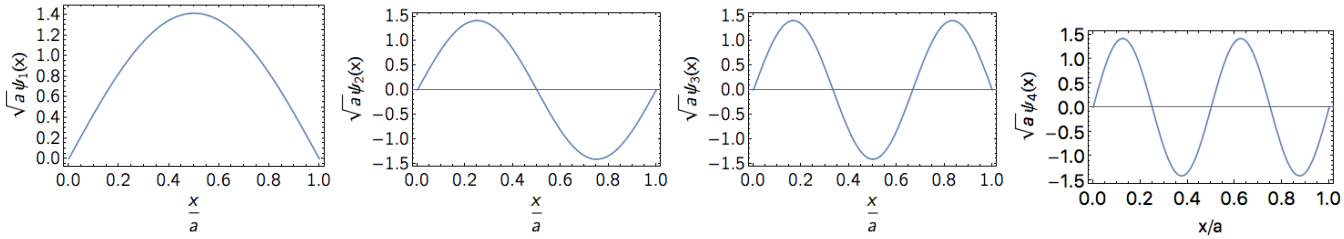


Figure 6: Wave functions for the 4 lowest energy states in the infinite square well potential.

under reflection around $x = a/2$.

5.3 Finite square well

Let us now consider a particle moving in the potential

$$V(x) = \begin{cases} 0 & \text{if } |x| < a \\ V_0 & \text{if } |x| > a. \end{cases} \tag{163}$$

The TISE for the wave function $\psi(x)$ reads

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = [E - V(x)]\psi(x) \ . \tag{164}$$

Let us first consider the case $E < V_0$. In this case the solution of (164) is

$$\psi(x) = \begin{cases} A\cos(kx) + B\sin(kx) & \text{if } |x| < a \ , \\ Ce^{-\kappa x} + C'e^{\kappa x} & \text{if } x > a \ , \\ De^{\kappa x} + D'e^{-\kappa x} & \text{if } x < -a \ , \end{cases} \tag{165}$$

where

$$E = \frac{\hbar^2 k^2}{2m} = V_0 - \frac{\hbar^2 \kappa^2}{2m}. \tag{166}$$

Now we impose

- Normalizability

$$\int_{-\infty}^{\infty} dx\ |\psi(x)|^2 = 1\ . \tag{167}$$

  This sets $C' = D' = 0$, i.e. imposes that the wave function vanishes at $x \to \pm\infty$.

- Continuity of $\psi(x)$ at $x = \pm a$, i.e. $\lim_{\epsilon\to 0} \psi(\pm a - \epsilon) = \lim_{\epsilon\to 0} \psi(\pm a + \epsilon)$

$$\begin{aligned} A\cos(ka) + B\sin(ka) &= Ce^{-\kappa a}\ , \\ A\cos(ka) - B\sin(ka) &= De^{-\kappa a}\ . \end{aligned} \tag{168}$$

- Continuity of $\psi'(x)$ at $x = \pm a$

$$\begin{aligned} Bk\cos(ka) - Ak\sin(ka) &= -C\kappa e^{-\kappa a}\ , \\ Bk\cos(ka) + Ak\sin(ka) &= D\kappa e^{-\kappa a}\ . \end{aligned} \tag{169}$$

Equations (168)and (169) have two types of solutions

(i) $B = 0$, $C = D$ and $k\tan(ka) = \kappa$, corresponding to *symmetric* wave functions $\psi(x) = \psi(-x)$.

(ii) $A = 0$, $C = -D$ and $k\cot(ka) = -\kappa$, corresponding to *antisymmetric* wave functions $\psi(x) = -\psi(-x)$.

The (anti)symmetry of energy eigenstates is a result of a *symmetry* of the problem under reflection around $x = 0$, i.e. $x \to -x$. This symmetry is called *parity*. Symmetric solutions are said to be *even* under the parity transformation (i.e. they map onto themselves), while antisymmetric solutions are *odd* under parity (i.e. they map onto minus themselves). What remains to be done is to solve the remaining equations for the wave numbers, e.g.

$$k\tan(ka) = \kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}. \tag{170}$$

We rewrite this slightly as

$$\tan(ka) = \sqrt{\frac{W^2}{k^2a^2} - 1}\ , \quad W = \sqrt{\frac{2mV_0a^2}{\hbar^2}}. \tag{171}$$

This equation does not have simple solutions, but we can understand the structure of solutions by plotting the two sides of the equation as functions of ka. This is done in Fig. 7. We see that for $W = 10$ there are 4 solutions to the equation. For larger values of W there will be more solutions, but there will always be at least one! We call these states *bound states*, because $|\psi(x)|^2$ drops off very quickly away from the square well, which means that the particle is most likely to be found inside the well. *So in one dimension a potential well will always have at least one bound state, no matter how small V_0 is.* Note however that the probability of finding the particle outside the well is not zero (as it would be classically for energies $E < V_0$)!

Let us now turn to the case $E > V_0$. Now the solutions to the TISE look like

$$\psi(x) = \begin{cases} A\cos(kx) + B\sin(kx) & \text{if } |x| < a\ , \\ C\cos(Kx) + C'\sin(Kx) & \text{if } x > a\ , \\ D\cos(Kx) + D'\sin(Kx) & \text{if } x < -a\ , \end{cases} \tag{172}$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 K^2}{2m} - V_0. \tag{173}$$

In this case the wave functions will not vanish at $x \to \pm\infty$ and the spectrum of energies will be continuous.

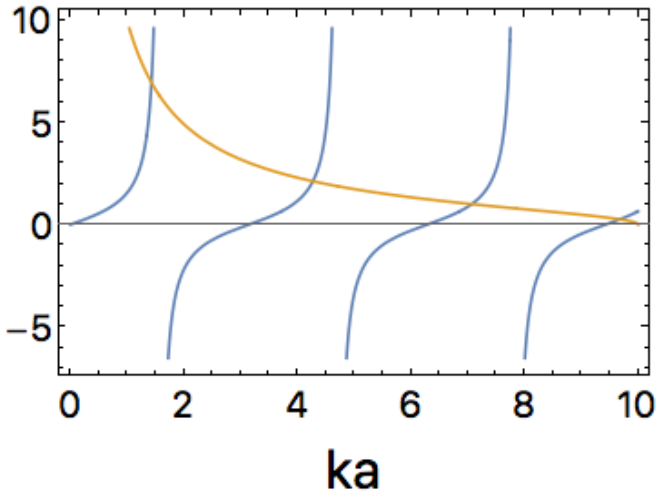


Figure 7: Solutions of eqn (171) for $W = 10$.

5.4 Split infinite square well

Next we consider a potential of the form

$$\begin{aligned} V(x) &= V_0\delta(x) + V_{\rm ISW}(x) \ , \\ V_{\rm ISW}(x) &= \begin{cases} 0 & \text{if } 0 < |x| < a/2 \\ \infty & \text{else.} \end{cases} \end{aligned} \tag{174}$$

The TISE reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \ . \tag{175}$$

If $V_0 = 0$ we are dealing with an infinite square well, which is now symmetric around $x = 0$. The odd-parity energy eigenstates can be read off from our previous solution

$$\psi_{2n}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi n}{a}x\right) \ , \qquad E_{2n} = \frac{\hbar^2\pi^2(2n)^2}{2ma^2} \ . \tag{176}$$

As $\psi_{2n}(0) = 0$ these wave functions also fulfil the TISE (175) in presence of the additional delta-function potential!

Using that $V(x)$ vanishes away from $x = 0$ we conclude that the even-parity eigenstates must have wave functions of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } 0 < x \le a/2 \ , \\ Ae^{-ikx} + Be^{ikx} & \text{if } -a/2 \le x < 0 \ . \end{cases} \tag{177}$$

The free parameters are fixed by noting that

- The wave functions must vanish at $\pm a/2$ for finite energy eigenstates, i.e. $\psi(\pm a/2) = 0$. This gives

$$B = -Ae^{ika} \ . \tag{178}$$

- The wave function must be continuous at $x = 0$. Our Ansatz fulfils this requirement.
- The derivative of the wave function at $x = 0$ is determined by integrating the TISE around $x = 0$

$$\int_{-\epsilon}^{\epsilon} dx \left[-\frac{\hbar^2\psi''(x)}{2m} + V_0\delta(x)\psi(x) - E\psi(x)\right] = 0 \ . \tag{179}$$

Using that the wave function is continuous at zero and taking the limit $\epsilon \to 0$ we obtain $\psi'(0^+) - \psi'(0^-) = \frac{2mV_0}{\hbar^2}\psi(0)$, which in turn implies

$$ik(A - B) = \frac{mV_0}{\hbar^2}(A + B) \ . \tag{180}$$

We see that the first derivative of the wave function is *discontinuous* at $x = 0$. This is a characteristic feature of delta-function potentials. If we regularize the delta function, e.g. by

$$\delta_\epsilon(x) = \frac{e^{-x^2/4\epsilon}}{\sqrt{4\pi\epsilon}}, \tag{181}$$

then the wave function and its derivative are continuous at $x = 0$. The discontinuity of the derivative arises only in the limit $\epsilon \to 0$. Substituting (178) leaves us with a quantization condition for k

$$k \cot(ka/2) = -\frac{mV_0}{\hbar^2} \ . \tag{182}$$

The most interesting case is when V_0 becomes very large. Then the right hand side of (182) is very large and k must be close to one of the singularities of $\cot(ka/2)$

$$k_{2n+1} \approx \frac{2n\pi}{a} - \frac{2n\pi}{a}\frac{2\hbar^2}{maV_0}. \tag{183}$$

For large V_0 our wave functions are thus approximately given by

$$\psi_{2n+1}(x) \approx \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi n}{a}|x|\right) \ , \qquad E_{2n+1} \approx \frac{\hbar^2\pi^2(2n)^2}{2ma^2} \ . \tag{184}$$

The corrections to the wave functions and energies are proportional to $1/V_0$. This implies that at large V_0 there are pairs of eigenstates with almost degenerate energies but opposite parities. Let us now prepare our system is the state corresponding to the wave function

$$\Psi(x, 0) = \frac{\psi_{2n}(x) - \psi_{2n+1}(x)}{\sqrt{2}}. \tag{185}$$

The probability density to find the particle at position x is

$$|\Psi(x, 0)|^2 \approx \begin{cases} \frac{4}{a}\sin^2\left(\frac{2\pi n}{a}x\right) & \text{if } -\frac{a}{2} \le x \le 0 \\ 0 & \text{else.} \end{cases} \tag{186}$$

So to a very good approximation the particle is on the left hand side of the potential well. The time evolution of the system is given by the time-dependent Schrödinger equation. Using our general result

$$|\psi(t)\rangle = \sum_n \langle E_n|\psi(0)\rangle e^{-\frac{i}{\hbar}E_n t}|E_n\rangle \ , \tag{187}$$

and going over to the position representation we have

$$\underbrace{\langle x|\psi(t)\rangle}_{\Psi(x,t)} = \sum_n \langle E_n|\psi(0)\rangle e^{-\frac{i}{\hbar}E_n t}\underbrace{\langle x|E_n\rangle}_{\psi_n(x)}. \tag{188}$$

For our particular choice of initial state this becomes

$$\Psi(x, t) = \frac{1}{\sqrt{2}}\left[e^{-\frac{i}{\hbar}E_{2n}t}\psi_{2n}(x) - e^{-\frac{i}{\hbar}E_{2n+1}t}\psi_{2n+1}(x)\right] \ . \tag{189}$$

Consider now the probability density to find the particle at position x at time $t^* = \pi\hbar/(E_{2n} - E_{2n+1})$. This is a late time as the splitting between the two energy levels is small. We have

$$|\Psi(x,t^*)|^2 = \frac{|\psi_{2n}(x) + \psi_{2n+1}(x)|^2}{2} \approx \begin{cases} \frac{4}{a}\sin^2\left(\frac{2\pi n}{a}x\right) & \text{if } 0 \le x \le \frac{a}{2} \\ 0 & \text{else.} \end{cases} \tag{190}$$

To a very good approximation the particle is now in the right hand side of the well! This is a purely quantum mechanical effect, which we refer to as *tunnelling* through a potential barrier.

5.5 Scattering of free particles

Next we consider a potential step

$$V(x) = \begin{cases} 0 & \text{if } |x| > a \\ V_0 & \text{if } |x| < a. \end{cases} \tag{191}$$

The corresponding TISE

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + [V(x) - E]\psi(x) = 0 \tag{192}$$

is solved by considering the regions $x < -a$, $|x| < a$ and $x > a$ separately. For $E < V_0$ energy eigenstates are of the form

$$\psi(x) = \begin{cases} De^{ikx} + re^{-ikx} & \text{if } x < -a \\ Ae^{-\kappa x} + Be^{\kappa x} & \text{if } |x| < a \\ te^{ikx} + Ce^{-ikx} & \text{if } x > a\ , \end{cases} \tag{193}$$

where k and κ are related to the energy eigenvalue by

$$E = \frac{\hbar^2 k^2}{2m} = V_0 - \frac{\hbar^2\kappa^2}{2m}. \tag{194}$$

We see that the wave functions do not vanish at $\pm\infty$ and are not normalizable to one. We now specify solutions such that $C = 0$ and $D = 1$ as these have a nice physical interpretation. For $C = 0$ there is no left-moving wave at $x > a$[1], and the wave functions can be interpreted as an incident plane wave with amplitude 1 that gets partially reflected by the barrier (re^{-ikx}) and partially transmitted (te^{ikx}).

The free parameters in (193) are fixed by the four requirements that the wave function and its first derivative are continuous at $x = \pm a$. This gives the following four equations for the four unknowns A, B, r, and t

$$\begin{aligned} e^{-ika} + re^{ika} &= Ae^{\kappa a} + Be^{-\kappa a}\ , \\ te^{ika} &= Ae^{-\kappa a} + Be^{\kappa a}\ , \\ ik[e^{-ika} - re^{ika}] &= \kappa[-Ae^{\kappa a} + Be^{-\kappa a}]\ , \\ ikte^{ika} &= \kappa[-Ae^{-\kappa a} + Be^{\kappa a}]. \end{aligned} \tag{195}$$

After some algebra we find

$$\begin{aligned} t &= \frac{2i\kappa k e^{-2ika}}{(k^2-\kappa^2)\sinh(2\kappa a) + 2ik\kappa\cosh(2\kappa a)}\ , \\ r &= \frac{e^{-2ika}(\kappa^2+k^2)\sinh(2\kappa a)}{(k^2-\kappa^2)\sinh(2\kappa a) + 2ik\kappa\cosh(2\kappa a)}. \end{aligned} \tag{196}$$

We note that

$$|r|^2 + |t|^2 = 1, \tag{197}$$

[1] e^{ikx} corresponds to a right-moving wave as can be seen by including the time dependence imposed by the TDSE: $e^{ikx - i\frac{\hbar k^2}{2m}t}$. The points of constant phase can be seen to move rightwards.

which corresponds to the conservation of probability in the scattering interpretation mentioned above. A simple way of seeing that $|r|^2 + |t|^2 = 1$ is to consider the probability currents for $x < -a$ and $x > a$. We have

$$J_{x<-a} = \frac{\hbar k}{m}[1 - |r|^2] \ , \qquad J_{x>a} = \frac{\hbar k}{m}|t|^2 \ . \tag{198}$$

These must be equal by conservation of probability (consider the integral form (142) of the continuity equation and take as the volume e.g. the interval $[-2a, 2a]$). The transmission probability is

$$|t|^2 = \frac{4k^2\kappa^2}{4\kappa^2k^2 + (k^2+\kappa^2)^2\sinh^2(2\kappa a)} \ . \tag{199}$$

Transmission includes the possibility that the incoming particle failed to interact with the potential barrier. To isolate the possibility of scattering to occur we write the amplitude of the outgoing wave as $t = 1 + T$, where the 1 corresponds to the possibility of passing through undisturbed and T representing actual forward scattering. The total *scattering cross section* is defined as the sum of the probabilities for forwards and backwards scattering

$$\sigma = |T|^2 + |r|^2 = |1 - t|^2 + |r|^2. \tag{200}$$

This is a good point to elaborate a bit more on continuity conditions for the derivative of the wave function. In our example the first derivative is continuous. Let us now however consider the limit $a \to 0$, $V_0 \to \infty$ such that $2aV_0 = V_\delta$ is kept fixed. Let us denote this limit as $\lim_\delta$. In this limit our potential is like a delta-function and hence no longer "nice" at $x = 0$. The derivative of the wave functions behaves as

$$\begin{aligned} \psi'(0^-) &= ik \lim_\delta (1 - r) = \frac{mV_\delta/\hbar^2}{ik - mV_\delta/\hbar^2} \ , \\ \psi'(0^+) &= ik \lim_\delta t = \frac{ik}{ik - mV_\delta/\hbar^2} \ . \end{aligned} \tag{201}$$

So in the limit the first derivative is no longer continuous. Its jump at $x = 0$ is

$$\psi'(0^+) - \psi'(0^-) = \frac{ik(2mV_\delta/\hbar^2)}{ik - mV_\delta/\hbar^2} = \frac{2mV_\delta}{\hbar^2}\psi(0). \tag{202}$$

5.6 Resonant Scattering

Scattering experiments are widely used to probe the internal structure of atomic nuclei and "elementary" particles. We will now consider a toy model that explains how the structure of the scattering cross section reflects the existence of long-lived bound states inside the nucleus. To that end we consider particles moving in a one dimensional potential of the form

$$V(x) = V_\delta \left[\delta(x + a) + \delta(x - a)\right] . \tag{203}$$

We aim to construct finite energy eigenstates of the form

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{if } x < -a \\ Ae^{ikx} + Be^{-ikx} & \text{if } |x| < a \\ te^{ikx} & \text{if } x > a. \end{cases} \tag{204}$$

The energy of such a solution is

$$E(k) = \frac{\hbar^2k^2}{2m}. \tag{205}$$

Such solutions can be interpreted in terms of a right-moving wave with unit amplitude that scatters off the potential and eventually generates a reflected left-moving wave at $x < -a$ and a transmitted right-moving wave at $x > a$. The wave functions (204) must fulfil the following conditions

- Continuity of the wave function at $x = \pm a$. This gives

$$\begin{aligned} e^{-ika} + re^{ika} &= Ae^{-ika} + Be^{ika} \ , \\ te^{ika} &= Ae^{ika} + Be^{-ika} \ . \end{aligned} \tag{206}$$

  These can be cast in matrix form

$$\underbrace{\begin{pmatrix} e^{-ika} & e^{ika} \\ e^{ika} & e^{-ika} \end{pmatrix}}_{M_1} \begin{pmatrix} A \\ B \end{pmatrix} = e^{ika} \begin{pmatrix} r \\ t \end{pmatrix} + e^{-ika} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{207}$$

- Jump discontinuity of the first derivatives at the positions of the delta-functions. These conditions are again obtained by integrating the TISE over infinitesimal intervals around $\pm a$, e.g.

$$\int_{a-\epsilon}^{a+\epsilon} dx \left[-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_\delta \delta(x-a)\psi(x) - E\psi(x) \right] = 0 \ . \tag{208}$$

  This gives two equations

$$\begin{aligned} \psi'(a+0) - \psi'(a-0) &= \frac{2m}{\hbar^2} V_\delta \psi(a) \ , \\ \psi'(-a+0) - \psi'(-a-0) &= \frac{2m}{\hbar^2} V_\delta \psi(-a) \ . \end{aligned} \tag{209}$$

  These two equations can be written in matrix form as

$$\underbrace{\begin{pmatrix} (v_0 - ik)e^{-ika} & (v_0 + ik)e^{ika} \\ (v_0 + ik)e^{ika} & (v_0 - ik)e^{ika} \end{pmatrix}}_{M_2} \begin{pmatrix} A \\ B \end{pmatrix} = ike^{ika} \begin{pmatrix} r \\ t \end{pmatrix} - ike^{-ika} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \tag{210}$$

  where we have defined

$$v_0 = \frac{2mV_\delta}{\hbar^2}. \tag{211}$$

Eliminating A and B we can extract a system of equations for only r and t

$$\left[M_2 M_1^{-1} - ik \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \begin{pmatrix} r \\ t \end{pmatrix} = e^{-2ika} \begin{pmatrix} k \csc(2ka) \\ -ik - v_0 - k \cot(2ka) \end{pmatrix}. \tag{212}$$

The solution of this system is

$$\begin{aligned} t &= \frac{4k^2}{(2k + iv_0)^2 + e^{4ika} v_0^2} \ , \\ r &= \frac{v_0[e^{-2ika}(v_0 - 2ik) - e^{2ika}(v_0 + 2ik)]}{(2k + iv_0)^2 + e^{4ika} v_0^2} \ . \end{aligned} \tag{213}$$

The total scattering cross section is defined as

$$\sigma = |t-1|^2 + |r|^2 = 2 + \frac{4k^2 \left(-4k^2 - v_0^2 \cos(4ka) + v_0^2 \right)}{8k^4 + 4k^2 v_0^2 - v_0^2 \left(v_0^2 - 4k^2 \right) \cos(4ka) + 4kv_0^3 \sin(4ka) + v_0^4} \ . \tag{214}$$

We see that at certain values of k (and hence at particular energies) the cross section is strongly enhanced. To understand the origin of this phenomenon it is useful to consider the limit of an impenetrable delta-function potential $V_\delta \to \infty$. In this case we have $v_0 a \gg 1$ and the "resonances" occur at

$$k_n a \approx \frac{\pi n}{2} \ , \quad n = 1, 2, 3 \ldots \tag{215}$$

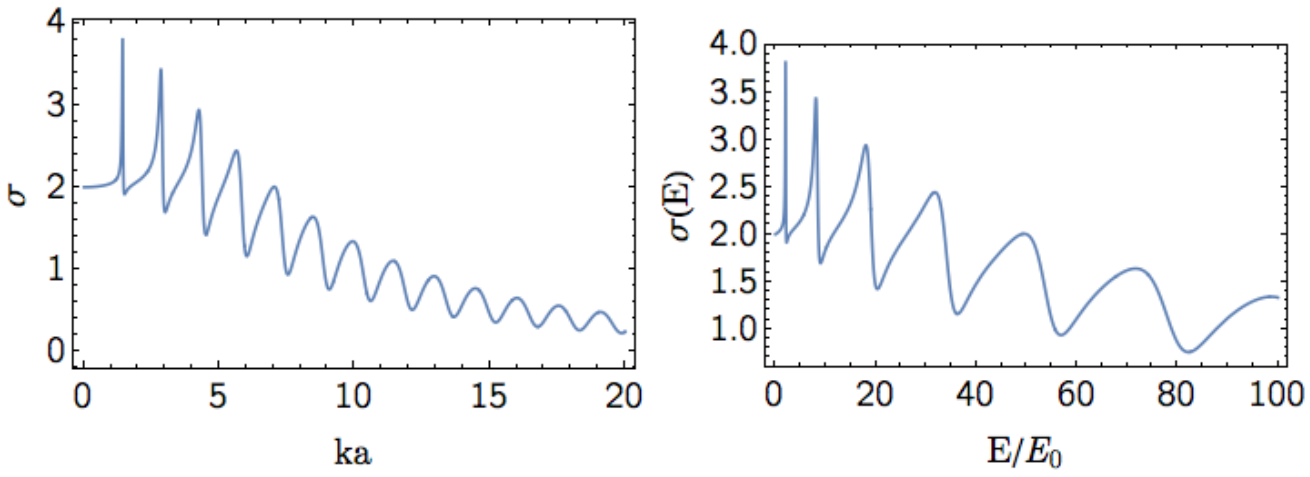


Figure 8: Left: Total scattering cross section σ as a function of ka for $v_0 a = 10$. Right: Total scattering cross section σ as a function of energy E for $v_0 a = 10$ ($E_0 = \hbar^2/(2ma^2)$).

These correspond to energies

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{8ma^2}. \tag{216}$$

For very large values of V_δ we basically have a infinite square well (as the wave functions must vanish at $\pm a$). We already know that in the latter stationary states occur at energies, *cf.* (160)

$$E_n^{\mathrm{ISW}} = \frac{\hbar^2 (\pi n)^2}{2m(2a)^2} = \frac{\hbar^2 (\pi n)^2}{8ma^2} \ , \tag{217}$$

where we have taken into account that the width of the well is $2a$. These are exactly the energies at which the total cross section has spikes! The interpretation is now clear: for special energies the cross section is large because the particle can get temporarily trapped between the barriers, until after some time it escapes to the left or the right. We say that there is a long-lived bound state between the barriers at that energy. So the structure of the total cross section tells us about the energy levels of such long-lived bound states. Long-lived bound states are related to certain types of radioactive decay.

In the case where the peaks in the cross section are very narrow, it follows from our explicit expression for σ that they are approximately of the form

$$\sigma(E \approx E_R) \approx \text{const} + \frac{2(\Gamma/2)^2}{(\Gamma/2)^2 + (E - E_R)^2} \ , \tag{218}$$

where E_R is the energy at which the peak is centred. The form (218) is called *Breit-Wigner* cross section and is used widely to fit experimental data. It can be shown that the parameter Γ is inversely related to the time it takes for the particle to escape from inside the well.



Eugene Wigner (Nobel Prize in Physics 1963).
"Where in the Schrödinger equation do you put the joy of being alive?"

Wigner is also known for not being given tenure at Princeton University in the 1930ies.

Homework 5: Wave Mechanics

2.7 Particles move in the potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases}.$$

Particles of mass m and energy $E > V_0$ are incident from $x = -\infty$. Show that the probability that a particle is reflected is

$$\left(\frac{k-K}{k+K}\right)^2,$$

where $k \equiv \sqrt{2mE}/\hbar$ and $K \equiv \sqrt{2m(E-V_0)}/\hbar$. Show directly from the time-independent Schrödinger equation that the probability of transmission is

$$\frac{4kK}{(k+K)^2}$$

and check that the flux of particles moving away from the origin is equal to the incident particle flux.

2.8 Show that the energies of bound, odd-parity stationary states of the square potential well

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 > 0 & \text{otherwise} \end{cases},$$

are governed by

$$\cot(ka) = -\sqrt{\frac{W^2}{(ka)^2} - 1} \quad \text{where} \quad W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad \text{and} \quad k^2 = 2mE/\hbar^2.$$

Show that for a bound odd-parity state to exist, we require $W > \pi/2$.

2.9 A free particle of energy E approaches a square, one-dimensional potential well of depth V_0 and width $2a$. Show that the probability of being reflected by the well vanishes when $Ka = n\pi/2$, where n is an integer and $K = (2m(E+V_0)/\hbar^2)^{1/2}$. Explain this phenomenon in physical terms.

2.10 A particle of energy E approaches from $x < 0$ a barrier in which the potential energy is $V(x) = V_\delta \delta(x)$. Show that the probability of its passing the barrier is

$$P_{\text{tun}} = \frac{1}{1 + (K/2k)^2} \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad K = \frac{2mV_\delta}{\hbar^2}.$$

2.11 Given that the wavefunction is $\psi = A\mathrm{e}^{\mathrm{i}(kz-\omega t)} + B\mathrm{e}^{-\mathrm{i}(kz+\omega t)}$, where A and B are constants, show that the probability current density is

$$\boldsymbol{J} = v\big(|A|^2 - |B|^2\big)\,\hat{\boldsymbol{z}},$$

where $v = \hbar k/m$. Interpret the result physically.

2.12 Consider a free particle in one dimension with Hamiltonian

$$H = \frac{\hat{p}^2}{2m}. \tag{219}$$

Let the wave function of the particle at time $t = 0$ be a Gaussian wave packet

$$\psi(x,0) = \langle x|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma^2} + \frac{i}{\hbar}p_0 x}\ . \tag{220}$$

Show that in the momentum representation we have

$$\langle p|\psi(0)\rangle = \int dx\ \langle p|x\rangle\langle x|\psi(0)\rangle = \left[\frac{2\sigma^2}{\pi\hbar^2}\right]^{\frac{1}{4}} e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}. \tag{221}$$

Comment on the relation between the forms of the state in the position and momentum representations as a function of σ. By solving the TDSE show that the probability distribution function at time t can be written in the form

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{2\pi\hbar^2|b(t)|^2}} e^{-\frac{\sigma^2}{2\hbar^2|b(t)|^2}(x-p_0 t/m)^2}\ , \tag{222}$$

and derive the form of the function $b(t)$. Explain what happens physically to the particle as time evolves.

6 Harmonic Oscillators

The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction. Sidney Coleman.

Harmonic oscillations are ubiquitous in Physics as they describe small excursions from points of equilibrium. QM harmonic oscillators are extremely important as they are the basic building blocks of relativistic Quantum Field Theories and the quantum theory of many-particle systems that describe solids.

The Hamiltonian for a one dimensional harmonic oscillator is

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{223}$$

The corresponding TISE in the position representation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{m\omega^2}{2}x^2\psi(x) = E\psi(x). \tag{224}$$

One way of approaching the QM harmonic oscillator is to solve this differential equation by the Frobenius method. Here we will follow a different approach and employ operator methods. We start by introducing

so called creation and annihilation operators by

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} \ , \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} \ . \end{aligned} \tag{225}$$

Here $a^\dagger$ is the Hermitian conjugate operator to a. Creation/annihilation operators fulfil the following commutation relations

$$\boxed{[a, a^\dagger] = -\frac{i}{2\hbar}[\hat{x}, \hat{p}] + \frac{i}{2\hbar}[\hat{p}, \hat{x}] = 1.} \tag{226}$$

The utility of these operators is that the Hamiltonian can be expressed in a simple way in terms of them. We have

$$a^\dagger a = \frac{m\omega}{2\hbar}\hat{x}^2 + \frac{1}{2m\hbar\omega}\hat{p}^2 - \frac{i}{2\hbar}[\hat{p}, \hat{x}] \ , \tag{227}$$

which tells us that

$$\boxed{H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).} \tag{228}$$

Here

$$\boxed{\hat{N} = a^\dagger a} \tag{229}$$

is referred to as the *number operator*. In order to proceed we will require the commutation relations of the creation/annihilation operators with the Hamiltonian (or equivalently the number operator)

$$[a, \hat{N}] = a \ , \qquad [a^\dagger, \hat{N}] = -a^\dagger. \tag{230}$$

These are established as follows

$$[a, \hat{N}] = aa^\dagger a - a^\dagger aa = [a, a^\dagger]a = a \ . \tag{231}$$

Now assume that we know an eigenstate $|E\rangle$ of H

$$H|E\rangle = E|E\rangle. \tag{232}$$

We will now show that both $a^\dagger|E\rangle$ and $a|E\rangle$ are eigenstates of H as well. Consider

$$Ha^\dagger|E\rangle = \left([H, a^\dagger] + a^\dagger H\right)|E\rangle = \left(\hbar\omega a^\dagger + a^\dagger E\right)|E\rangle = (E + \hbar\omega)\, a^\dagger|E\rangle. \tag{233}$$

That's a bingo: $a^\dagger|E\rangle$ is an eigenstate with energy $E + \hbar\omega$. Similarly we have

$$Ha|E\rangle = \left([H, a] + aH\right)|E\rangle = \left(-\hbar\omega a + aE\right)|E\rangle = (E - \hbar\omega)\, a|E\rangle. \tag{234}$$

So $a|E\rangle$ is an eigenstate with energy $E - \hbar\omega$. Finally we consider the "length" $\langle E|a^\dagger a|E\rangle$ of the ket vector $a|E\rangle$

$$0 \leq \langle E|a^\dagger a|E\rangle = \langle E|\frac{H}{\hbar\omega} - \frac{1}{2}|E\rangle = \frac{E}{\hbar\omega} - \frac{1}{2}. \tag{235}$$

This tells us that the energy eigenvalues are bounded from below

$$E \geq \frac{\hbar\omega}{2}. \tag{236}$$

This means that there is an eigenstate with lowest energy E_0, which we denote by $|0\rangle$. Using (234) we have

$$Ha|0\rangle = (E_0 - \hbar\omega)a|0\rangle, \tag{237}$$

so either $a|0\rangle$ is an eigenstate with energy $E_0 - \hbar\omega$ or $a|0\rangle = 0$. The former is impossible because E_0 is by construction to lowest energy eigenvalue, so we must have

$$a|0\rangle = 0. \tag{238}$$

This is turn tell us that the ground state energy is

$$H|0\rangle = \frac{\hbar\omega}{2}|0\rangle \Rightarrow E_0 = \frac{\hbar\omega}{2}. \tag{239}$$

This is the first interesting result: the ground state energy of the QM harmonic oscillator is not zero, but $E_0 = \frac{\hbar\omega}{2}$. This is called the *zero-point energy*. Using (233) repeatedly we can construct eigenstates of the form

$$|n\rangle = \frac{1}{N_n}(a^\dagger)^n|0\rangle \ , \tag{240}$$

where N_n is a normalization constant. The energy of the states (240) is $E_n = E_0 + n\hbar\omega$ as each $a^\dagger$ adds an energy $\hbar\omega$ by virtue of (233), i.e.

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right).} \tag{241}$$

We now observe that

$$\begin{aligned} [a, (a^\dagger)^n] &= a(a^\dagger)^n - (a^\dagger)^n a = [a, a^\dagger](a^\dagger)^{n-1} + a^\dagger[a, a^\dagger](a^\dagger)^{n-2} + (a^\dagger)^2[a, a^\dagger](a^\dagger)^{n-3} + \dots \\ &= n(a^\dagger)^{n-1}, \end{aligned} \tag{242}$$

which implies that

$$a|n\rangle = \alpha_n|n-1\rangle \ . \tag{243}$$

The constant α_n is most easily calculated by considering

$$\begin{aligned} \langle n|a^\dagger a|n\rangle &= |\alpha_n|^2 \\ &= \langle n|\hat{N}|n\rangle = n. \end{aligned} \tag{244}$$

Using that we can choose our normalization constants to be real we thus have

$$\boxed{a|n\rangle = \sqrt{n}|n-1\rangle.} \tag{245}$$

The analogous relation for the creation operator is

$$\boxed{a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.} \tag{246}$$

It is established by noting that

$$a^\dagger|n\rangle = \beta_n|n+1\rangle \tag{247}$$

and then calculating

$$\langle n|aa^\dagger|n\rangle = |\beta_n|^2 = \langle n|\hat{N} + [a, a^\dagger]|n\rangle = n = 1. \tag{248}$$

Using (246) repeatedly we have

$$(a^\dagger)^n|0\rangle = \sqrt{n!}|n\rangle \ , \tag{249}$$

which gives the normalization constant

$$\boxed{N_n = \sqrt{n!}.} \tag{250}$$

Nice.

6.1 Ground state of the Quantum Harmonic Oscillator

We now turn to a more detailed analysis of the ground state and its properties. Our starting point is the fact the $|0\rangle$ is annihilated by a

$$a|0\rangle = 0 = \left[\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right]|0\rangle. \tag{251}$$

In the position representation this becomes

$$\begin{aligned}
0 &= \langle x|a|0\rangle = \langle x|\left[\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right]|0\rangle \\
&= \int dx'\ \langle x|\left[\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right]|x'\rangle\langle x'|0\rangle \\
&= \sqrt{\frac{m\omega}{2\hbar}}\int dx'\ \underbrace{\langle x|\hat{x}|x'\rangle}_{x\delta(x-x')}\langle x'|0\rangle + \frac{i}{\sqrt{2m\omega\hbar}}\int dx'\ \underbrace{\langle x|\hat{p}|x'\rangle}_{-i\hbar\frac{d}{dx}\delta(x-x')}\langle x'|0\rangle \\
&= \left[\sqrt{\frac{m\omega}{2\hbar}}x + \frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{d}{dx}\right]\underbrace{\langle x|0\rangle}_{\psi_0(x)}\ .
\end{aligned} \tag{252}$$

This is a first order differential equation for the ground state wave function $\psi_0(x)$. Its normalized solution is

$$\boxed{\psi_0(x) = \frac{1}{(2\pi\ell^2)^{\frac{1}{4}}}e^{-\frac{x^2}{4\ell^2}}\ , \qquad \ell = \sqrt{\frac{\hbar}{2m\omega}}.} \tag{253}$$

We see that the ground state wave function is a Gaussian centred around zero. Its energy $E_0 = \frac{\hbar\omega}{2}$ is larger than zero, in contrast to the lowest energy configuration of a classical harmonic oscillator. The existence of a zero-point energy is a direct consequence of the Heisenberg uncertainty relation. In order to have zero energy our quantum mechanical particle would need to have neither potential energy, i.e. be localized at $x = 0$, nor kinetic energy, i.e. have zero momentum. These two requirements cannot be met simultaneously because of the uncertainty relation.

We now turn to the calculation of ground state expectation values. We have

$$\begin{aligned}
\langle 0|\hat{x}|0\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle 0|a + a^\dagger|0\rangle = 0\ , \\
\langle 0|\hat{p}|0\rangle &= -i\sqrt{\frac{m\hbar\omega}{2}}\langle 0|a - a^\dagger|0\rangle = 0\ ,
\end{aligned} \tag{254}$$

where we have used that $a|0\rangle = 0 = \langle 0|a^\dagger$. This means that on average the particle in the ground state of our harmonic oscillator is located at $x = 0$ and has zero momentum. The variances are

$$\begin{aligned}
\langle 0|\hat{x}^2|0\rangle &= \frac{\hbar}{2m\omega}\langle 0|(a + a^\dagger)^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa^\dagger|0\rangle = \frac{\hbar}{2m\omega}\langle 0|[a, a^\dagger]|0\rangle = \frac{\hbar}{2m\omega}\ , \\
\langle 0|\hat{p}^2|0\rangle &= -\frac{m\hbar\omega}{2}\langle 0|(a - a^\dagger)^2|0\rangle = \frac{m\hbar\omega}{2}\langle 0|aa^\dagger|0\rangle = \frac{m\hbar\omega}{2}.
\end{aligned} \tag{255}$$

Putting everything together we have

$$\boxed{\Delta x\Delta p = \frac{\hbar}{2}.} \tag{256}$$

This means that the ground state of the harmonic oscillator saturates the Heisenberg uncertainty relation, i.e. it is a state of *minimal uncertainty*.

6.2 Excited states of the Quantum Harmonic Oscillator

We now turn to the wave functions for excited states. For the first excited state we have

$$\begin{aligned}\psi_1(x) = \langle x|1\rangle = \langle x|a^\dagger|0\rangle &= \langle x|\left[\sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right]|0\rangle \\ &= \left[\frac{x}{2\ell} - \ell\frac{d}{dx}\right]\langle x|0\rangle \\ &= \frac{1}{(2\pi\ell^2)^{\frac{1}{4}}}\frac{x}{\ell}e^{-\frac{x^2}{4\ell^2}} \ . \end{aligned} \tag{257}$$

For the higher excited states we have the following *recurrence relation*

$$\begin{aligned}\psi_n(x) = \langle x|n\rangle &= \frac{1}{\sqrt{n}}\langle x|a^\dagger|n-1\rangle \\ &= \frac{1}{\sqrt{n}}\left[\frac{x}{2\ell} - \ell\frac{d}{dx}\right]\underbrace{\langle x|n-1\rangle}_{\psi_{n-1}(x)}. \end{aligned} \tag{258}$$

Using this repeatedly we have

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left[\frac{x}{2\ell} - \ell\frac{d}{dx}\right]^n\psi_0(x) \equiv \frac{1}{\sqrt{n!}}f_n(x)\psi_0(x) \ , \tag{259}$$

where $f_n(x)$ is some polynomial in x. Substituting (259) into (258) we obtain a recurrence relation for $f_n(x)$

$$f_n(x) = \frac{x}{\ell}f_{n-1}(x) - \ell f'_{n-1}(x) \ , \quad f_0(x) = 1 \ . \tag{260}$$

Comparing this with the recurrence relation of the so-called *Hermite polynomials* $H_n(z)$

$$H_n(z) = 2zH_{n-1}(z) - H'_{n-1}(z) \ , \quad H_0(z) = 1 \ , \tag{261}$$

we conclude that

$$f_n(x) = \frac{1}{2^{n/2}}H_n\left(\frac{x}{\sqrt{2}\ell}\right). \tag{262}$$

This gives our final result

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{n!2^n}}\ H_n\left(\frac{x}{\sqrt{2}\ell}\right)\ \psi_0(x).} \tag{263}$$

The first few Hermite polynomials are

$$H_0(z) = 1 \ , \quad H_1(z) = 2z \ , \quad H_2(z) = 4z^2 - 2 \ , \quad H_3(z) = 8z^3 - 12z. \tag{264}$$

From the properties of the Hermite polynomials it follows that

- $\psi_{2n}(x)$ are even under parity $x \to -x$, i.e. $\psi_{2n}(-x) = \psi_{2n}(x)$.
- $\psi_{2n+1}(x)$ are odd under parity $x \to -x$, i.e. $\psi_{2n+1}(-x) = -\psi_{2n+1}(x)$.
- $\psi_n(x)$ has n-1 nodes.

Expectation values in excited states of the harmonic oscillator can be calculated from the following

$$\begin{aligned}\langle n|a|n\rangle &= 0 \ , \qquad \langle n|a^\dagger|n\rangle = 0 \ , \\ \langle n|a^\dagger a|n\rangle &= n \ , \qquad \langle n|aa^\dagger|n\rangle = n+1 \ , \qquad \langle n|(a^\dagger)^2|n\rangle = 0 = \langle n|a^2|n\rangle. \end{aligned} \tag{265}$$

Using these we can easily show that

$$\begin{aligned}\langle n|\hat{x}|n\rangle &= 0 = \langle n|\hat{p}|n\rangle \ , \\ \langle n|\hat{x}^2|n\rangle &= \frac{\hbar}{m\omega}\big(n+\frac{1}{2}\big) \ , \quad \langle n|\hat{p}^2|n\rangle = \hbar m\omega\big(n+\frac{1}{2}\big)\end{aligned} \tag{266}$$

The product of uncertainties is thus

$$\Delta x \ \Delta p = \hbar\big(n+\frac{1}{2}\big) \ . \tag{267}$$

This tells us that only the ground state is a state of minimal uncertainty, and the uncertainties are larger in highly excited states.

6.3 What oscillates in the quantum harmonic oscillator?

Let us now consider a harmonic oscillator initially prepared in a state $|\psi(0)\rangle$

$$|\psi(0)\rangle = \sum_{n=0}^{\infty} \underbrace{\langle n|\psi(0)\rangle}_{a_n} \ |n\rangle \ . \tag{268}$$

The TDSE tells us that at time t the state of the system will be

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} a_n \ e^{-i\omega t(n+\frac{1}{2})} \ |n\rangle \ . \tag{269}$$

The average position of our particle as a function of time is then given by the expectation value

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \sum_{n,m=0}^{\infty} a_m^* a_n e^{i\omega t(m-n)} \langle m|\hat{x}|n\rangle \ . \tag{270}$$

Matrix elements of the position operator are readily worked out using (245), (246) and $\hat{x} = \ell[a + a^\dagger]$

$$\langle m|\hat{x}|n\rangle = \ell\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right] . \tag{271}$$

Substituting (271) into (270) we have

$$\begin{aligned}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \ell\sum_{n=1}^{\infty}\sqrt{n}\left[a_n a_{n-1}^* e^{-i\omega t} + a_{n-1}a_n^* e^{i\omega t}\right] \\ &= \sum_{n=1}^{\infty} b_n \cos(\omega t + a_n) \ ,\end{aligned} \tag{272}$$

where $2\sqrt{n}\ell a_n^* a_{n-1} = b_n \exp(i\phi_n)$. Eqn (272) proves that if we prepare the harmonic oscillator in a generic initial state $|\psi(0)\rangle$ the expectation value of position oscillates with frequency ω. This is reassuring.

6.4 Quantum vs classical harmonic oscillator

The solution of the equations of motion for the classical harmonic oscillator is

$$x(t) = x_0 \sin(\omega t) \ , \quad E = \frac{m\omega^2}{2}x_0^2 \ . \tag{273}$$

Defining the probability density of finding the classical harmonic oscillator at position x by

$$P_{\rm cl}(x)dx = 2\frac{dt}{T} \ , \quad T = \frac{2\pi}{\omega} \ , \tag{274}$$

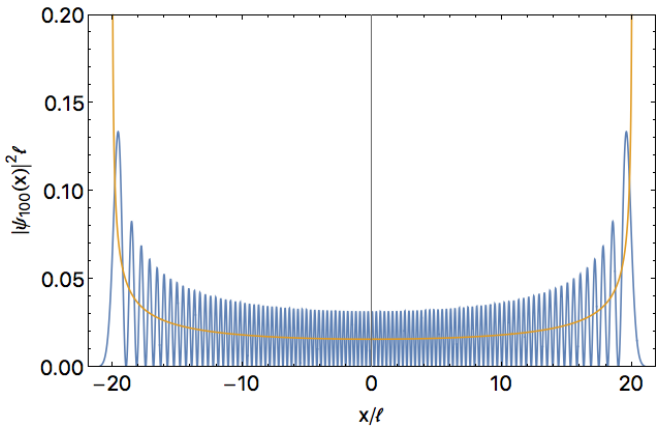


Figure 9: Probability distribution in a stationary state of the harmonic oscillator with $n = 100$.

we have

$$P_{\rm cl}(x) = \frac{1}{\pi\sqrt{x_0^2 - x^2}} = \frac{1}{2\pi\ell\sqrt{\frac{E}{\hbar\omega} - \frac{x^2}{4\ell^2}}} \tag{275}$$

In Fig. 9 we compare $P_{\rm cl}(x)$ to the probability distribution of a quantum harmonic oscillator at the same energy $E_{100} = 100.5\hbar\omega$. We observe that the quantum mechanical probability is a strongly oscillatory function with oscillations occurring on a length scale $\sim \ell/\sqrt{n}$. Averaging the quantum mechanical probability distribution over a very small range approaches the classical probability distribution in the large-n limit.

Aside 4: Coherent States

There are other states in the harmonic oscillator problem that are of great interest. Consider the eigenvalue equation for the annihilation operator

$$a|\alpha\rangle = \alpha|\alpha\rangle. \tag{276}$$

These are called *coherent states* for reasons that will become clear shortly. Recalling that

$$a = \frac{\hat{x}}{2\ell} + \frac{i\ell}{\hbar}\hat{p}\ , \tag{277}$$

we can turn (276) into a differential equation by going to the position representation

$$\begin{aligned} \langle x|a|\alpha\rangle &= \alpha\langle x|\alpha\rangle \\ &= \frac{x}{2\ell}\langle x|\alpha\rangle + \ell\frac{d}{dx}\langle x|\alpha\rangle. \end{aligned} \tag{278}$$

This is solved by

$$\Phi_\alpha(x) = \langle x|\alpha\rangle = \frac{1}{(2\pi\ell^2)^{1/4}} e^{-\frac{(x-2\ell\alpha)^2}{4\ell^2}}\ . \tag{279}$$

So the wave functions of coherent states are Gaussians centred at positions $2\ell\alpha$. We can express the coherent states in terms of the energy eigenstates (which after all form a basis) as follows. Using the eigenvalue equation together with (246) we obtain a recurrence relation

$$\langle n|a|\alpha\rangle = \alpha\ \langle n|\alpha\rangle = \sqrt{n+1}\langle n+1|\alpha\rangle. \tag{280}$$

This is solved by

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle. \tag{281}$$

This provides us with the desired expansion in terms of energy eigenstates

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \langle 0|\alpha\rangle \ |n\rangle. \tag{282}$$

We note that coherent states are particular superpositions involving *all* energy eigenstates. We have

$$\langle 0|\alpha\rangle = \int_{-\infty}^{\infty} dx \ \Phi_\alpha(x)\Psi_0^*(x) = e^{-\frac{\alpha^2}{2}}. \tag{283}$$

What makes coherent states special is their time evolution. Using the expansion in terms of energy eigenstates we have

$$|\alpha, t\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \langle 0|\alpha\rangle \ e^{-\frac{i}{\hbar}E_n t}|n\rangle. \tag{284}$$

Using that $E_n = \hbar\omega(n + 1/2)$ we have

$$\begin{aligned} |\alpha, t\rangle &= e^{-i\frac{\omega t}{2}} \sum_{n=0}^{\infty} \frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}} \frac{\langle 0|\alpha e^{-i\omega t}\rangle}{\langle 0|\alpha e^{-i\omega t}\rangle} \langle 0|\alpha\rangle \ |n\rangle, \\ &= e^{-i\frac{\omega t}{2}} \frac{e^{-\alpha^2/2}}{e^{-(\alpha e^{-i\omega t})^2/2}} |\alpha e^{-i\omega t}\rangle \ , \end{aligned} \tag{285}$$

where we have used (283) for both $\langle 0|\alpha\rangle$ and $\langle 0|\alpha e^{-i\omega t}\rangle$. The corresponding wave functions are

$$\Phi_\alpha(x, t) = \Phi_{\alpha_t}(x) e^{-i\frac{\omega t}{2}} e^{-\frac{\alpha^2}{2}(1-e^{2i\omega t})}. \tag{286}$$

Here comes the joke: the probability density $|\Phi_\alpha(x, t)|^2$ of a coherent state looks like a Gaussian wave-packet that oscillates with frequency ω while *precisely retaining its shape*!

Aside 5: Solving the Schrödinger equation numerically

Most Schrödinger equations cannot be solved exactly in the way we have done in our various examples. Therefore one typically resorts to numerical solutions. To be specific, let's consider the following example

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \lambda\hat{x}^4 \equiv H_0 + \lambda\hat{x}^4 \ , \quad \lambda > 0. \tag{287}$$

Let's say that we are interested in determining the ground state wave function of this Hamiltonian. One way of doing this is to use our knowledge of the eigenstates of the harmonic oscillator part H_0

$$H_0|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle. \tag{288}$$

Using that these states form an orthonormal basis of the space of quantum states we have

$$\mathbf{1} = \sum_{n=0}^{\infty} |n\rangle\langle n|, \tag{289}$$

and therefore

$$H = \mathbf{1}H\mathbf{1} = \sum_{n,m} \langle m|H|n\rangle \ |m\rangle\langle n|. \tag{290}$$

The eigenstates $|\psi_n\rangle$ of H can also be expressed in this basis

$$|\psi_n\rangle = \sum_m \langle m|\psi_n\rangle \ |m\rangle. \tag{291}$$

The matrix elements of the Hamiltonian in this basis are

$$\langle m|H|n\rangle \ = \hbar\omega(n+\frac{1}{2})\delta_{n,m} + \lambda\langle m|\hat{x}^4|n\rangle. \tag{292}$$

The matrix elements of the position operator can be determined either numerically by working out the integrals

$$\langle m|\hat{x}^4|n\rangle = \int_{-\infty}^{\infty} dx \ \left[\psi_m^{(0)}(x)\right]^* x^4 \psi_n^{(0)}(x), \tag{293}$$

where $\psi_n^{(0)}(x)$ are the harmonic oscillator wave functions, or by using our creation/annihilation operator algebra

$$\begin{aligned}
\langle m|\hat{x}^4|n\rangle &= \ell^4\langle m|(a+a^\dagger)^4|n\rangle \\
&= \ell^4\Big[\sqrt{n(n-1)(n-2)(n-3)}\delta_{m,n-4} + (4n-2)\sqrt{n(n-1)}\delta_{m,n-2} \\
&\quad +(6n^2+6n+3)\delta_{m,n} + \sqrt{(n+1)(n+2)}(4n+6)\delta_{m,n+2} \\
&\quad +\sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{m,n+4}\Big] \equiv \ell^4 V_{mn}.
\end{aligned} \tag{294}$$

The idea is now to *truncate* the sums in (290) by introducing a *cutoff* N. This turns H into an $(N+1)\times(N+1)$ matrix

$$H_{nm} = \hbar\omega\left[(n+\frac{1}{2})\delta_{n,m} + \underbrace{\frac{\lambda\ell^4}{\hbar\omega}}_{\mu} V_{nm}\right], \quad n,m = 0,\ldots,N. \tag{295}$$

We now simply diagonalize the (dimensionless) matrix $H/(\hbar\omega)$ numerically and obtain approximate values for the energies and eigenstates of H. We increase the cutoff N until the ground state energy and wave function no longer change within our desired numerical accuracy. For example, taking $\mu = 0.1$ and $N = 10$ gives

$$\begin{aligned}
E_0 &\approx 0.668812\hbar\omega \ , \\
|\psi_0\rangle &\approx -0.986914|0\rangle + 0.160316|2\rangle - 0.0133936|4\rangle - 0.0086538|6\rangle + 0.0064238|8\rangle - 0.00223485|10\rangle.
\end{aligned} \tag{296}$$

Increasing the cutoff to $N = 20$ gives

$$\begin{aligned}
E_0 &\approx 0.668773\hbar\omega \ , \\
|\psi_0\rangle &\approx -0.986896|0\rangle + 0.160386|2\rangle - 0.0134396|4\rangle - 0.00875891|6\rangle + 0.00682899|8\rangle \\
&\quad -0.00299289|10\rangle + 0.000832743|12\rangle - 0.0000103442|14\rangle - 0.000169943|16\rangle \\
&\quad +0.000129011|18\rangle - 0.0000507885|20\rangle
\end{aligned} \tag{297}$$

You get the idea. In general we choose an appropriate basis of states in which to express our Hamiltonian of interest and carry out the analogous procedure.

Homework 6: The simple harmonic oscillator

3.1 After choosing units in which everything, including $\hbar = 1$, the Hamiltonian of a harmonic oscillator may be written $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2)$, where $[\hat{x}, \hat{p}] = \mathrm{i}$. Show that if $|\psi\rangle$ is a ket that satisfies $H|\psi\rangle = E|\psi\rangle$, then

$$\frac{1}{2}(\hat{p}^2 + \hat{x}^2)(\hat{x} \mp \mathrm{i}\hat{p})|\psi\rangle = (E \pm 1)(\hat{x} \mp \mathrm{i}\hat{p})|\psi\rangle.$$

Explain how this algebra enables one to determine the energy eigenvalues of a harmonic oscillator.

3.2 Given that $\hat{a}|n\rangle = \alpha|n-1\rangle$ and $E_n = (n + \frac{1}{2})\hbar\omega$, where the annihilation operator of the harmonic oscillator is

$$\hat{a} \equiv \frac{m\omega\hat{x} + \mathrm{i}\hat{p}}{\sqrt{2m\hbar\omega}},$$

show that $\alpha = \sqrt{n}$. Hint: consider $|\hat{a}|n\rangle|^2$.

3.3 The pendulum of a grandfather clock has a period of 1 s and makes excursions of 3 cm either side of dead centre. Given that the bob weighs 0.2 kg, around what value of n would you expect its non-negligible quantum amplitudes to cluster?

3.4 Show that the minimum value of $E(p, x) \equiv p^2/2m + \frac{1}{2}m\omega^2x^2$ with respect to the real numbers p, x when they are constrained to satisfy $xp = \frac{1}{2}\hbar$, is $\frac{1}{2}\hbar\omega$. Explain the physical significance of this result.

3.5 How many nodes are there in the wavefunction $\langle x|n\rangle$ of the nth excited state of a harmonic oscillator?

3.6 Show that for a harmonic oscillator that wavefunction of the second excited state is $\langle x|2\rangle = \text{constant} \times (x^2/\ell^2 - 1)\mathrm{e}^{-x^2/4\ell^2}$, where $\ell \equiv \sqrt{\hbar/2m\omega}$ and find the normalising constant.

3.7 Use

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) = \ell(\hat{a} + \hat{a}^\dagger)$$

to show for a harmonic oscillator that in the energy representation the operator $\hat{x}$ is

$$\hat{x}_{jk} = \ell \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots & & & & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & & & & & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots & & & & \\ & & \sqrt{3} & \cdots & & & & & \\ \cdots & & \cdots & & \cdots & & \cdots & & \\ & & & \cdots & 0 & \sqrt{n-1} & \cdots & & \\ & & & & \sqrt{n-1} & 0 & \sqrt{n} & & \\ & & & & & \sqrt{n} & 0 & \sqrt{n+1} & \cdots \\ & & & & & & \sqrt{n+1} & 0 & \\ \cdots & & \cdots & & \cdots & & \cdots & & \cdots \end{pmatrix}$$

Calculate the same entries for the matrix $\hat{p}_{jk}$.

3.8 At $t = 0$ the state of a harmonic oscillator of mass m and frequency ω is

$$|\psi\rangle = \frac{1}{2}|N-1\rangle + \frac{1}{\sqrt{2}}|N\rangle + \frac{1}{2}|N+1\rangle.$$

Calculate the expectation value of x as a function of time and interpret your result physically in as much detail as you can.

Homework 7: More problems on basic quantum mechanics

3.9 A three-state system has a complete orthonormal set of states $|1\rangle, |2\rangle, |3\rangle$. With respect to this basis the operators $\hat{H}$ and $\hat{B}$ have matrices

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \hat{B} = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where ω and b are real constants.
(a) Are $\hat{H}$ and $\hat{B}$ Hermitian?
(b) Write down the eigenvalues of $\hat{H}$ and find the eigenvalues of $\hat{B}$. Solve for the eigenvectors of both $\hat{H}$ and $\hat{B}$. Explain why neither matrix uniquely specifies its eigenvectors.
(c) Show that $\hat{H}$ and $\hat{B}$ commute. Give a basis of eigenvectors common to $\hat{H}$ and $\hat{B}$.

3.10 A system has a time-independent Hamiltonian that has spectrum $\{E_n\}$. Prove that the probability P_k that a measurement of energy will yield the value E_k is is time-independent. Hint: you can do this either from Ehrenfest's theorem, or by differentiating $\langle E_k, t|\psi\rangle$ w.r.t. t and using the TDSE.

3.11 Let $\psi(x)$ be a properly normalised wavefunction and $\hat{Q}$ an operator on wavefunctions. Let $\{q_r\}$ be the spectrum of $\hat{Q}$ and $\{u_r(x)\}$ be the corresponding correctly normalised eigenfunctions. Write down an expression for the probability that a measurement of Q will yield the value q_r. Show that $\sum_r P(q_r|\psi) = 1$. Show further that the expectation of Q is $\langle Q\rangle \equiv \int_{-\infty}^{\infty} \psi^* \hat{Q}\psi \,\mathrm{d}x$.

3.12 (a) Find the allowed energy values E_n and the associated normalized eigenfunctions $\phi_n(x)$ for a particle of mass m confined by infinitely high potential barriers to the region $0 \le x \le a$.
(b) For a particle with energy $E_n = \hbar^2 n^2 \pi^2 / 2ma^2$ calculate $\langle x\rangle$.
(c) Without working out any integrals, show that

$$\langle (x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \frac{a^2}{4}.$$

Hence find $\langle (x - \langle x\rangle)^2\rangle$ using the result that $\int_0^a x^2 \sin^2(n\pi x/a)\,\mathrm{d}x = a^3(1/6 - 1/4n^2\pi^2)$.
(d) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical average values $\langle x\rangle_{\mathrm{C}}$ and $\langle (x - \langle x\rangle)^2\rangle_{\mathrm{C}}$, and show that for high values of n the quantum and classical results tend to each other.

3.13 A **Fermi oscillator** has Hamiltonian $\hat{H} = \hat{f}^\dagger \hat{f}$, where $\hat{f}$ is an operator that satisfies

$$\hat{f}^2 = 0, \quad \hat{f}\hat{f}^\dagger + \hat{f}^\dagger \hat{f} = 1.$$

Show that $\hat{H}^2 = \hat{H}$, and thus find the eigenvalues of $\hat{H}$. If the ket $|0\rangle$ satisfies $\hat{H}|0\rangle = 0$ with $\langle 0|0\rangle = 1$, what are the kets (a) $|a\rangle \equiv \hat{f}|0\rangle$, and (b) $|b\rangle \equiv \hat{f}^\dagger|0\rangle$?
In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion in an excitation of a Fermi oscillator. Explain the connection between the spectrum of

$\hat{f}^\dagger \hat{f}$ and the Pauli exclusion principle (which states that zero or one fermion may occupy a particular quantum state).

SOME OPTIONAL (!) OFF-SYLLABUS STUFF YOU MAY FIND INTERESTING

3.14 Numerical solutions of the Schrödinger equation By following the discussion given in the lecture notes construct numerical solutions for the first 10 eigenstates $|\phi_n\rangle$ of the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \lambda\hat{x}^4.$$

for $\frac{\lambda\ell^4}{\hbar\omega} = 0.1$. You can download a MATHEMATICA file for doing this from the course webpage. Now use the eigenvectors to obtain an expression for the ground state of the harmonic oscillator Hamiltonian ($\lambda = 0$) in terms of the eigenstates of H

$$|0\rangle \approx \sum_{n=0}^{N} \langle\phi_n|0\rangle \ |\phi_n\rangle.$$

Now assume that we initially prepare our system in the state $|\Phi(0)\rangle = |0\rangle$ and then consider time evolution under the Hamiltonian H. We have

$$|\Phi(t)\rangle \approx \sum_{n=0}^{N} \langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}|\phi_n\rangle. \tag{298}$$

We now want to determine the probability density $|\langle x|\Phi(t)\rangle|^2$ to find the particle at position x at time t. To do this we express $|\Phi(t)\rangle$ in terms of harmonic oscillator wave functions $\psi_k(x)$

$$\begin{aligned}\langle x|\Phi(t)\rangle &\approx \sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle x|\phi_n\rangle = \sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle x|\sum_{k=0}^{\infty}|k\rangle\langle k|\phi_n\rangle \\ &\approx \sum_{k=0}^{N}\sum_{n=0}^{N}\langle\phi_n|0\rangle \ e^{-\frac{i}{\hbar}E_n t}\langle k|\phi_n\rangle \ \psi_k(x). \end{aligned} \tag{299}$$

In the last step we have cut off the sum over k in the resolution of the identity, which is justified because $\langle k|\phi_n\rangle\langle\phi_n|0\rangle$ are negligible for large k. We have explicit expression for the harmonic oscillator wave functions and know $\langle k|\phi_n\rangle$ and E_n from our numerics. We therefore can plot $P(x,t) = |\langle x|\Phi(t)\rangle|^2$ for any given time. In order to keep our discussion very general we note that we essentially have two dimensionful quantities in our problem

- A time scale $1/\omega$.
- A length scale ℓ.

We use these scales to introduce dimensionless variables parametrizing the time and position by $x = z\ell$, $t = \tau/\omega$. The probability to observe our particle in the interval $[x, x+dx]$ is $P(x,t)dx = p(z,\tau)dz$, where

$$p(z,\tau) = |\langle z\ell|\Phi(\tau/\omega)\rangle|^2\ell.$$

The nice thing is that $p(z,\tau)$ no longer contains any dimensionful quantities

$$p(z,\tau) \approx \left|\frac{e^{-z^2/4}}{(2\pi)^{\frac{1}{4}}}\sum_{k=0}^{N}\sum_{n=0}^{N}\langle\phi_n|0\rangle \ \langle k|\phi_n\rangle \ e^{-i(E_n/\hbar\omega)\tau}\frac{H_k(z/\sqrt{2})}{\sqrt{k!2^k}}\right|^2. \tag{300}$$

Plot $p(x,\tau)$ as a function of z for some values of τ.