

Chapter 1

Quantum Kinematics

1.1 The Two-Slit Experiment

We begin this course with the classic two-slit experiment, which is one of the most fundamental experiments which helped to establish the fundamental principles of quantum mechanics. This serves both as an introduction or reminder to the basis for quantum physics and will be the key example we return to and generalise in increasing sophistication throughout the course.

The setup of the experiment is illustrated in Fig. 1.1. Particles (usually electrons) are emitted from the source on the left-hand side. They travel through the grating and then the intensity is measured on the screen at the right-hand side. If the grating only contained one

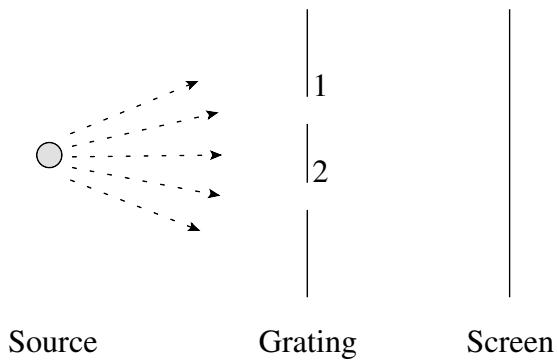


Figure 1.1: The two-slit experiment: particles are fired from the source on the left-hand side and then the intensity of the beam is measured on the screen at the right-hand side. The profiles predicted by classical and quantum physics are described in the text.

slit, the intensity measured on the screen would be given by the distributions P_1 or P_2 shown in Fig. 1.2(a). Classically the particles which reach the screen travel through either slit 1 or slit 2 and the final distribution seen should be the sum of P_1 and P_2 , shown in Fig. 1.2(b). However, the pattern observed in experiments

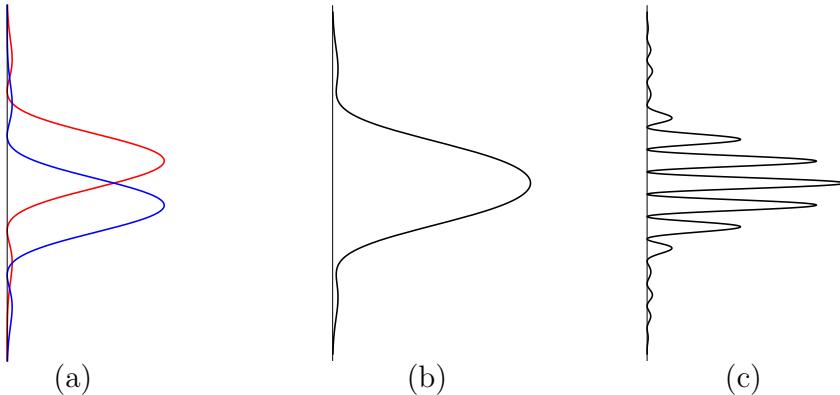


Figure 1.2: If the grating had only one slit, the pattern on the screen would appear as P_1 (red) or P_2 (blue) shown in (a). Classically then, one expects the sum of these two distributions, shown in (b). Quantum mechanics instead requires the amplitudes, ϕ to be summed before squaring, predicting the distribution shown in (c). This is the distribution which is experimentally observed.

is actually that shown in Fig. 1.2(c). This is instead consistent with the observed patterns in waves (e.g. water or sound)¹.

We can interpret the relative intensity of particles observed to hit the screen as being proportional to the relative probability that an initial particle ends up at that point. We understand probabilities to be given as the square of “amplitudes”, so P_1 and P_2 above are given by $|\phi_1|^2$ and $|\phi_2|^2$ for some $\phi_{1,2}$. The classical prediction is given by $|\phi_1|^2 + |\phi_2|^2$. In contrast, the quantum prediction is that it is given by $|\phi_1 + \phi_2|^2$; the amplitudes are summed *before* squaring. The difference between the final two results is the interference term. This is real but can take either sign, which is why there are places where the probability goes to zero – in physics terms, these are points of destructive interference.

During this course, we will calculate the probabilities of particular final states given an initial state for more and more complex systems, through increasingly sophisticated calculations.

1.2 Mathematical Framework

We will now introduce the mathematical definitions and notation that we will use throughout the course. Some of these are quite abstract.

¹Analytical expressions for the intensity can be found in arXiv:1110.2346. They are given by Fresnel functions.

States and linearity

We write any possible final state for a system as a “ket”: $|\psi\rangle$ where ψ can be a list of properties e.g. $|x, t\rangle$. The space of all such possible states form a “Hilbert space”: a complex linear vector space, \mathcal{H} , with a complex inner (dot) product. The overall normalisation of a state carries no physics meaning because $|\psi\rangle$ and $c|\psi\rangle$, $c \neq 0$, share the same eigenvalues with respect to any operator (observable).

The linearity of the Hilbert Space means that given any two states $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$, the state

$$|\psi_3\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle, \quad c_1, c_2 \in \mathbb{C}, \quad (1.1)$$

is also in \mathcal{H} . Constructing a third state in this way is a **linear superposition** of states.

Dual space

The (complex) inner product is defined such that

$$\begin{aligned} \langle\phi|\psi\rangle &= \langle\psi|\phi\rangle^* \in \mathbb{C}. \\ \langle\psi|\psi\rangle &\geq 0, \end{aligned} \quad (1.2)$$

(and $\langle\psi|\psi\rangle = 0 \Rightarrow |\psi\rangle = 0$ uniquely).

Although not absolutely necessary (as inner product sufficient) can define a dual space to \mathcal{H} , \mathcal{H}^* which means that every state $|\psi\rangle$ in \mathcal{H} has a **dual** or *adjoint* vector, written as the bra $\langle\psi|$ in \mathcal{H}^* . Formally the inner product is then a map $\mathcal{H}^* \times \mathcal{H} \rightarrow \mathbb{C}$. The inner product allows us to define a normalisation of a state as

$$\| |\psi\rangle \|^2 \equiv \langle\psi|\psi\rangle = 1. \quad (1.3)$$

However, since we are free to multiply by any constant this has no physical meaning. We therefore usually *choose* to normalise all states to 1 (this avoids clumsy factors when we want to calculate probabilities).

For consistency we must take the duality as anti-linear, for

$$\begin{aligned} \langle\phi|\psi_3\rangle &= c_1\langle\phi|\psi_1\rangle + c_2\langle\phi|\psi_2\rangle \\ &= [c_1^*\langle\psi_1|\phi\rangle + c_2^*\langle\psi_2|\phi\rangle]^*, \end{aligned} \quad (1.4)$$

which means that the dual vector of $|\psi\rangle$ is given by

$$\langle\psi_3| = c_1^*\langle\psi_1| + c_2^*\langle\psi_2|, \quad (1.5)$$

i.e. the constants are complex-conjugated, an antilinear superposition.

Example If we return to the two-slit experiment, the Hilbert space has two states, $|1\rangle$ and $|2\rangle$, corresponding to whether or not the particle travels through slit number 1 or 2. The state of any particle in the experiment will in general be a linear combination of these:

$$|f\rangle = c_1|1\rangle + c_2|2\rangle. \quad (1.6)$$

There are many further examples of two-state systems in nature such as electron spin and neutral-kaon mixing.

Probability

In quantum physics, we no longer have the sense of definiteness which exists in classical physics. Instead, we deal mostly with probabilities. Using the states above, the probability that a system will be observed in a final state $|\phi\rangle$ when it was observed initially in a state $|\psi\rangle$ is

$$P(\psi \rightarrow \phi) = |\langle\phi|\psi\rangle|^2. \quad (1.7)$$

The complex number given by the inner product $\langle\phi|\psi\rangle$ is called the **probability amplitude**. The amplitude for $|\psi\rangle \rightarrow |\phi\rangle$ followed by $|\phi\rangle \rightarrow |\chi\rangle$ is $\langle\chi|\phi\rangle\langle\phi|\psi\rangle$. (eg particle goes through slit 1, $|\phi\rangle = |1\rangle$.) Therefore

$$P(\psi \rightarrow \phi, \phi \rightarrow \chi) = |\langle\chi|\phi\rangle\langle\phi|\psi\rangle|^2 = |\langle\chi|\phi\rangle|^2|\langle\phi|\psi\rangle|^2 = P(\psi \rightarrow \phi)P(\phi \rightarrow \chi), \quad (1.8)$$

as we would expect.

The difference arises when we wish to add probabilities. The amplitude for either $|\psi\rangle \rightarrow |\phi\rangle$ or $|\psi\rangle \rightarrow |\chi\rangle$ is $\langle\chi|\psi\rangle + \langle\phi|\psi\rangle$. This gives the probability:

$$\begin{aligned} P(\psi \rightarrow \phi \text{ or } \chi) &= |\langle\chi|\psi\rangle + \langle\phi|\psi\rangle|^2 \\ &= |\langle\chi|\psi\rangle|^2 + |\langle\phi|\psi\rangle|^2 + 2\text{Re}(\langle\chi|\psi\rangle\langle\phi|\psi\rangle^*) \\ &\neq P(\psi \rightarrow \phi) + P(\psi \rightarrow \chi). \end{aligned} \quad (1.9)$$

The difference is down to the interference term at the end of the first line. This has fundamental, physical effects. For example, that term can have negative sign.

For the two-slit experiment, the amplitude for a particle to pass through state $|1\rangle$, ie slit 1 is $\langle f|1\rangle\langle 1|i\rangle$ (similarly for slit 2). Adding amplitudes gives probability

$$\begin{aligned} |\langle f|i\rangle|^2 &= |\langle f|1\rangle\langle 1|i\rangle + \langle f|2\rangle\langle 2|i\rangle|^2 \\ &= |\langle f|1\rangle\langle 1|i\rangle|^2 + |\langle f|2\rangle\langle 2|i\rangle|^2 + 2\text{Re}((\langle f|1\rangle\langle 1|i\rangle)(\langle f|2\rangle\langle 2|i\rangle)^*). \end{aligned} \quad (1.10)$$

As before the last term in the expansion is responsible for the parts of the screen where no electrons are observed; these are places $|f\rangle$ where the probability goes to

zero, even though neither the probability of hitting $|f\rangle$ via slit 1, $|\langle f|1\rangle\langle 1|i\rangle|^2$, or the probability of hitting $|f\rangle$ via slit 2, $|\langle f|2\rangle\langle 2|i\rangle|^2$ are zero individually. This explains the pattern² seen in Fig. 1.2.

You might think then that we only need to add a detector on each of the slits to measure the two non-zero probabilities separately, and then the sum cannot be zero. However, observing the particles in this way changes the experiment, and we would indeed get a different final answer. In classical physics, we do not usually have to account for the effect of the act of observing has on a system (watching a football does not change its direction). Indeed, this was suggested by Dirac as a possible means to define what we mean by “big” and “small”.

Thus we may take **measurement** (or ‘observation’) to be the interaction of the (quantum) system with a macroscopic system (and not due to any intervention of a human observer³).

In/distinguishability: The result above, with interference, is correct provided we cannot distinguish which slit the particle has travelled through. If we could distinguish which slit the particle had passed through (or wave if we imagine polarised filters for example), we return to the classical probability. Thus we have

$$\begin{aligned} \text{classically} &\equiv \text{outcomes distinguishable} \\ \text{quantum mechanically} &\equiv \text{outcomes indistinguishable}. \end{aligned}$$

This issue of indistinguishability is actually a deep concept. It also means that for any given particle in the initial state, we cannot say which slit it will travel through, or where/if it will hit the screen. We can only calculate the probability of a given final state and then, provided we repeat the experiment often enough, we can still predict macroscopic properties of the system. In the case of the two-slit experiment, we can still predict the final pattern on the screen.

1.3 Basis states and completeness

We now return to the Hilbert space introduced in section 1.2. There we said that this was formed from the space of all such possible states. Here we go further and define a set of basis states, $\{|n\rangle\}$, such that for any $|\psi\rangle \in \mathcal{H}$, we may write

$$|\psi\rangle = \sum_n \psi_n |n\rangle \tag{1.11}$$

²This result is still being verified experimentally, the latest result being for antimatter (positrons), arXiv:1808.08901.

³See eg Griffiths, Afterword for a brief discussion.

for some complex numbers ψ_n . These become the components of $|\psi\rangle$ in the basis $\{|n\rangle\}$. We may choose the basis vectors to be *orthonormal*, such that

$$\langle m|n\rangle = \delta_{mn}. \quad (1.12)$$

Then we can recover the components by calculating

$$\langle m|\psi\rangle = \sum_n \psi_n \langle m|n\rangle = \psi_m. \quad (1.13)$$

We recognise $\langle m|\psi\rangle$ as the probability amplitude for the state $|\psi\rangle$ to go to the basis state $|m\rangle$. We may rewrite Eq. (1.11) as

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle. \quad (1.14)$$

This must hold for all states $|\psi\rangle \in \mathcal{H}$, we have the so-called *completeness relation*

$$\sum_n |n\rangle \langle n| = \hat{1}, \quad (1.15)$$

where $\hat{1}$ is the identity or unit operator. We will use this relation again and again throughout this course. This represents the fact that at any time, a state must be in some linear superposition of the basis states. It is also necessary for the probabilistic interpretation which requires that $\sum_n P(\psi \rightarrow n) = 1$. We have

$$\sum_n P(\psi \rightarrow n) = \sum_n |\langle n|\psi\rangle|^2 = \sum_n \langle\psi|n\rangle \langle n|\psi\rangle = \langle\psi|\psi\rangle = 1. \quad (1.16)$$

(We have also used our choice of normalised states. Note alternative notation for norm of state $\| |\psi\rangle \| \equiv \langle\psi|\psi\rangle$.)

Example In any two-state system (such as the two-slit experiment), we may choose to write the two states as vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.17)$$

The completeness relation is then the statement that the sum of the outer products of the vectors is the identity:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.18)$$

1.4 Observables and Operators

An observable in quantum mechanics corresponds to a property of a system which can be measured to determine the state of that system at a given time. In practice, this can be done for example via Geiger counters or photo-detectors, but in this course we will not be concerned with the means of the measurement, only with the results. Examples of observables are position, angular momentum and energy.

Consider an observable which must take **real** values ξ_n in the basis states $|n\rangle$.

Ansatz for an operator, $\hat{\xi}$:

$$\hat{\xi} = \sum_n \xi_n |n\rangle\langle n|, \quad (1.19)$$

(called the **spectral representation** of the operator).

This satisfies the following properties:

1. $\hat{\xi}$ is a **linear** operator:

$$\hat{\xi}(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1\hat{\xi}|\psi_1\rangle + c_2\hat{\xi}|\psi_2\rangle,$$

by linearity of the Hilbert space.

2. $\hat{\xi}$ is a **hermitian** operator:

$$\begin{aligned} \langle\psi|\hat{\xi}^\dagger|\phi\rangle &\underset{\substack{\text{definition of} \\ \text{conjugate}^\dagger}}{\equiv} \langle\phi|\hat{\xi}|\psi\rangle^* = \left(\sum_n \xi_n \langle\phi|n\rangle\langle n|\psi\rangle \right)^* \\ &= \sum_n \xi_n \langle\phi|n\rangle^* \langle n|\psi\rangle^* \quad \xi_n \text{ real} \quad (1.20) \\ &= \sum_n \xi_n \langle\psi|n\rangle\langle n|\phi\rangle \\ &= \langle\psi|\hat{\xi}|\phi\rangle. \end{aligned}$$

True $\forall |\psi\rangle, |\phi\rangle$ so $\hat{\xi}^\dagger = \hat{\xi}$ ie hermitian.

3. $|n\rangle$ are **eigenstates** of $\hat{\xi}$, with eigenvalues ξ_n :

$$\hat{\xi}|n\rangle = \sum_m \xi_m |m\rangle\langle m|n\rangle = \xi_n |n\rangle. \quad (1.21)$$

4. If the states $|n\rangle$ are also eigenstates of a second observable, $\hat{\eta}$, with eigenvalues η_n , then

$$\hat{\xi}\hat{\eta}|n\rangle = \xi_n \eta_n |n\rangle = \eta_n \xi_n |n\rangle = \hat{\eta}\hat{\xi}|n\rangle \quad \forall |n\rangle, \quad (1.22)$$

and hence $\hat{\xi}$ and $\hat{\eta}$ commute, $[\hat{\xi}, \hat{\eta}] = 0$.

Measurement

When we make a measurement according to the operator $\hat{\xi}$, we measure the eigenvalue with respect to that operator. The state $|\psi\rangle$ of the system **collapses** into an eigenstate $|n\rangle$ of $\hat{\xi}$. The probability that we measure the value ξ_n is given by $|\langle n|\psi\rangle|^2$.

We can also construct the average value obtained over many measurements of the same initial state (i.e. not sequential measurements of a single state) as:

$$\begin{aligned}\langle \xi \rangle \equiv \bar{\xi} &\equiv \sum_n \xi_n |\langle n|\psi\rangle|^2 \\ &= \sum_n \xi_n \langle\psi|n\rangle\langle n|\psi\rangle \\ &= \langle\psi|\hat{\xi}|\psi\rangle.\end{aligned}\tag{1.23}$$

This is called the **expectation value** of $\hat{\xi}$ in the state $|\psi\rangle$.

We can think of the measurement process as projecting $|\psi\rangle$ onto a specific eigenstate $|n\rangle$ and define a projection operator for the state $|n\rangle$ to be:

$$\hat{P}_n = |n\rangle\langle n|.\tag{1.24}$$

It is easily checked that this has the correct properties of a projection operator: $\hat{P}_n^2 = \hat{P}_n$ and $\sum_n \hat{P}_n = \hat{1}$.

After a measurement has yielded an eigenvalue ξ_n , the state is no longer $|\psi\rangle$, but $|\psi\rangle \rightarrow \hat{P}_n|\psi\rangle$ with probability

$$||\hat{P}_n|\psi\rangle||^2 = \langle\psi|n\rangle\langle n|n\rangle\langle n|\psi\rangle = |\langle n|\psi\rangle|^2, \text{ as expected}.\tag{1.25}$$

This is the origin of the term collapses, as all other components of the state $|\psi\rangle$ in the basis have been lost.

Degeneracy

It is possible that there may be more than one physical state which has the same eigenvalue of a given observable. This is known as a degeneracy and we label the multiple states by adding another index (or more), e.g.

$$\hat{\xi}|n, m\rangle = \xi_n |n, m\rangle \quad \forall m \in M_n,\tag{1.26}$$

where M_n is a particular set. The corresponding projection operator is then given by:

$$\hat{P}_n = \sum_{m \in M_n} |n, m\rangle\langle n, m|.\tag{1.27}$$

To project onto a single state would require a second measurement of a further observable which leads to the definition of a maximally commuting set of observables. We do not discuss this further in this course.

1.5 Change of Basis

The choice of basis states is not usually unique, and we may find it helpful to change from one basis to another, $\{|n\rangle\} \rightarrow \{|n'\rangle\}$. (An alternative notation for $|n'\rangle$ is $|\bar{n}\rangle$.) As the original states form a basis, we may express the new states in terms of them by inserting the completeness operator

$$|n'\rangle = \sum_m |m\rangle \langle m|n'\rangle = \sum_m |m\rangle U_{mn}, \quad (1.28)$$

where $U_{mn} = \langle m|n'\rangle$. Dirac named the U_{mn} transformation coefficients. The use of notation usually used for matrices is deliberate as this is just a linear transformation.

If the new basis is also orthonormal we have

$$\delta_{mn} = ' \langle m|n\rangle' = \sum_l ' \langle m|l\rangle \langle l|n\rangle' = \sum_l U_{ml}^\dagger U_{ln} \quad (1.29)$$

because $' \langle m|n\rangle' = \langle n|m\rangle'^* = (U_{nm})^* = (U_{mn}^T)^* \equiv U_{mn}^\dagger$. This means U_{mn} is the mn element of a unitary matrix

$$U^\dagger U = I, \quad (1.30)$$

(or $UU^\dagger = I$ as the transformation is non-singular, inverse exists, so $U^\dagger = U^{-1}$)⁴.

We can define a corresponding operator \hat{U} such that

$$|n'\rangle = \hat{U}|n\rangle, \quad (1.31)$$

which means that

$$U_{mn} = \langle m|\hat{U}|n\rangle. \quad (1.32)$$

This operator must also be unitary

$$\hat{U}^\dagger \hat{U} = \hat{I} \quad (1.33)$$

as

$$\begin{aligned} \delta_{mn} &= \sum_l U_{lm}^* U_{ln} \\ &= \sum_l \langle l|\hat{U}|m\rangle^* \langle l|\hat{U}|n\rangle = \sum_l \langle m|\hat{U}^\dagger|l\rangle \langle l|\hat{U}|n\rangle \\ &= \langle m|\hat{U}^\dagger \hat{U}|n\rangle. \end{aligned} \quad (1.34)$$

⁴This is an ‘active’ transformation, as $|n'\rangle = \sum_m |m\rangle U_{mn} = \sum_m U_{nm}^{*-1} |m\rangle$ which is essentially an inverse passive transformation.

Unitary operators are not in general observables because they don't necessarily have real eigenvalues.

1.6 Continuous Variables – position and wavenumber

We have so far discussed a finite number of eigenstates for a given observable. We will now generalise this to continuous variables, which you can consider to be the limit as $N \rightarrow \infty$ of N discrete variables. As a concrete example, consider position x . If we generalise the two-slit experiment of section 1.1 to an N -slit experiment, then the basis of states is $|n\rangle$ with $n = 1, \dots, N$ and we have

$$P(i \rightarrow f) = |\langle f|i \rangle|^2, \quad \text{with} \quad \langle f|i \rangle = \sum_{n=1}^N \langle f|n \rangle \langle n|i \rangle. \quad (1.35)$$

Position basis

To take the limit of infinitely many slits, we introduce the continuous label x . Usual transition to continuous variables

$$|n\rangle \rightarrow |x\rangle, \quad \sum_n \rightarrow \int dx, \quad \delta_{mn} \rightarrow \delta(x - x'). \quad (1.36)$$

The component of $|\psi\rangle$ in the basis $|x\rangle$ now becomes a function of x , which we write as $\psi(x)$. The continuous equivalent of Eq. (1.11) is

$$|\psi\rangle = \int_a^b \psi(x) |x\rangle dx. \quad (1.37)$$

The orthonormality condition for the basis, Eq. (1.12), becomes

$$\langle x'|x \rangle = \delta(x - x'). \quad (1.38)$$

This leads to the relation

$$\langle x|\psi\rangle = \int_a^b \psi(x) \langle x|x'\rangle dx' = \psi(x). \quad (1.39)$$

Therefore we write $\psi(x) = \langle x|\psi\rangle$ and $\psi^*(x) = \langle \psi|x\rangle$. Returning to the original expression for $|\psi\rangle$, Eq. (1.37), we now have

$$|\psi\rangle = \int_a^b dx |x\rangle \langle x|\psi\rangle. \quad (1.40)$$

This holds for all states $|\psi\rangle$, and hence we have the continuous equivalent of the completeness relation:

$$\hat{1} = \int_a^b dx |x\rangle\langle x|. \quad (1.41)$$

This again represents the fact that the particle must be somewhere in the x -region.

We can now use this result to show:

$$1 = \langle\psi|\psi\rangle = \int_a^b dx \langle\psi|x\rangle\langle x|\psi\rangle = \int_a^b dx \psi^*(x)\psi(x). \quad (1.42)$$

So can interpret the square of the probability amplitude, $|\psi(x)|^2$, as a probability density: $|\psi(x)|^2 dx$ is the probability that the particle is between x and $x + dx$.

So $\psi(x)$ is the spatial wave function of wave mechanics.

Analogously to the discrete operator in Eq. (1.19), we may define the (continuous) position operator as

$$\hat{x} = \int_a^b dx x |x\rangle\langle x|, \quad (1.43)$$

(spectral resolution, so by definition Hermitian). It is easily checked that this gives

$$\hat{x}|x\rangle = \int_a^b dx' x' |x'\rangle\langle x'|x\rangle = \int_a^b dx' x' |x'\rangle\delta(x' - x) = x|x\rangle, \quad (1.44)$$

as it should. It was necessary here to introduce the dummy integration variable x' in order to distinguish the operator definition of \hat{x} from the state we're considering, $|x\rangle$. This is extremely important. Each insertion of an integral definition of an operator like Eq. (1.43), or of the completeness condition, Eq. (1.41), must come with a new, different variable. When working with these equations, it is always worth taking time to double-check you've done this correctly.

The expectation value of \hat{x} in the state $|\psi\rangle$ is

$$\langle\psi|\hat{x}|\psi\rangle = \int_a^b dx \langle\psi|\hat{x}\rangle x \langle x|\psi\rangle = \int_a^b dx x \psi^*(x)\psi(x). \quad (1.45)$$

So far, we have made no comments about the integration limits a and b . These are the allowed values of x , and need not necessarily be finite. Then, for example, the transition amplitude from an initial state $|i\rangle$ to some final state $|f\rangle$ becomes

$$\langle f|i\rangle = \int_{-\infty}^{\infty} dx \langle f|x\rangle\langle x|i\rangle. \quad (1.46)$$

Fourier Transform Basis

A common alternative to the position basis above is the so-called Fourier Transform basis. This consists of states $|k\rangle$ such that⁵

$$|k\rangle \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{+ikx} |x\rangle. \quad (1.47)$$

The completeness relation, though, gives

$$|k\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x|k\rangle. \quad (1.48)$$

Combining the two therefore gives

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \implies \langle k|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-ikx}. \quad (1.49)$$

We can use this to derive the inner product between two states $|k\rangle$ and $|k'\rangle$:

$$\langle k'|k\rangle = \int_{-\infty}^{\infty} dx \langle k'|x\rangle \langle x|k\rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{i(-k'+k)x} = \delta(k' - k). \quad (1.50)$$

(This implies that the transformation is unitary – one orthonormal basis has been transformed to another.)

We can now construct the operator \hat{k} as usual:

$$\hat{k} = \int dk k |k\rangle \langle k|, \quad (1.51)$$

This directly leads to

$$\hat{k}|k\rangle = k|k\rangle, \quad (1.52)$$

as in the case for \hat{x} . By definition, \hat{k} is Hermitian. It follows that

$$\begin{aligned} \hat{k}|x\rangle &= \int dk k |k\rangle \langle k|x\rangle = \frac{1}{\sqrt{2\pi}} \int dk k |k\rangle e^{-ikx} \\ &= \frac{i}{\sqrt{2\pi}} \frac{\partial}{\partial x} \int dk |k\rangle e^{-ikx} \\ &= i \frac{\partial}{\partial x} \int dk |k\rangle \langle k|x\rangle \\ &= i \frac{\partial}{\partial x} |x\rangle. \end{aligned} \quad (1.53)$$

⁵Note that later we will associate k with the wave number and take the momentum $p = \hbar k$.

This then gives $\langle \psi | \hat{k} | x \rangle = i\partial/\partial x \langle \psi | x \rangle$, with the corresponding complex conjugate

$$\langle x | \hat{k} | \psi \rangle = -i \frac{\partial}{\partial x} \psi(x). \quad (1.54)$$

Finally, the product formed with \hat{k} between two states is then given by

$$\langle \phi | \hat{k} | \psi \rangle = \int dx \langle \phi | x \rangle \langle x | \hat{k} | \psi \rangle = \int dx \phi^*(x) \left(-i \frac{\partial}{\partial x} \right) \psi(x). \quad (1.55)$$

The equivalent in the Fourier basis of the definition of $\psi(x)$ in the position basis is

$$\begin{aligned} \tilde{\psi}(k) &= \langle k | \psi \rangle \\ &= \int dx \langle k | x \rangle \langle x | \psi \rangle \\ &= \int \frac{dx}{\sqrt{2\pi}} e^{-ikx} \psi(x) \quad ie \text{ Fourier transform}. \end{aligned} \quad (1.56)$$

May also show (which you should check):

$$\begin{aligned} \langle k | \hat{k} | \psi \rangle &= k \tilde{\psi}(k), \\ \langle \phi | \hat{k} | \psi \rangle &= \int dk \tilde{\phi}^*(k) k \tilde{\psi}(k), \\ \langle k | \hat{x} | \psi \rangle &= i \frac{\partial}{\partial k} \tilde{\psi}(k) \\ \langle \phi | \hat{x} | \psi \rangle &= \int dk \tilde{\phi}^*(k) \left(i \frac{\partial}{\partial k} \right) \tilde{\psi}(k). \end{aligned} \quad (1.57)$$

We summarise the results for \hat{x} and \hat{k} acting on the state vector $|\psi\rangle$ in table 1.1.

Basis	\hat{x}	\hat{k}
$\langle x $	x	$-i\partial/\partial x$
$\langle k $	$i\partial/\partial k$	k

Table 1.1: Summary of the action of \hat{x} and \hat{k} on $|\psi\rangle$.

The commutator is given by

$$[\hat{x}, \hat{k}] = i\hat{1}, \quad (1.58)$$

as for example

$$\begin{aligned} \langle x | [\hat{x}, \hat{k}] | \psi \rangle &= \langle x | (\hat{x}\hat{k} - \hat{k}\hat{x}) | \psi \rangle \\ &= x \left(-i \frac{\partial}{\partial x} \psi(x) \right) - \left(-i \frac{\partial}{\partial x} (x\psi(x)) \right) = i\psi(x). \end{aligned} \quad (1.59)$$

and as this is true $\forall |\psi\rangle$, then the result follows. As this is non-zero, the two operators do not correspond to simultaneous observables.

This result also leads to the Heisenberg uncertainty principle

$$\Delta x \Delta k \geq \frac{1}{2}, \quad (1.60)$$

where $\Delta\xi \equiv \langle \hat{\xi}^2 \rangle - \langle \hat{\xi} \rangle^2$.

Later identify

$$p = \hbar k \quad \text{or} \quad \hat{p} = \hbar \hat{x}, \quad (1.61)$$

(use this in example sheet I).

3-dimensions

For ease of notation, all of the above has been performed in one dimension. It can be easily generalised to three dimensions by replacing the 1-d integrals with ones in $3 - d$. For example:

$$\langle \vec{r}' | \vec{r} \rangle = \delta^{(3)}(\vec{r} - \vec{r}'), \quad (1.62)$$

$$\int_{-\infty}^{\infty} d^3 r | \vec{r} \rangle \langle \vec{r} | = \hat{I} = \int_{-\infty}^{\infty} d^3 k | \vec{k} \rangle \langle \vec{k} |, \quad (1.63)$$

$$\tilde{\psi}(\vec{k}) = \int \frac{d^3 r}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{r}} \psi(\vec{r}). \quad (1.64)$$

In particular, note that there is a factor of $\sqrt{2\pi}$ for *each* dimension of the integral when moving to the Fourier basis.

Notation: $\vec{x} \equiv \vec{r}$, components x_i or r_i .

1.7 Time as a Continuum

Having generalised from two slits to infinitely many slits, the next generalisation of the two-slit experiment is to infinitely many gratings, see Fig. 1.3. We will start with a finite number, N , and then take the limit as the $N \rightarrow \infty$ while keeping the total time constant as we did with the number of slits. This will give a description of time as a continuum. As before, we denote the initial and final states as $|i\rangle$ and $|f\rangle$ respectively. Let the n -th grating be passed at position x_n at time t_n , which we write as state $|x_n, t_n\rangle$. At fixed time t_1 , there is a completeness relation in x_1 (as the particle must be somewhere at time t_1) and so we can write the transition amplitude $\langle f | i \rangle$ as

$$\langle f | i \rangle = \int dx_1 \langle f | x_1, t_1 \rangle \langle x_1, t_1 | i \rangle. \quad (1.65)$$

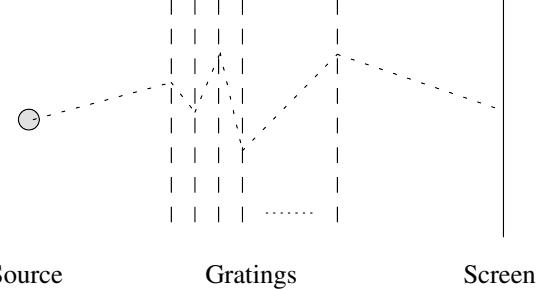


Figure 1.3: A sketch of the generalised two-slit experiment, now with N gratings (each with infinitely many slits).

We can now do the same for t_2, \dots, t_N :

$$\begin{aligned} \langle f|i\rangle &= \int dx_1 \int dx_2 \langle f|x_2, t_2\rangle \langle x_2, t_2|x_1, t_1\rangle \langle x_1, t_1|i\rangle \\ &= \dots \\ &= \int dx_1 \dots \int dx_N \langle f|x_N, t_N\rangle \dots \langle x_2, t_2|x_1, t_1\rangle \langle x_1, t_1|i\rangle. \end{aligned} \quad (1.66)$$

As N increases, the time intervals between each slice get smaller as we keep the total time constant. This fixes each path more precisely. However, we also generate more and more integrals as the number of possible paths increases.

Given $|i\rangle = |x_a, t_a\rangle$ and $|f\rangle = |x_b, t_b\rangle$, we can take the gratings at equal intervals and define

$$t_n = t_a + n\epsilon; \quad \text{where} \quad \epsilon = \frac{t_b - t_a}{N+1}, \quad (1.67)$$

such that

$$(x_0, t_0) = (x_a, t_a), \quad \text{and} \quad (x_{N+1}, t_{N+1}) = (x_b, t_b). \quad (1.68)$$

We can then compactly write Eq. (1.66) as

$$\langle x_b, t_b|x_a, t_a\rangle = \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=1}^{N+1} \langle x_n, t_n|x_{n-1}, t_{n-1}\rangle \right). \quad (1.69)$$

The first bracket integrates over all combinations of points, i.e. the paths, while the second bracket gives the amplitude for each of those paths.

The $\epsilon \rightarrow 0$ limit of Eq. (1.69) is written

$$\langle x_b, t_b|x_a, t_a\rangle = \int_{x_a}^{x_b} \mathcal{D}x \langle x_b, t_b|x_a, t_a\rangle \Big|_{x(t)}, \quad (1.70)$$

where $\mathcal{D}x$ represents that the integral is over all paths $x(t)$ which begin at $x = x_a$ and end at $x = x_b$. $\langle x_b, t_b|x_a, t_a\rangle|_{x(t)}$ is the amplitude along the continuous path $x(t)$.

Intuitive re-writing

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \sim \exp[i\epsilon\phi(x_n, x_{n-1}, t_n, t_{n-1})], \quad (1.71)$$

where $\epsilon = t_n - t_{n-1}$ and ϕ is a real function, ie a phase.

We call this the transition amplitude along the path $x(t)$.

- $\epsilon \rightarrow 0$, amplitude constant.
- ϕ only depends on $x_n, t_n, x_{n-1}, t_{n-1}$, ie locality.
- regard transition $|x_{n-1}, t_{n-1}\rangle \rightarrow |x_n, t_n\rangle$ as a change of basis, with unitary operator \hat{U}

$$|x_n, t_n\rangle = \hat{U}^\dagger |x_{n-1}, t_{n-1}\rangle,$$

(\dagger for convention). We write

$$\hat{U} = \hat{1} + i\epsilon\hat{\phi} + O(\epsilon^2) \approx e^{i\epsilon\hat{\phi}},$$

where \hat{U} unitary $\Rightarrow \hat{\phi}$ Hermitian. (This is actually always possible for a unitary operator.) So write

$$\hat{\phi}|x_n, t_n\rangle \sim \phi(x_n, x_{n-1}, t_n, t_{n-1})|x_n, t_n\rangle,$$

giving

$$|x_{n-1}, t_{n-1}\rangle \sim e^{i\epsilon\phi}|x_n, t_n\rangle,$$

leading to the result.

So

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle|_{x(t)} &\sim \prod_{n=1}^{N+1} e^{i\epsilon\phi(x_n, x_{n-1}, t_n, t_{n-1})} \\ &\sim \exp \left\{ i \sum_{n=1}^{N+1} (t_n - t_{n-1}) \phi(x_n, x_{n-1}, t_n, t_{n-1}) \right\} \end{aligned} \quad (1.72)$$

or as $N \rightarrow \infty$

$$\langle x_b, t_b | x_a, t_a \rangle|_{x(t)} = \exp \left\{ i \int_{t_a}^{t_b} dt \phi(x(t), \dot{x}(t), t) \right\}, \quad (1.73)$$

The precise mathematical formulation of this limit is actually very difficult to construct. The results are only meaningful after careful normalisation which we will construct in the next section.

To identify ϕ with *something* now need some classical mechanics.

Key Concepts

1. Probabilities in quantum systems are expressed as squares of probability amplitudes. When summing over different states, the amplitudes are summed before they are squared. This gives interference effects not present in classical systems, which have been experimentally verified.
2. In a quantum system, we cannot determine the precise behaviour of any single component. However, we can still make (correct) predictions for the behaviour of the system as a whole derived from the relevant probability amplitudes.
3. We describe quantum systems in terms of the relevant Hilbert space of states, which is an abstract vector space. Each Hilbert space \mathcal{H} has a dual space \mathcal{H}^* . \mathcal{H} is complete, allowing us to obtain the completeness relation

$$\hat{1} = \sum_n |n\rangle\langle n|.$$

4. When we make a measurement of an observable on a state, this projects a state onto the measured eigenstate. This act of making the measurement therefore fundamentally alters the state of the system.
5. Eigenstates are not necessarily discrete. There are analogues for continuous variables of e.g. the completeness relation and expectation value. The most common continuous variables encountered are position and time. A good interpretation of these is to consider the two-slit experiment with N slits or N gratings and then take the limit $N \rightarrow \infty$.

Chapter 2

Quantum Dynamics

In order to mathematically define the path integral of the previous section, we will use the quantum action. We therefore begin this section by revisiting the classical theory.

2.1 Revision of Classical Dynamics

In Lagrangian dynamics, the **action** for a path $x(t)$ is

$$S[x(t)] = \int_{t_a}^{t_b} L(x, \dot{x}, t) dt, \quad (2.1)$$

where L is the Lagrangian of the system. For a non-relativistic point particle in a potential V in one dimension this is given by

$$L(x, \dot{x}, t) = T - V = \frac{1}{2}m\dot{x}^2 - V(x, t). \quad (2.2)$$

Classical dynamics is based upon the **Principle of least action** (equivalent to Newton's equations) which is the statement that the classical path $\bar{x}(t)$ is an extremum of the functional S :

$$\left. \frac{\delta S}{\delta x} \right|_{x=\bar{x}} = 0. \quad (2.3)$$

The notation $\delta S/\delta x$ is the functional derivative of the functional S with respect to x . We compute this by considering a small variation in the path $x(t)$ (like you would consider a small variation in the variable x in normal differentiation). We write consider the path given by $x(t) + \delta x(t)$, where $\delta x(t)$ is taken to be small so that we can neglect terms of order $\delta x(t)^2$ and above. The corresponding change in

S is

$$\begin{aligned}
\delta S &= S[x + \delta x] - S[x] = \int_{t_a}^{t_b} dt \left(L(x + \delta x, \dot{x} + \delta \dot{x}, t) - L(x, \dot{x}, t) \right) \\
&= \int_{t_a}^{t_b} dt \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) + \mathcal{O}(\delta x^2) \\
&= \left[\frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_a}^{t_b} - \int_{t_a}^{t_b} dt \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right) \delta x + \mathcal{O}(\delta x^2),
\end{aligned} \tag{2.4}$$

using integration by parts. Usually the endpoints are fixed ($\delta x(t_a) = 0 = \delta x(t_b)$) so the square bracket vanishes leaving Lagrange's equation for the classical path:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0. \tag{2.5}$$

We define the action on the classical path $S_{\text{cl}} = S[\bar{x}(t)]$. This is a function of the endpoints x_a, t_a and x_b, t_b (as well as through the integral limits, also implicitly in \bar{x}).

Hamilton's principal function

We will now vary the final spatial point $(x_b, t_b) \rightarrow (x_b, t_b) + (\delta x_b, \delta t_b)$, but keep the initial points (x_a, t_a) fixed. Regarding as a variation in the path, then from the last line of Eq. (2.4) we find (choosing $\delta t_b = 0$)

$$\delta S_{\text{cl}} = \frac{\partial L}{\partial \dot{x}} \delta x \Big|_{t_b}^{t_b} + 0, \tag{2.6}$$

because the original path already satisfied Eq. (2.5). Using the definition of the canonical momentum p conjugate to x : $p = \partial L / \partial \dot{x}$ we therefore have

$$\frac{\partial S_{\text{cl}}}{\partial x_b} = p_b, \tag{2.7}$$

p_b is the classical momentum at the endpoint.

We will now consider varying t_b and keeping x_b fixed. As $x_b = x(t_b)$ then $0 = \delta x_b(t_b) + \dot{x}(t_b)\delta t_b$ or $\delta x(t_b) = -\dot{x}_b \delta t_b$. (Particle arrives at the same x_b at time $t_b + \delta t_b$.) So we have two variations, from δt_b and $\delta x(t_b)$.

The first contribution is from the end point of the integral, Eq. (2.1), while the second is as before, Eq. (2.6). Hence we have

$$\begin{aligned}
\delta S_{\text{cl}} &= L_b \delta t_b + p_b \delta x(t_b) \\
&= (L_b - p_b \dot{x}_b) \delta t_b = -E_b \delta t_b.
\end{aligned} \tag{2.8}$$

where $E_b \equiv H$ is the energy function or the Hamiltonian at b . This gives

$$E_b = -\partial S_{\text{cl}}/\partial t_b, \quad (2.9)$$

or

$$E \left(x_b, \frac{\partial S_{\text{cl}}}{\partial x_b}, t_b \right) + \frac{\partial S_{\text{cl}}}{\partial t_b} = 0. \quad (2.10)$$

This is the Hamiltonian-Jacobi equation (or keeping p_b , Eq. (2.7) equations).

Hamilton's principle function, ie solution of the H-J equation, here denoted by S_{cl} , is the action up to a constant.

A different derivation is given in the course 'Hamiltonian Dynamics' where it follows from a canonical transformation of variables to a constant Hamiltonian.

Example 1: The Free Particle The Lagrangian for a free particle is given by

$$L = \frac{1}{2}m\dot{x}^2 \Rightarrow \ddot{x} = 0, \quad (2.11)$$

and hence

$$\bar{x} = x_a + v(t - t_a), \quad \text{where } v = \frac{x_b - x_a}{t_b - t_a} = \dot{\bar{x}}, \quad (2.12)$$

so v is the constant velocity of the particle. Then

$$S_{\text{cl}} = S[\bar{x}] = \int_{t_a}^{t_b} \frac{1}{2}m\dot{x}^2 dt = \frac{1}{2}m \frac{(x_b - x_a)^2}{(t_b - t_a)}. \quad (2.13)$$

This gives

$$p_b = \frac{\partial S_{\text{cl}}}{\partial x_b} = mv, \quad \text{and} \quad E_b = -\frac{\partial S_{\text{cl}}}{\partial t_b} = \frac{1}{2}mv^2. \quad (2.14)$$

Example 2: The Simple Harmonic Oscillator The Lagrangian for the simple harmonic oscillator and the corresponding equation of motion are

$$L = \frac{1}{2}m(\dot{x}^2 - \omega^2 x^2) \quad \text{and} \quad \ddot{x} + \omega^2 x = 0. \quad (2.15)$$

Writing $T = t_b - t_a$ and imposing $\bar{x}(t_a) = x_a$ and $\bar{x}(t_b) = x_b$, we find

$$\bar{x}(t) = x_b \frac{\sin \omega(t - t_a)}{\sin \omega T} + x_a \frac{\sin \omega(t_b - t)}{\sin \omega T}. \quad (2.16)$$

This then gives

$$S[\bar{x}] = \frac{m\omega}{2 \sin \omega T} [(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b], \quad (2.17)$$

so the Hamilton-Jacobi equations are

$$p_b = m\dot{\bar{x}} \Big|_{t=t_b}, \quad E_b = \frac{m}{2} \left(\dot{\bar{x}}^2 + \omega^2 \bar{x}^2 \right) \Big|_{t=t_b}. \quad (2.18)$$

See problem sheet II.

2.2 The Amplitude for a Path

We now return to constructing an amplitude for a path $x(t)$ which we wrote in Eq. (1.73) as

$$\langle x_b, t_b | x_a, t_a \rangle \Big|_{x(t)} \sim \exp \left\{ i \int_{t_a}^{t_b} dt \phi(x(t), \dot{x}(t), t) \right\}. \quad (2.19)$$

In order to determine ϕ , we go back to the classical case because we should always recover the known results by taking the classical limit of the quantum results. The classical action is the Lagrangian integrated over a path, which suggests that our phase ϕ should be proportional to the Lagrangian L . We find that this recovers the results that we expect. We must also include a constant such that the exponent is dimensionless. The dimensions of the action

$$[S] = [t][E] = [x][p]. \quad (2.20)$$

We therefore introduce a dimensionful constant \hbar and write

$$\langle x_b, t_b | x_a, t_a \rangle \Big|_{x(t)} = e^{iS[x(t)]/\hbar}. \quad (2.21)$$

Notes:

- We have still to determine the overall normalisation constant; this will be absorbed in our definition of $\mathcal{D}x$.
- If our action is modified by a constant, $S \rightarrow S + c$, c constant, all amplitudes will change by the same phase $e^{ic/\hbar}$ and so any physical result will be unchanged.
- The size of quantum fluctuations is set by the size where the variations in the exponent are $\mathcal{O}(1)$. This gives $\delta S \sim \mathcal{O}(\hbar)$.
- This formulation is an assumption, but backed up with very good experimental confirmation.

2.3 The Feynman Path Integral

The result of the previous section gives the following expression for the transition amplitude:

$$\langle x_b, t_b | x_a, t_a \rangle = \underbrace{\int_{x_a}^{x_b} \mathcal{D}x}_{\text{sum over all paths}} \underbrace{e^{iS[x(t)]/\hbar}}_{\substack{\text{amplitude} \\ \text{for each path}}}. \quad (2.22)$$

In practice, in order to evaluate the integral in Eq. (2.22), we use the limiting procedure described in Eq. (58) and (1.71). This means that we define the measure through

$$\int_{x_a}^{x_b} \mathcal{D}x = \lim_{N \rightarrow \infty} A_N \prod_{n=1}^N \int_{-\infty}^{\infty} dx_n, \quad (2.23)$$

where

$$A_N = \nu(\epsilon)^{N+1}, \quad (2.24)$$

i.e. a normalising factor $\nu(\epsilon)$ for **each discrete interval**.

Given this formalism, we are free to insert a complete set of states into the transition amplitude:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \int dx_c \langle x_b, t_b | x_c, t_c \rangle \langle x_c, t_c | x_a, t_a \rangle \\ &= \int dx_c \int_{x_a}^{x_b} \mathcal{D}x \int_{x_a}^{x_c} \mathcal{D}x' \exp \left\{ \frac{i}{\hbar} \left(\int_{t_c}^{t_b} L dt + \int_{t_a}^{t_c} L dt \right) \right\}. \end{aligned} \quad (2.25)$$

This can be interpreted as splitting the path into two and summing over all possible places to do that, see Fig. 2.1. This method of splitting will prove useful for

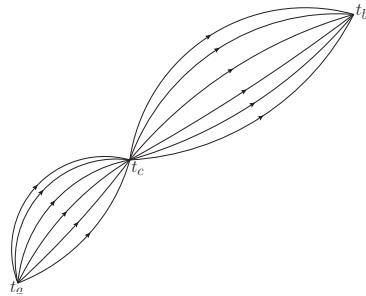


Figure 2.1: We can insert a complete set of states labelled $|x_c, t_c\rangle$ to split any path in two.

evaluating the factors of ν .

2.4 Connection to the Classical Limit

For quantum processes, we are usually in a situation where you can consider t_b and t_a to be close, and also x_a and x_b to be close. The action $S[x(t)]$ is taken to be of

order of \hbar meaning the fluctuations in the exponent are of order 1. This means that paths far from the classical path may be important¹.

In contrast, in classical processes, the intervals between t_b and t_a and between x_b and x_a are often much larger; and crucially in general we have $S[x(t)] \gg \hbar$. In fact, formally, the classical limit is obtained by taking $\hbar \rightarrow 0$.

Consider paths which are a small perturbation of a given path $x(t)$. Given that the magnitude of S is so large, one expects that δS will also be large even when δx is small. This means that the integrand, $\exp(i\delta S/\hbar)$, will oscillate violently and contributions from nearby paths will cancel out. There is though one special path, the classical path $\bar{x}(t)$, which is exactly defined as the path where the terms of order δx are zero. Therefore the change in δS is of order $(\delta x)^2$, and this means nearby paths *can* add constructively². Therefore, in the limit $\hbar \rightarrow 0$, the classical path gives the dominant contribution and we arrive at the classical principle of least action! In this situation, we therefore have

$$\langle x_b, t_b | x_a, t_a \rangle \sim e^{iS_{\text{cl}}/\hbar}. \quad (2.26)$$

This is known as the semi-classical approximation.

2.5 Momentum and Energy

Momentum

Now consider a small change in the final endpoint of the path: $x_b \rightarrow x_b + \delta x_b$. We will not change t_b . The resultant change in phase of the integrand, $\delta S_{\text{cl}}/\hbar$, is defined to be $k_b \delta x_b$, where k_b is the wavenumber. Now we have from Eq. (2.7) (Hamiltonian-Jacobi equation) $\delta S_{\text{cl}} = p_b \delta x_b$, so as b is arbitrary

$$p = \hbar k, \quad (2.27)$$

or which naturally converts to operator language as $\hat{p} = \hbar \hat{k}$. Returning to the results for \hat{k} in Table 1.1

$$[\hat{x}, \hat{p}] = i\hbar, \quad (2.28)$$

the famous Heisenberg uncertainty principle.

If we use momentum rather than wavenumber, this also effects the normalisation of the wavefunctions

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad \text{and} \quad \langle p | x \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}. \quad (2.29)$$

¹See Mackenzie, arXiv:quant-ph/0004090 section 3 for a brief discussion.

²If you have studied a course in advanced complex methods, this is exactly the argument underlying the saddle point method. The classical path is the path of steepest descent.

The extra factor of \hbar in the square-root corrects the normalisation of the states $|p\rangle$ since they now have a factor of $1/\hbar$ in the exponent.

Energy

We may instead vary t_b while keeping x_b fixed. The change in phase, $\delta S_{\text{cl}}/\hbar$, is now defined to be $-\omega_b \delta t_b$, where ω_b is the frequency. The change in the action is now given by $\delta S_{\text{cl}} = -E_b \delta t_b$ (see Eq. 2.8) which gives as b is arbitrary

$$E = \hbar\omega. \quad (2.30)$$

2.6 Gaussian Integrals

In this course, we will frequently be faced with Gaussian integrals. Before continuing we first collect some useful results which we will use.

For proofs see the problem sheet.

Basic Gaussian integrals

The most basic Gaussian integral is

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \quad (2.31)$$

where a is real and positive. One method to derive this is to square the integral (with another dummy variable y) and then switch to polar coordinates. If a is a complex number, this integral still converges to the same result provided the real part of a is greater than zero.

Gaussian integrals with positive powers of x^2 may be evaluated by differentiating with respect to a . Two examples are:

$$\int_{-\infty}^{\infty} dx x^2 e^{-ax^2} = \frac{1}{2a} \sqrt{\frac{\pi}{a}} \quad \text{and} \quad \int_{-\infty}^{\infty} dx x^4 e^{-ax^2} = \frac{3}{4a^2} \sqrt{\frac{\pi}{a}}. \quad (2.32)$$

Integrals over integrands with odd powers of x multiplying the exponential vanish by anti-symmetry.

If the exponent has a linear term, it is necessary to complete the square to evaluate the integral. One gets:

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \int_{-\infty}^{\infty} dx e^{-a(x-b/2a)^2+b^2/4a} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}, \quad (2.33)$$

again provided the real part of a is greater than zero. This shift is also valid if b is complex, although the evaluation now involves closing a rectangular contour instead of a simple change of variables. We have, for example,

$$\int_{-\infty}^{\infty} dx e^{-ax^2+ikx} = \sqrt{\frac{\pi}{a}} e^{-k^2/4a}. \quad (2.34)$$

This result shows that the Fourier transform of a Gaussian function is itself a Gaussian function!

Again, one can obtain results with additional factors of x^k by differentiating with respect to a and/or b , e.g.

$$\begin{aligned} \int_{-\infty}^{\infty} dx xe^{-ax^2+bx} &= \frac{b}{2a} \sqrt{\frac{\pi}{a}} e^{b^2/4a} \\ \int_{-\infty}^{\infty} dx x^2 e^{-ax^2+bx} &= \frac{1}{2a} \left(1 + \frac{b^2}{2a}\right) \sqrt{\frac{\pi}{a}} e^{b^2/4a}. \end{aligned} \quad (2.35)$$

We will also require results with purely imaginary quadratic terms in the exponent.

Interlude: Note on Principal value of \sqrt{z}

For complex numbers we need to define $z^{1/2}$ (more generally z^α). $z = 0$ is a *branch point* as setting $z = re^{i\phi}$ then for a path circling the origin, z changes by $e^{2\pi i/2}$, ie $z^{1/2}$ is ambiguous.

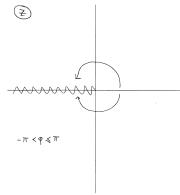


Figure 2.2: Principal value of $z^{1/2}$.

To avoid this take a *branch cut* from 0 to $-\infty$ (convention). By definition you cannot cross this, see Fig. 2.2. We *define* z by

$$z = re^{i\phi}, \quad -\pi < \phi \leq \pi. \quad (2.36)$$

Then $\sqrt{z} = r^{1/2} e^{i\phi/2}$. Here we are interested in

$$\sqrt{-i} \equiv \sqrt{e^{-i\pi/2}} = e^{-i\pi/4}, \quad \sqrt{i} \equiv \sqrt{e^{i\pi/2}} = e^{i\pi/4}. \quad (2.37)$$

Of particular interest for us here is

$$\frac{1}{\sqrt{-i}} = \frac{1}{e^{-i\pi/4}} = e^{i\pi/4} = \sqrt{i}, \quad (2.38)$$

as we shall use many times. Note however that not all operations are allowed for example $\sqrt{-i} = \sqrt{-1}\sqrt{i} = i\sqrt{i}$ is *wrong*. For $\sqrt{-i} = e^{-i\pi/4} = (1-i)/\sqrt{2}$, while $i\sqrt{i} = e^{i\pi/2}e^{i\pi/4} = e^{3i\pi/4} = -(1-i)/\sqrt{2}$. It is easy to find contradictions.

Fresnel integrals

The simplest is the Fresnel integral:

$$\int_{-\infty}^{\infty} dx e^{iax^2} = \sqrt{\frac{\pi}{-ia}} \equiv \sqrt{\frac{i\pi}{a}} \equiv e^{i\pi/4} \sqrt{\frac{\pi}{a}}, \quad (2.39)$$

where again a is real and positive. For $-ve$ a take the complex conjugate. (The result is still valid for complex a provided the imaginary part is strictly positive.)

To evaluate this, from Fig. 2.3 you first consider the integral from 0 to R and

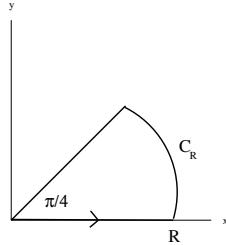


Figure 2.3: Manipulating the Fresnel integral.

evaluate the integral round the contour consisting of this, the straight line at an angle of $\pi/4$ to the real axis and the arc of the circle joining the two to first give $\int_{-\infty}^{\infty} dx e^{iax^2} = e^{i\pi/4} 2 \int_0^R dr e^{-ar^2} + O(1/R)$.

Repeating the procedure of completing the square again yields

$$\int_{-\infty}^{\infty} dx e^{iax^2+ikx} = e^{i\pi/4} \sqrt{\frac{\pi}{a}} e^{-ik^2/4a}. \quad (2.40)$$

2.7 The Free Particle

We will now evaluate the path integral explicitly for the simplest case, that of the free particle. We start with discrete space intervals and will eventually take the

continuum limit. We will use many Gaussian integrals.

The free particle Lagrangian is

$$L = T = \frac{1}{2}m\dot{x}^2 \simeq \frac{1}{2}m\left(\frac{x_{n+1} - x_n}{\epsilon}\right)^2 \quad (2.41)$$

in the discrete approximation. This then gives

$$\langle x_b, t_b | x_a, t_a \rangle = \underbrace{\lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right)}_{I_N} \exp \left\{ \frac{i\epsilon}{\hbar} \frac{m}{2} \sum_{n=0}^N \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 \right\}, \quad (2.42)$$

where $A_N = (\nu(\epsilon))^{N+1}$, Eq. (2.24), is a normalisation constant, which remains to be fixed.

Basic double Gaussian integral

The integrals are a series of nested Gaussian integrals. Each is of the form

$$I = \int_{-\infty}^{\infty} du e^{i(x-u)^2/a} e^{i(u-y)^2/b}. \quad (2.43)$$

We evaluate this by completing the square. A further useful trick is to use translation invariance, here seen by a change of variable $u \rightarrow u + y$ when the integrand is now a function of $x - y$ (rather than x and y separately). Now

$$\frac{1}{a}(x - y - u)^2 + \frac{1}{b}u^2 = \left(\frac{1}{a} + \frac{1}{b} \right) \left(u - \frac{x - y}{a(\frac{1}{a} + \frac{1}{b})} \right)^2 + \frac{(x - y)^2}{a + b}. \quad (2.44)$$

Shifting u again and using Eq. (2.39) we find

$$I = \sqrt{\frac{i\pi ab}{a+b}} \exp \left[i \frac{(x-y)^2}{a+b} \right]. \quad (2.45)$$

Nested Gaussian integrals

We now return to Eq. (2.42) and will evaluate the integrals one at a time. First set $c = 2\hbar\epsilon/m$ and change variables $x_n \rightarrow x'_n = x_n/\sqrt{c}$. Then we have

$$\begin{aligned} I_N &= c^{N/2} \int dx'_1 \dots dx'_N e^{i[(x'_1 - x'_0)^2 + (x'_2 - x'_1)^2 + \dots]} \\ &= c^{N/2} \sqrt{\frac{i\pi 1}{1+1}} \int dx'_2 \dots dx'_N e^{i[(x'_2 - x'_0)^2/2 + (x'_3 - x'_2)^2 + \dots]} \\ &= c^{N/2} \sqrt{\frac{i\pi 1}{2}} \sqrt{\frac{i\pi 2}{3}} \dots \sqrt{\frac{i\pi N}{N+1}} e^{i[(x'_{N+1} - x'_0)^2/(N+1)]} \\ &= \left(\frac{2\pi i\epsilon\hbar}{m} \right)^{N/2} \frac{1}{\sqrt{N+1}} \exp \left\{ i \frac{m}{2\epsilon\hbar(N+1)} (x_b - x_a)^2 \right\}. \end{aligned} \quad (2.46)$$

The evaluation

Thus

$$\langle x_b, t_b | x_a, t_a \rangle = \lim_{N \rightarrow \infty} A_N \left(\frac{2\pi i \epsilon \hbar}{m} \right)^{\frac{N+1}{2}} \sqrt{\frac{m}{2\pi i \hbar (N+1) \epsilon}} \exp \left\{ i \frac{m(x_b - x_a)^2}{2\epsilon \hbar (N+1)} \right\}. \quad (2.47)$$

By definition $(N+1)\epsilon = t_b - t_a = T$. If we now choose ($A_N = \nu(\epsilon)^{N+1}$)

$$\nu(\epsilon) = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \quad \text{such that} \quad A_N \left(\frac{2\pi i \epsilon \hbar}{m} \right)^{\frac{N+1}{2}} = 1, \quad (2.48)$$

(so the limit exists, ie independent of N) we find

$$\langle x_b, t_b | x_a, t_a \rangle = \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left\{ i \frac{m}{2\hbar} \frac{(x_b - x_a)^2}{T} \right\}. \quad (2.49)$$

Re-writing using the classical action

Recall from eq. (2.13) that the classical action for a free particle is

$$S_{\text{cl}} = \frac{m}{2} \frac{(x_b - x_a)^2}{T}. \quad (2.50)$$

We have therefore shown that

$$\langle x_b, t_b | x_a, t_a \rangle = F_0(T) e^{iS_{\text{cl}}/\hbar}, \quad \text{where} \quad F_0(T) = \sqrt{\frac{m}{2\pi i \hbar T}}. \quad (2.51)$$

The notation for the prefactor specifically emphasises that it is now independent of x_a or x_b .

Notes

1. If we then consider variations in (x_b, t_b) (as before) then $\delta S_{\text{cl}} = p(t_b) \delta x_b$, Eq. (2.7) and $\delta S_{\text{cl}} = -E_b \delta t_b$, Eq. (2.8)

$$\langle x_b + \delta x, t_b + \delta t | x_a, t_a \rangle = \langle x_b, t_b | x_a, t_a \rangle e^{(i/\hbar)(p_b \delta x_b - E_b \delta t_b)}. \quad (2.52)$$

This represents a plane wave with momentum p_b and energy $E_b = p_b^2/(2m)$ as expected from the Hamilton-Jacobi equations, Eq. (2.18).

[This also justifies the use of a plane wave in the ‘slit’ question in example sheet I.]

2. We will return to the free particle amplitude again later in the course. It is called the *free-particle Green function*, written

$$G_0(x_b - x_a, t_b - t_a) \equiv \langle x_b, t_b | x_a, t_a \rangle \quad t_b > t_a. \quad (2.53)$$

This makes it clear that it only depends on the differences of the endpoints.

In momentum space:

[FT convention changes!]

$$\begin{aligned} \tilde{G}_0 &= \int_{-\infty}^{\infty} dx e^{ipx/\hbar} G_0(x, t) \\ &= \exp\left(-i \frac{p^2 t}{2m\hbar}\right) = \exp\left(-i \frac{Et}{\hbar}\right), \end{aligned} \quad (2.54)$$

where $E = p^2/2m$ which is a plane wave with classical energy E as expected.

[See also example sheet III.]

3. The normalisation constant $\nu(\epsilon)$ chosen in Eq. (2.48) diverges as $\epsilon \rightarrow 0$. This means the amplitude diverges for infinitesimal time intervals. This occurs because the amplitude at finite times must be finite and this is proportional to

$$\lim_{N \rightarrow \infty} \left(\nu(\epsilon) \sqrt{\frac{2\pi i \hbar \epsilon}{m}} \right). \quad (2.55)$$

This condition means we must have

$$\nu(\epsilon) = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} (1 + \mathcal{O}(\epsilon)), \quad (2.56)$$

and so the only freedom is in the $\mathcal{O}(\epsilon)$ term which goes to zero in the limit $\epsilon \rightarrow 0$.

4. As $\langle x_b, t_b | x_a, t_a \rangle$ is a Gaussian in $x_b - x_a$ with width $\hbar(t_b - t_a)/m$ and unit area with the above normalisation, we recover the orthonormality condition as $t_b \rightarrow t_a$:

$$\langle x_b, t_b | x_a, t_a \rangle \xrightarrow[t_b \rightarrow t_a]{\longrightarrow} \delta(x_b - x_a), \quad (2.57)$$

[A representation of the δ -function is $\lim_{\epsilon \rightarrow 0} \delta_\epsilon(x) \rightarrow \delta(x)$ where $\delta_\epsilon(x) = \sqrt{a/(\pi\epsilon)} \exp(-(a/\epsilon)x^2)$ proved by considering $\int dx f(x)\delta_\epsilon(x)$.]

5. This normalisation also gives the correct completeness condition:

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{-\infty}^{\infty} dx \langle x_b, t_b | x, t \rangle \langle x, t | x_a, t_a \rangle. \quad (2.58)$$

(Use splitting, see Fig. 2.1 and Gaussian result for amplitude.) See example sheet III.

Alternative derivation

There is an alternative derivation which makes the x -independence of the prefactor more explicit. We will consider the quantum fluctuations about the classical path by writing $x(t) = \bar{x}(t) + \eta(t)$, where $\bar{x}(t)$ is the classical path with boundary conditions $x(t_a) = x_a$, $x(t_b) = x_b$ and $\eta(t)$ satisfies $\eta(t_a) = 0 = \eta(t_b)$. We find

$$S[x] = \frac{m}{2} \int_{t_a}^{t_b} dt (\dot{\bar{x}}^2 + \dot{\eta}^2) - 2 \int_{t_a}^{t_b} dt \eta \ddot{\bar{x}} + 2[\eta \dot{\bar{x}}]_{t_a}^{t_b}. \quad (2.59)$$

The last two terms vanish because $\ddot{\bar{x}} = 0$ and $\eta(t_a) = 0 = \eta(t_b)$. As \bar{x} is a fixed path, $dx_n = d\eta_n$ for all n and this gives:

$$\int_{x_a}^{x_b} \mathcal{D}x = \int_0^0 \mathcal{D}\eta. \quad (2.60)$$

We therefore have:

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x e^{iS[x(t)]/\hbar} = e^{iS_{\text{cl}}/\hbar} \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar}. \quad (2.61)$$

The limits on the η -integral merely indicate the boundary conditions. We know that η has no dependence on x_a and x_b and so the η -integral can only depend on t_a and t_b . By translational invariance, we can further deduce that it depends only on their difference and write it as

$$F_0(T) \equiv \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} = \langle 0, t_b | 0, t_a \rangle = \langle 0, T | 0, 0 \rangle. \quad (2.62)$$

The integral can be evaluated explicitly, see example sheet III. Alternatively we have

$$\begin{aligned} \langle 0, T | 0, 0 \rangle &= \int_{-\infty}^{\infty} dx \langle 0, T | x, t \rangle \langle x, t | 0, 0 \rangle \\ \Rightarrow F_0(T) &= \int_{-\infty}^{\infty} dx F_0(T-t) \exp\left(\frac{imx^2}{2\hbar(T-t)}\right) F_0(t) \exp\left(\frac{imx^2}{2\hbar t}\right) \\ &= \sqrt{\frac{2\pi i \hbar (T-t)t}{mT}} F_0(T-t) F_0(t). \end{aligned} \quad (2.63)$$

By inspection $F_0(t) \propto 1/\sqrt{t}$ (or take the limit at large times $T \gg t$ to give $F_0(T-t) \simeq F_0(T)$) and we find

$$F_0(t) = \sqrt{\frac{m}{2\pi i \hbar t}} \quad (2.64)$$

as before. Note we have not performed any discretisation of the path integral here. Although discretisation is often the most convenient method to perform the calculation, it is not essential.

2.8 The Harmonic Oscillator

The Lagrangian for the harmonic oscillator is given by:

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2. \quad (2.65)$$

Once again we will write $x = \bar{x} + \eta$ where \bar{x} is the classical path satisfying $\bar{x}(t_a) = x_a$, $\bar{x}(t_b) = x_b$ and η is the deviation from this satisfying $\eta(t_a) = 0 = \eta(t_b)$. We then find

$$\begin{aligned} S[\bar{x} + \eta] &= \frac{m}{2} \int_{t_a}^{t_b} dt [(\dot{\bar{x}} + \dot{\eta})^2 - \omega^2(\bar{x} + \eta)^2] \\ &= S[\bar{x}] + S[\eta] + m \int_{t_a}^{t_b} dt (\dot{\bar{x}}\dot{\eta} - \omega^2\bar{x}\eta) \\ &= S_{\text{cl}} + S[\eta] + m[\eta\dot{\bar{x}}]_{t_a}^{t_b} - m \int_{t_a}^{t_b} dt \eta(\ddot{\bar{x}} + \omega^2\bar{x}) \\ &= S_{\text{cl}} + S[\eta]. \end{aligned} \quad (2.66)$$

One can show that this result is true for any action where the Lagrangian is quadratic in x .

As in the case of the free particle, we have $\mathcal{D}x = \mathcal{D}\eta$ and therefore

$$\langle x_b, t_b | x_a, t_a \rangle = e^{iS_{\text{cl}}/\hbar} \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} \equiv F_\omega(T) e^{iS_{\text{cl}}/\hbar}, \quad (2.67)$$

where we have again used the fact that the η -integral has no dependence on the position endpoints x_a and x_b to deduce F_ω depends only on the time interval:

$$F_\omega(T) = \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} = \langle 0, T | 0, 0 \rangle. \quad (2.68)$$

The normalisation factor can be evaluated directly by discretising the path integral in x -space or by expanding $\eta(t)$ in a Fourier series, see Feynman and Hibbs section 3.11.

Here, however, we will use the constraint arising from the completeness relation:

$$\langle 0, T | 0, 0 \rangle = \int_{-\infty}^{\infty} dx \langle 0, T | x, t \rangle \langle x, t | 0, 0 \rangle. \quad (2.69)$$

We know from Eq. (2.17) and example sheet II that the classical action is

$$S_{\text{cl}} = \frac{m\omega}{2 \sin \omega T} [(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b]. \quad (2.70)$$

This implies

$$\begin{aligned} F_\omega(T) &= \int_{-\infty}^{\infty} dx F_\omega(T-t) \exp\left(\frac{i m \omega x^2}{2\hbar} \frac{\cos \omega(T-t)}{\sin \omega(T-t)}\right) F_\omega(t) \exp\left(\frac{i m \omega x^2}{2\hbar} \frac{\cos \omega t}{\sin \omega t}\right) \\ &= F_\omega(T-t) F_\omega(t) \sqrt{\frac{2\pi i \hbar \sin \omega(T-t) \sin \omega t}{m \omega \sin \omega T}}. \end{aligned} \quad (2.71)$$

Again by inspection $F_\omega(t) \propto 1/\sqrt{\sin \omega t}$ (or take the limit $T \gg t$ so $F_\omega(T-t) \approx F_\omega(T)$ and $\sin \omega(T-t) \approx \sin \omega T$) and hence

$$F_\omega(t) = \sqrt{\frac{m \omega}{2\pi i \hbar \sin \omega t}}. \quad (2.72)$$

Another important check is that we should reproduce the free particle result when $\omega \rightarrow 0$ and indeed we recover

$$F_\omega(t) \xrightarrow[\omega \rightarrow 0]{} \sqrt{\frac{m}{2\pi i \hbar t}} = F_0(T). \quad (2.73)$$

2.9 The Forced Harmonic Oscillator

The forced harmonic oscillator has an additional linear term in x :

$$L = \frac{1}{2}m(\dot{x}^2 - \omega^2 x^2) + J(t)x, \quad (2.74)$$

where the external force $J(t)$ is non-zero but arbitrary for $t_a \leq t \leq t_b$. The equation of motion for the classical path becomes

$$\ddot{\bar{x}} + \omega^2 \bar{x} = \frac{J}{m}. \quad (2.75)$$

The action still splits into two independent parts in the usual way:

$$\begin{aligned} S[\bar{x} + \eta, J] &= \frac{m}{2} \int dt \left((\dot{\bar{x}} + \dot{\eta})^2 - \omega^2 (\bar{x} + \eta)^2 + \frac{2J}{m} (\bar{x} + \eta) \right) \\ &= S_{\text{cl}}[\bar{x}, J] + S[\eta, 0] + m[\dot{\bar{x}}\eta]_{t_a}^{t_b} - m \int dt \eta (\ddot{\bar{x}} + \omega^2 \bar{x} - (J/m)) \\ &= S_{\text{cl}}[\bar{x}, J] + S[\eta, 0]. \end{aligned} \quad (2.76)$$

(as $\eta(t_a) = 0 = \eta(t_b)$). A very minor modification of the steps for the unforced harmonic oscillator yields:

$$\langle x_b, t_b | x_a, t_a \rangle = F_\omega(T) e^{i S_{\text{cl}}[\bar{x}, J]/\hbar}. \quad (2.77)$$

This is now the classical action for the forced harmonic oscillator, $S_{\text{cl}}[\bar{x}, J]$ (see example sheet II, ghastly!). However the prefactor term, $F_\omega(T)$, is the same as for the unforced harmonic oscillator because the η -term in the split action is independent of J .

2.10 Phase space path integral

Phase space path integral

We will now consider the infinitesimal amplitude for the case of a general potential:

$$L = \frac{1}{2}m\dot{x}^2 - V(x, t). \quad (2.78)$$

The infinitesimal amplitude is given by

$$\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle = \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp \left\{ \frac{i\epsilon}{\hbar} \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 - V(x_n, t_n) \right] \right\}. \quad (2.79)$$

We take the free particle normalisation as the potential is higher order in ϵ , see eg Eq. (2.56). This can also be explicitly checked for the harmonic oscillator, ie Eq. (2.73) where now

$$F_\omega(\epsilon) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega\epsilon}} \rightarrow \sqrt{\frac{m}{2\pi i\hbar\epsilon}} = F_0(\epsilon). \quad (2.80)$$

Now **linearise** the quadratic kinetic term with the identity, ie **Gaussian momentum integral**, or the **Gaussian p -integral**

$$\begin{aligned} & \exp \left\{ \frac{im\epsilon}{2\hbar} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 \right\} \\ &= \sqrt{\frac{2\pi\hbar i\epsilon}{m}} \int_{-\infty}^{+\infty} \frac{dp_n}{2\pi i\hbar} \exp \left\{ -\frac{i\epsilon}{2m\hbar} p_n^2 + \frac{i}{\hbar} p_n (x_{n+1} - x_n) \right\}, \end{aligned} \quad (2.81)$$

which gives

$$\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle = \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \exp \left\{ \frac{ip_n}{\hbar} (x_{n+1} - x_n) - \frac{i\epsilon}{2m\hbar} p_n^2 - \frac{i\epsilon}{\hbar} V(x_n, t_n) \right\} \quad (2.82)$$

One can take this to construct an alternative representation of the path integral known as the **phase space path integral**. Sewing the infinitesimal steps together gives

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_N \langle x_b, t_b | x_N, t_N \rangle \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle \dots \langle x_1, t_1 | x_a, t_a \rangle \\ &= \lim_{N \rightarrow \infty} \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=0}^N \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle \right) \\ &= \lim_{N \rightarrow \infty} \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=0}^N \int \frac{dp_n}{2\pi\hbar} \right) \\ &\quad \times \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{n=0}^N \left[p_n \left(\frac{x_{n+1} - x_n}{\epsilon} \right) - \frac{p_n^2}{2m} - V(x_n, t_n) \right] \right\} \\ &\equiv \int \mathcal{D}x \int \mathcal{D}p \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt (p\dot{x} - H(x, p, t)) \right\}, \end{aligned} \quad (2.83)$$

where H is the classical Hamiltonian. There is now a natural measure in x and p . Also taking the trace, ie setting $x_b = x_a = x$ and integrating over x gives symmetry in x and p phase space.

Another derivation of the free-particle amplitude

The result above gives another derivation of the free-particle amplitude:

$$\begin{aligned} & \langle x_b, t_b | x_a, t_a \rangle \\ &= \lim_{N \rightarrow \infty} \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=0}^N \int \frac{dp_n}{2\pi\hbar} \right) \\ & \quad \times \exp \left\{ \frac{i}{\hbar} \sum_{n=0}^N \left(p_n(x_{n+1} - x_n) - \frac{\epsilon p_n^2}{2m} \right) \right\} \end{aligned} \quad (2.84)$$

Integrating out the x -integrals first gives ($T = t_b - t_a$)

$$\begin{aligned} & \langle x_b, t_b | x_a, t_a \rangle \\ &= \lim_{N \rightarrow \infty} \left(\prod_{n=0}^N \int \frac{dp_n}{2\pi\hbar} \right) \left(\prod_{n=1}^N \delta(p_n - p_{n-1}) \right) \\ & \quad \times \exp \left\{ \frac{i}{\hbar} \left(p_N x_b - p_0 x_a - \frac{\epsilon}{2m} \sum_{n=0}^N p_n^2 \right) \right\} \\ &= \lim_{N \rightarrow \infty} \int_{-\infty}^{\infty} \frac{dp_0}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} p_0(x_b - x_a) - \frac{i}{2m\hbar} (N+1)\epsilon p_0^2 \right\} \\ &= \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left\{ i \frac{m}{2\hbar T} (x_b - x_a)^2 \right\}, \end{aligned} \quad (2.85)$$

where we re-wrote the sum in the first line

$$\sum_{n=0}^N p_n(x_{n+1} - x_n) = p_N x_b - p_0 x_a - \sum_{n=1}^N x_n(p_n - p_{n-1}), \quad (2.86)$$

in order to perform the N integrals over the x_n . The delta function integrals over N momenta p_n leave just one momentum integral and $(N+1)\epsilon = T$.

2.11 Time evolution operator

Momentum normalisation

In section 1.6, we had results for

$$|p\rangle = \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{+ipx/\hbar} |x\rangle, \quad (2.87)$$

giving

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad \text{and} \quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}. \quad (2.88)$$

The extra factor of \hbar in the square-root corrects the normalisation of the states $|p\rangle$, in particular

$$\begin{aligned} \langle p'|p\rangle &= \int_{-\infty}^{+\infty} dx \langle p'|x\rangle \langle x|p\rangle = \int_{-\infty}^{+\infty} \frac{dx}{2\pi\hbar} e^{i(-p'+p)x/\hbar} \\ &= \delta(p' - p), \end{aligned} \quad (2.89)$$

and

$$\int_{-\infty}^{+\infty} dp |p\rangle \langle p| = \hat{1}. \quad (2.90)$$

since they now have a factor of $1/\hbar$ in the exponent.

These are time independent, but can, of course, be considered at a particular time, say t_0 .

Time evolution operator

Let us return to Eq. (2.82) to write

$$\begin{aligned} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \exp \left\{ \frac{ip_n}{\hbar} (x_{n+1} - x_n) \right\} \exp \left\{ -\frac{i\epsilon}{2m\hbar} p_n^2 \right\} \\ &\quad \times \exp \left\{ -\frac{i\epsilon}{\hbar} V(x_n, t_n) \right\}. \end{aligned} \quad (2.91)$$

We now introduce a basis of time-independent momentum and position eigenstates satisfying

$$\hat{p}|p_n\rangle = p_n|p_n\rangle, \quad \text{and} \quad \hat{x}|x_n\rangle = x_n|x_n\rangle, \quad (2.92)$$

and use the results in Eq. (2.88) to write

$$\begin{aligned} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \int_{-\infty}^{\infty} dp_n \underbrace{\langle x_{n+1} | p_n \rangle \langle p_n | x_n \rangle}_{\text{exponential factors}} \exp \left\{ -\frac{i\epsilon}{2m\hbar} p_n^2 \right\} \exp \left\{ -\frac{i\epsilon}{\hbar} V(x_n, t_n) \right\}, \end{aligned} \quad (2.93)$$

where although the states are time independent, we can consider them all to be inserted at time t_0 . Then

$$\begin{aligned} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \int_{-\infty}^{\infty} dp_n \langle x_{n+1} | \exp \left\{ -\frac{i\epsilon}{2m\hbar} \hat{p}^2 \right\} | p_n \rangle \langle p_n | \exp \left\{ -\frac{i\epsilon}{\hbar} V(\hat{x}, t_n) \right\} | x_n \rangle \\ &= \langle x_{n+1} | \exp \left\{ -\frac{i\epsilon}{2m\hbar} \hat{p}^2 \right\} \exp \left\{ -\frac{i\epsilon}{\hbar} V(\hat{x}, t_n) \right\} | x_n \rangle. \end{aligned} \quad (2.94)$$

The exponentials do not commute, however as we neglect $O(\epsilon^2)$ higher terms we can simply expand

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \dots}, \quad (2.95)$$

to add the operators (truncated Baker-Campbell-Hausdorff formula)

$$\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle = \langle x_{n+1} | \exp \left\{ -\frac{i\epsilon}{\hbar} H(\hat{x}, \hat{p}, t_n) \right\} | x_n \rangle, \quad (2.96)$$

where

$$H(\hat{x}, \hat{p}, t) = \frac{\hat{p}^2}{2m} + V(\hat{x}, t) \equiv \hat{H}(t). \quad (2.97)$$

This is the quantum-mechanical analogue of the classical Hamiltonian.

We now put t_{n+1} and t_n back in the exponent

$$\begin{aligned} & \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle \\ &= \langle x_{n+1} | \exp \left\{ -\frac{i}{\hbar} ((t_{n+1} - t_0) - (t_n - t_0)) \hat{H}(t_0) \right\} | x_n \rangle \\ &= \langle x_{n+1} | \exp \left\{ -\frac{i}{\hbar} (t_{n+1} - t_0) \hat{H}(t_0) \right\} \exp \left\{ \frac{i}{\hbar} (t_n - t_0) \hat{H}(t_0) \right\} | x_n \rangle, \end{aligned} \quad (2.98)$$

where t_0 is a further time, which lies infinitesimally close to both t_{n+1} and t_n and can be taken as the time when the states were inserted. We have also approximated $\hat{H}(t_n)$ by $\hat{H}(t_0)$.

Motivated by Eq. (2.98), we write

$$\begin{aligned} |x, t\rangle &= \exp \left\{ \frac{i}{\hbar} (t - t_0) \hat{H}(t_0) \right\} |x\rangle \\ &\equiv \hat{U}^\dagger(t, t_0) |x\rangle, \quad \text{say}. \end{aligned} \quad (2.99)$$

Properties of time evolution operator

Now seek an operator $\hat{U}(t, t_0)$ for **finite** $t - t_0$, with the properties

- \hat{U} unitary as transformation $|x\rangle \rightarrow |x, t\rangle$ basis change, so

$$\hat{U}^\dagger(t, t_0) = \hat{U}^{-1}(t, t_0). \quad (2.100)$$

- Boundary condition: $\hat{U}(t_0, t_0) = \hat{1}$
- Product rule (so we can build a finite time interval from many infinitesimal time intervals)

$$\hat{U}(t, t') \hat{U}(t', t_0) = \hat{U}(t, t_0). \quad (2.101)$$

Implies can also reverse process: set $t = t_0$ in above, $\hat{U}^{-1}(t, t_0) = \hat{U}(t_0, t)$.

\hat{U} is called the **time evolution operator**.

Differential equation

Thus

$$\hat{U}(t + \delta t, t_0) = \hat{U}(t + \delta t, t)\hat{U}(t, t_0) = e^{-i/\hbar\delta t\hat{H}(t)}\hat{U}(t, t_0), \quad (2.102)$$

upon using Eq. (2.99). Expanding gives

$$i\hbar \frac{\partial \hat{U}(t, t_0)}{\partial t} = \hat{H}(t) \hat{U}(t, t_0). \quad (2.103)$$

Explicit time independent (conservative) Hamiltonian

If additionally we have a conservative system, \hat{H} independent of time, (usual case) then have time translation invariance

$$\hat{U}(t, t_0) \equiv \hat{U}(t - t_0). \quad (2.104)$$

For this case we take many time steps – product of U s (or equivalently trivially solve Eq. (2.103)) giving the result for finite $t - t_0$ of

$$\hat{U}(t, t_0) = \exp \left\{ -\frac{i}{\hbar}(t - t_0)\hat{H} \right\}. \quad (2.105)$$

This will be the usual case we consider here.

Explicit time dependent Hamiltonian

It can be shown that in general $\hat{U}(t, t_0)$ obeys

$$\hat{U}(t, t_0) = T \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}(t') \right\}. \quad (2.106)$$

(generalisation of time independent Hamiltonian case, T is time ordering see later).

2.11.1 A useful result

This means that Eq. (2.99) holds for finite $t - t_0$, ie

$$|x, t\rangle = \hat{U}^\dagger(t, t_0)|x\rangle, \quad \langle x, t| = \langle x|\hat{U}(t, t_0), \quad (2.107)$$

(active transformation so inverse action on basis), which means that setting $t = t_0$

$$|x, t_0\rangle \equiv |x\rangle. \quad (2.108)$$

So

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \langle x_b | \hat{U}(t_b, t_0) \hat{U}^\dagger(t_a, t_0) | x_a \rangle \\ &= \langle x_b | \hat{U}(t_b, t_0) \hat{U}(t_0, t_a) | x_a \rangle \\ &= \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle. \end{aligned} \quad (2.109)$$

2.12 Schrödinger equation

Now

$$\psi(x, t) = \langle x, t | \psi \rangle = \langle x | \hat{U}(t, t_0) | \psi \rangle, \quad (2.110)$$

giving from Eq. (2.103),

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \langle x | H(\hat{x}, \hat{p}, t) \hat{U}(t, t_0) | \psi \rangle. \quad (2.111)$$

But $\langle x | \hat{x} = x \langle x |$, $\langle x | \hat{p} = -i\hbar \partial / \partial x \langle x |$, so

$$\begin{aligned} i\hbar \frac{\partial \psi(x, t)}{\partial t} &= H \left(x, -i \frac{\partial}{\partial x}, t \right) \psi(x, t) \\ &\equiv \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t). \end{aligned} \quad (2.112)$$

This is of course **Schrödinger's Equation** – derived as a consequence of the path integral formalism.

The argument is reversible. One can derive Feynman's path integral representation from the Schrödinger equation. In this case, you must assume Schrödinger's equation. This is the path taken by many text books.

2.13 The Schrödinger and Heisenberg Pictures

From Eq. (2.110) we can define a time-dependent state vector $|\psi, t\rangle$ through

$$|\psi, t\rangle = \hat{U}(t, t_0) |\psi\rangle. \quad (2.113)$$

Again setting $t = t_0$ we have

$$|\psi, t_0\rangle \equiv |\psi\rangle, \quad (2.114)$$

From Eq. (2.103), this automatically satisfies the Schrödinger equation:

$$\hat{H} |\psi, t\rangle = i\hbar \frac{\partial}{\partial t} |\psi, t\rangle. \quad (2.115)$$

There is a choice in where we include the time-dependence: either in the state vector or the position eigenstates. In the *Schrödinger picture*, $|\psi, t\rangle$ and $|x\rangle$ are the state vector and the position eigenstate. In the *Heisenberg picture* $|\psi\rangle$ and $|x, t\rangle$ are the equivalent quantities. Both pictures, of course, give the same result.

The Schrödinger Picture

- The state vector $|\psi, t\rangle$ is time dependent; the position eigenstate $|x\rangle$ is time independent
- Operators e.g.

$$\hat{x} = \int dx x|x\rangle\langle x|, \quad (2.116)$$

are time independent

- Sometimes add an S suffix: e.g. \hat{x}_S .

The Heisenberg Picture

- The state vector $|\psi\rangle$ is time independent; the position eigenstate $|x, t\rangle$ is time dependent
- Operators e.g. for \hat{x}

$$\hat{x}(t) = \int dx x|x, t\rangle\langle x, t|, \quad (2.117)$$

are time independent. So using Eq. (2.107) gives

$$\hat{x}(t) = \hat{U}^\dagger(t, t_0)\hat{x}\hat{U}(t, t_0). \quad (2.118)$$

- Sometimes add an H suffix: e.g. $\hat{x}_H(t)$

Further notes

- Similarly for other operators \hat{O}
- All Heisenberg picture states/operators coincide with the Schrödinger picture states/operators at $t = t_0$
- $\psi(x, t)$ unchanged in either picture as

$$\psi(x, t) = \langle x, t|\psi\rangle = \langle x|\psi, t\rangle \quad (2.119)$$

- Expectation values are unchanged

$$\begin{aligned} \underbrace{\langle \psi | \hat{O}(t) | \psi \rangle}_{\text{Heisenberg picture}} &= \langle \psi, t | \hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) \hat{O} \hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) | \psi, t \rangle \\ &= \underbrace{\langle \psi, t | \hat{O} | \psi, t \rangle}_{\text{Schroedinger picture}}. \end{aligned} \quad (2.120)$$

- Now that we have defined the time-evolution of operators, we can derive an equation of motion for them (i.e. their evolution in time). For the position operator we have

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{O}(t) &= \left(i\hbar \frac{\partial \hat{U}^\dagger}{\partial t} \right) \hat{O} \hat{U} + \hat{U}^\dagger \hat{O} \left(i\hbar \frac{\partial \hat{U}}{\partial t} \right) \\
&= -\hat{U}^\dagger \hat{H} \hat{O} \hat{U} + \hat{U}^\dagger \hat{x} \hat{H} \hat{U} \\
&= -\hat{U}^\dagger \hat{H} \hat{U} \hat{U}^\dagger \hat{O} \hat{U} + \hat{U}^\dagger \hat{x} \hat{U} \hat{U}^\dagger \hat{H} \hat{U} \\
&= -\hat{H}_H \hat{O}(t) + \hat{O}(t) \hat{H}_H \\
&= [\hat{O}(t), \hat{H}_H(t)],
\end{aligned} \tag{2.121}$$

where

$$\hat{H}_H(t) = \hat{U}^\dagger(t, t_0) H(\hat{x}, \hat{p}, t) \hat{U}(t, t_0) = H(\hat{x}(t), \hat{p}(t), t). \tag{2.122}$$

Of course, practically, we shall only consider here the case of a time independent Hamiltonian, when $\hat{H}_H = \hat{H}(\hat{x}, \hat{p})$, giving simply

$$i\hbar \frac{\partial}{\partial t} \hat{O}(t) = [\hat{O}(t), \hat{H}]. \tag{2.123}$$

This is the **Heisenberg equation of motion** for the time-evolution of the position operator in the Heisenberg picture.

We describe an operator, \hat{O} as *conserved* if $\partial \hat{O}(t)/\partial t = 0$ which is equivalent to $[\hat{O}(t), \hat{H}] = 0$. For example, momentum is conserved if and only if $[\hat{p}, \hat{H}] = 0$.

For the rest of this course, we will largely adopt the Heisenberg picture.

2.14 Transition Amplitude as Green function

We commented in Section 2.7 (Eq. (2.53)), that the transition amplitude, Eq. (2.109)

$$\langle x_b, t_b | x_a, t_a \rangle = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle, \tag{2.124}$$

is a Green function.

Retarded Green function

Here we show that it is the **retarded Green function** for the Schrödinger Equation. We begin from the completeness relation again:

$$\psi(x, t) = \langle x, t | \psi \rangle = \int dx' \langle x, t | x', t' \rangle \langle x', t' | \psi \rangle. \tag{2.125}$$

Therefore, if we define

$$G(x, x'; t, t') = \begin{cases} \langle x, t | x', t' \rangle & t > t' \\ 0 & t < t' \end{cases}, \quad (2.126)$$

then we have

$$\theta(t - t')\psi(x, t) = \int dx' G(x, x'; t, t')\psi(x', t') \quad \forall t, t'.. \quad (2.127)$$

The (Heaviside) θ -function ensures that we only consider paths in which the particle moves forward in time. We will revisit this when we move to relativistic quantum mechanics.

Since $\psi(x, t)$ is a solution of the Schrödinger equation, we find

$$\begin{aligned} & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) - i\hbar \frac{\partial}{\partial t} \right) \theta(t - t')\psi(x, t) \\ &= 0 - i\hbar \left(\frac{\partial}{\partial t} \theta(t - t') \right) \psi(x, t) = -i\hbar \delta(t - t')\psi(x, t). \end{aligned} \quad (2.128)$$

as $(\partial/\partial t)\theta(t) = \delta(t)$. We now need to solve Eq. (2.127) and Eq. (2.128). As these equations are true for all for all $\psi(x, t)$, this implies

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) - i\hbar \frac{\partial}{\partial t} \right) G(x, x'; t, t') = -i\hbar \delta(t - t')\delta(x - x'). \quad (2.129)$$

This can be seen by multiplying on the right by $\psi(x', t')$ and integrating over x' and then using Eq. (2.127) to give Eq. (2.128).

We have therefore shown that the function G as defined in Eq. (2.126) is indeed a Green function for the Schrödinger equation.

Energy eigenstate representation

In the case of time-independent Hamiltonians it is useful to expand in a basis of energy eigenstates, $|n\rangle$:

$$\hat{H}|n\rangle = E_n|n\rangle \quad (2.130)$$

and we also define the shorthand $u_n(x) \equiv \langle x|n\rangle$. Then for $t > 0$, the Green function is

$$\begin{aligned} G(x, y; t) &\equiv \langle x, t | y, 0 \rangle = \langle x | e^{-it\hat{H}/\hbar} | y \rangle \\ &= \sum_n \langle x | e^{-it\hat{H}/\hbar} | n \rangle \langle n | y \rangle \\ &= \sum_n e^{-itE_n/\hbar} u_n(x) u_n^*(y). \end{aligned} \quad (2.131)$$

Furthermore note that we G contains **all** the information about the wavefunctions/energy eigenstates, which is possibly why path integrals are more complicated than say solving the Schrödinger equation.

We now define the Fourier Transform of $G(x, y; t)$ with respect to t as $\tilde{G}(x, y; E)$ given by

$$\tilde{G}(x, y; E) = \int_{-\infty}^{\infty} dt e^{itE/\hbar} G(x, y; t) e^{it(i\epsilon)/\hbar}. \quad (2.132)$$

The $i\epsilon \equiv i0^+$ prescription is introduced to ensure that the integral converges for positive real energies at the upper limit. Substituting in Eq. (2.131) gives

$$\begin{aligned} \tilde{G}(x, y; E) &= \sum_n \int_0^{\infty} dt e^{it(E-E_n)/\hbar} u_n(x) u_n^*(y) e^{it(i\epsilon)/\hbar} \\ &= i\hbar \sum_n \frac{u_n(x) u_n^*(y)}{E - E_n + i\epsilon}. \end{aligned} \quad (2.133)$$

Bound states correspond to poles in $\tilde{G}(x, y; E)$ which lie just below the real axis in the complex E -plane. This ensures that when we perform the inverse Fourier transform,

$$G(x, y; t) = \int_{-\infty}^{+\infty} \frac{dE}{2\pi} e^{-i/\hbar Et} \tilde{G}(x, y; E), \quad (2.134)$$

we close in the upper-half E plane for $t < 0$ (Jordan's Lemma) to recover the retarded or causal Green function (i.e. $G(x, y; t) = 0$ for $t < 0$).

[Technical note: $i\epsilon$ prescription also helps in path integral. e.g. for SHO, $E_n \rightarrow E_n - i\epsilon$, so $\omega \rightarrow \omega - i\epsilon$ ($\omega > 0$). Then $\omega^2 \rightarrow \omega^2 - 2i\epsilon$ so $S[x] \rightarrow S[x] + i\epsilon m \int dt x^2$, so damping factor $\exp(-\epsilon m/\hbar \int dt x^2)$.]

The trace

If we take $x = y$, and integrate over x (i.e. trace) we find

$$\begin{aligned} \int_{-\infty}^{\infty} dx \langle x, t | x, 0 \rangle &= \int dx G(x, x; t) \\ &= \sum_n e^{-itE_n/\hbar} \int dx |u_n(x)|^2 \\ &= \sum_n e^{-itE_n/\hbar} \end{aligned} \quad (2.135)$$

for orthonormal energy eigenfunctions $u_n(x)$. Then if we know $G(x, y; t)$ we can use this expression to deduce the energy eigenvalues.

For example, consider the harmonic oscillator:

$$\int_{-\infty}^{\infty} dx \langle x, t | x, 0 \rangle = \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega t}} \exp \left\{ \frac{im\omega}{2\hbar \sin \omega t} 2x^2 (\cos \omega t - 1) \right\}, \quad (2.136)$$

where we have substituted the classical action from Eq. (2.17). Performing the Gaussian integral gives

$$\begin{aligned} \int_{-\infty}^{\infty} dx \langle x, t | x, 0 \rangle &= \frac{1}{2i} \frac{1}{\sin \frac{\omega t}{2}} \\ &= \frac{e^{-i\omega t/2}}{1 - e^{-i\omega t}} = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} \\ &= \sum_n e^{-itE_n/\hbar}. \end{aligned} \quad (2.137)$$

It therefore follows that $E_n = (n + 1/2)\hbar\omega$. The eigenfunctions may also be deduced in this way (see example sheet).

2.15 Statistical Mechanics

We have

$$F = -kT \ln Z, \quad \beta = 1/kT. \quad (2.138)$$

- The Helmholtz free energy, F , determines thermodynamic properties of the system, e.g,

$$F = U - TS, \quad dU = Tds - pdV, \quad (2.139)$$

giving

$$S = - \left. \frac{\partial F}{\partial T} \right|_V, \quad p = - \left. \frac{\partial F}{\partial V} \right|_T, \quad (2.140)$$

- Z is the (microscopic) partition function, defined by

$$Z = \sum_n e^{-\beta E_n} = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle \equiv \text{tr} e^{-\beta \hat{H}}. \quad (2.141)$$

So e.g. $U = \langle \hat{H} \rangle = -\partial/\partial\beta \ln Z = \partial/\partial\beta(\beta F)$

Now we have already derived

$$\int_{-\infty}^{+\infty} dx \langle x, t | x, 0 \rangle = \sum_n e^{-i/\hbar E_n t}. \quad (2.142)$$

So comparing gives

$$Z = \int_{-\infty}^{+\infty} dx \langle x, -i\beta\hbar | x, 0 \rangle. \quad (2.143)$$

- Propagator at $-ve$ imaginary time related to partition function

- Discussed for one degree of freedom (1-dof).

For $N \sim 10^{26} \sim$ Avogadro's number, then 10^{26} path integrals for $\langle \vec{x}, -i\beta\hbar | \vec{x}, 0 \rangle$.

For non-interacting particles $Z \rightarrow Z^N$

- Classical limit (for completeness)

Trace is basis independent in Eq. (2.141); or use \hat{U} in Eq. (2.143) to give

$$\begin{aligned} Z &= \int dx \langle x | e^{-\beta H(\hat{x}, \hat{p})} | x \rangle = \int dx \langle x | e^{-\beta(\hat{p}^2/2m + V(\hat{x}))} | x \rangle \\ &= \int dx \langle x | e^{-\beta\hat{p}^2/2m} e^{-\beta V(\hat{x})} | x \rangle + O(\hbar) \quad \text{as } [\hat{x}, \hat{p}] = i\hbar \\ &= \int dx dp \langle x | e^{-\beta\hat{p}^2/2m} | p \rangle \langle p | e^{-\beta V(\hat{x})} | x \rangle + O(\hbar) \\ &= \int dx dp \langle x | p \rangle \langle p | x \rangle e^{-\beta H(x, p)} + O(\hbar) \end{aligned} \quad (2.144)$$

But $\langle x | p \rangle = e^{i/\hbar px} / \sqrt{2\pi}$ so we finally have

$$Z = \int \frac{dx dp}{2\pi\hbar} e^{-\beta H(x, p)} + O(\hbar). \quad (2.145)$$

(Note: this is *not* a path integral!) Classical phase space partition function, with correct normalisation $2\pi\hbar = h$

- For path integral, write $t = -i\tau$

[Alternatively $t = -i\hbar\tau$]

Then $L = \frac{1}{2}m(dx/dt)^2 - V(x) = -[\frac{1}{2}m(dx/d\tau)^2 + V(x)] \equiv -L_E$ (Euclidean).

Particle now moves in an inverted potential

Also $i/\hbar \int_0^t dt dL \rightarrow i/\hbar \int_0^{\hbar\beta} (-id\tau)(-L_E)$.

So

$$Z = \int dx \int_x^x Dx(\tau) e^{-i/\hbar \int_0^{\hbar\beta} d\tau L_E}. \quad (2.146)$$

$[\hbar\beta$ interplay between temperature and quantum effects.]

- If don't take trace, then have *density matrix*

$$\rho(x, y) = \sum_n e^{-\beta E_n} u_n(x) u_n^*(y). \quad (2.147)$$

Contains all knowledge of statistical system

- SHO example – as before

$$\begin{aligned} Z &= \int_{-\infty}^{+\infty} dx \langle x, -i\hbar\beta | x, 0 \rangle = \frac{1}{2i} \frac{1}{\sin(-\frac{1}{2}i\hbar\beta)} \\ &= \frac{1}{2 \sinh(\frac{1}{2}\hbar\omega\beta)}. \end{aligned} \quad (2.148)$$

Expand out as before to give $E_n = (n + \frac{1}{2})\hbar\omega$.

2.16 Single Particle in an Electromagnetic Field

Heaviside–Lorentz units – background information

We use here Heaviside–Lorentz units, as they get the units correct (e.g. x and ct in equations); the $4\pi s$ are in the solutions not the field equations and for QFT simply set $c \rightarrow 1$, ‘natural units’.

Conversion factors from SI units to Heaviside–Lorentz units

$$\vec{E} = \sqrt{\epsilon_0} \vec{E}_{SI}, \quad \vec{B} = c\sqrt{\epsilon_0} \vec{B}_{SI}, \quad (2.149)$$

and

$$\rho = \frac{1}{\sqrt{\epsilon_0}} \rho_{SI}, \quad \vec{j} = \frac{1}{\sqrt{\epsilon_0}} \vec{j}_{SI}, \quad [e = \frac{1}{\sqrt{\epsilon_0}} e_{SI}], \quad (2.150)$$

($c = 1/\sqrt{\epsilon_0\mu_0}$) giving Maxwell’s equations as

$$\begin{aligned} \vec{\nabla} \cdot \vec{E} &= \rho \\ \vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} &= 0 \\ \vec{\nabla} \cdot \vec{B} &= 0 \\ \vec{\nabla} \times \vec{B} &= \frac{1}{c} \vec{j} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t}. \end{aligned} \quad (2.151)$$

For the potentials $\phi(\vec{r}, t)$ which is the electric potential (also known as the ‘scalar’ or ‘electrostatic’ potential) and $\vec{A}(\vec{r}, t)$ which is the magnetic vector potential we have

[notation: either \vec{r} or \vec{x}]

$$\phi = \sqrt{\epsilon_0} \phi_{SI}, \quad \vec{A} = c\sqrt{\epsilon_0} \vec{A}_{SI}. \quad (2.152)$$

Then

$$\vec{E} = -\vec{\nabla} \phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \quad \text{and} \quad \vec{B} = \vec{\nabla} \times \vec{A}. \quad (2.153)$$

Lagrangian

The Lagrangian for a particle of charge e in an electromagnetic field is

$$L(\vec{r}, \dot{\vec{r}}, t) = \frac{1}{2}m\dot{\vec{r}}^2 - e\phi + \frac{e}{c}\dot{\vec{r}} \cdot \vec{A}, \quad (2.154)$$

giving for the Lorentz force

[Check this]

$$\vec{F} = m\ddot{\vec{r}} = e \left[\vec{E} + \frac{\dot{\vec{r}}}{c} \times \vec{B} \right].$$

This gives the following classical Hamiltonian:

$$H(\vec{r}, \vec{p}, t) = \frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 + e\phi, \quad (2.155)$$

which you should also check. [Remember that $p_i = \partial L / \partial \dot{r}_i$ and $H(\vec{r}, \vec{p}) = \vec{p} \cdot \dot{\vec{r}} - L$.]

[See also 'Hamiltonian Dynamics']

Gauge Invariance

Classically, the \vec{E} and \vec{B} fields (and then the classical path) are unchanged under the *gauge transformation*

$$\vec{A} \rightarrow \vec{A} + \vec{\nabla}\chi \quad \text{and} \quad \phi \rightarrow \phi - \frac{1}{c} \frac{\partial \chi}{\partial t}, \quad (2.156)$$

for any function $\chi(\vec{r}, t)$. This reflects a degree of freedom within the mathematical description.

The Lagrangian, however, *does* change under this transformation:

$$L \rightarrow L + \frac{e}{c} \left(\frac{\partial \chi}{\partial t} + \dot{\vec{r}} \cdot \vec{\nabla}\chi \right) = L + \frac{e}{c} \frac{d\chi}{dt}. \quad (2.157)$$

However, adding a total derivative to the Lagrangian doesn't change the Lagrange equations of motion as extra term in Lagrangian equation of motion gives

$$\frac{d}{dt} \frac{\partial}{\partial \dot{r}_i} \left(\frac{d\chi}{dt} \right) - \frac{\partial}{\partial r_i} \left(\frac{d\chi}{dt} \right) = \frac{d}{dt} \frac{\partial \chi}{\partial r_i} - \frac{d}{dt} \frac{\partial \chi}{\partial r_i} = 0. \quad (2.158)$$

This means that any classical physics is *gauge invariant*.

But the action changes by the addition of some boundary terms

$$\begin{aligned} S &= \int_{t_a}^{t_b} dt L \rightarrow S + \int_{t_a}^{t_b} dt \frac{d\chi}{dt} \\ &= S + \frac{e}{c} (\chi(\vec{r}_b, t_b) - \chi(\vec{r}_a, t_a)). \end{aligned} \quad (2.159)$$

(So, alternatively, can say that as endpoints fixed then $\delta S = 0$ gives unaltered equations of motion.) This therefore also changes the transition amplitude

$$\langle \vec{r}_b, t_b | \vec{r}_a, t_a \rangle \rightarrow \exp \left\{ \frac{ie}{\hbar c} (\chi(\vec{r}_b, t_b) - \chi(\vec{r}_a, t_a)) \right\} \int_{\vec{r}_a}^{\vec{r}_b} \mathcal{D}\vec{r} e^{\frac{i}{\hbar} S}. \quad (2.161)$$

We therefore deduce that

$$|\vec{r}, t\rangle \rightarrow \exp \left\{ -\frac{ie}{\hbar c} \chi(\vec{r}, t) \right\} |\vec{r}, t\rangle, \quad (2.162)$$

is an independent phase change *locally* at every point in space and time. The transition probability though, $|\langle \vec{r}_b, t_b | \vec{r}_a, t_a \rangle|^2$, is of course, unchanged. This is a symmetry of the theory, and is known as a $U(1)$ local gauge symmetry.

2.17 The Aharonov-Bohm Effect

This quantum effect was first observed in 1960.

The setup is again the double slit experiment, where now there is a magnetic field in the centre (e.g. a long thin solenoid), see Fig. 2.4. The magnetic field, \vec{B} , is

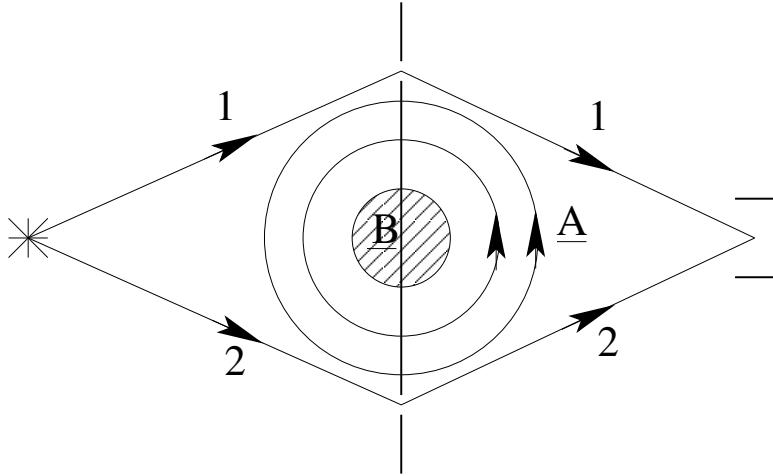


Figure 2.4: The set-up for the Aharonov-Bohm Effect. There is a long thin solenoid in the centre (shaded area). The field lines of the magnetic potential are the circles around this.

non-zero in the shaded area only (say pointing out of paper) and we will assume the particles are shielded from it perfectly. The \vec{B} field corresponds to a magnetic vector potential \vec{A} whose field lines form circle around the solenoid as shown.

In the absence of the field, we add the amplitudes as usual to get

$$e^{\frac{i}{\hbar} S[1]} + e^{\frac{i}{\hbar} S[2]} = e^{\frac{i}{\hbar} S[1]} \left(1 + e^{\frac{i}{\hbar} (S[2] - S[1])} \right). \quad (2.163)$$

Interference then arises from the relative phase $\delta\phi = (S[2] - S[1])/\hbar$.

We now add the (time-independent) magnetic field, and following the previous section, this adds an \vec{A} -term to the Lagrangian:

$$L \rightarrow L + \frac{e}{c} \dot{\vec{r}} \cdot \vec{A}. \quad (2.164)$$

Then

$$\begin{aligned} S &\rightarrow S + \frac{e}{c} \int_{t_a}^{t_b} dt \frac{d\vec{r}}{dt} \cdot \vec{A} \\ &= S + \frac{e}{c} \int_{\vec{r}_a}^{\vec{r}_b} d\vec{r} \cdot \vec{A}, \end{aligned} \quad (2.165)$$

where the integral with measure $d\vec{r}$ represents a line integral along path 1 or 2.

As the action changes and changes differently for every path, this alters the phase of each path and therefore also the relative phase. We find

$$\begin{aligned} \delta\phi &= \frac{e}{\hbar c} \left(\int_{C_2} \vec{A} \cdot d\vec{r} - \int_{C_1} \vec{A} \cdot d\vec{r} \right) \\ &= \frac{e}{\hbar c} \oint_C \vec{A} \cdot d\vec{r} \equiv \frac{e}{\hbar c} \Phi, \end{aligned} \quad (2.166)$$

where C is the closed path formed of path 2 and path 1 reversed.

The magnetic field is zero everywhere along this path, but the closed path does enclose the region of magnetic field. Stokes' theorem gives

$$\begin{aligned} \Phi &= \oint_C \vec{A} \cdot d\vec{r} = \int_S \vec{\nabla} \times \vec{A} \cdot d\vec{S} \\ &= \int_S \vec{B} \cdot d\vec{S}, \end{aligned} \quad (2.167)$$

valid for any surface S bounded by the closed curve C .

This gives Φ is the total magnetic flux flowing between the two paths. This means the interference pattern shifts due to the relative phase shift $(e/\hbar c)\Phi$ when the field is turned on, even though the particle doesn't pass through any region of non-zero magnetic field, and therefore doesn't feel any electromagnetic forces!

The phase change Φ is gauge-invariant: if $\vec{A} \rightarrow \vec{A} + \vec{\nabla}\chi$,

$$\Phi \rightarrow \Phi + \oint_C \vec{\nabla}\chi \cdot d\vec{r} = \Phi + \oint_C d\chi = \Phi + 0 = \Phi. \quad (2.168)$$

The effect is periodic: there is no effect if $\delta\phi = 2\pi n$ which corresponds to

$$\Phi = 2\pi n \frac{\hbar c}{e} = n \frac{hc}{e}, \quad n = 0, \pm 1, \pm 2, \dots \quad (2.169)$$

Discretised form of path integral – need ‘mid point’ rule i.e. $(x_n + x_{n+1})/2$ rather than just x_n for \vec{A} in velocity dependent potential. See example sheet VI.

2.18 Transition Elements

We have derived the transition amplitude

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x e^{\frac{i}{\hbar} S[x]}. \quad (2.170)$$

We are also interested in the path integral weighted by a function(al) of $x(t)$. The simplest example is ($t_a < t < t_b$)

$$\begin{aligned} \langle x(t) \rangle &\equiv \int_{x_a}^{x_b} \mathcal{D}x x(t) e^{\frac{i}{\hbar} S[x]} \\ &= \int_{-\infty}^{\infty} dx \int_x^{x_b} \mathcal{D}x'' \int_{x_a}^x \mathcal{D}x' \exp \left\{ \frac{i}{\hbar} \int_t^{t_b} L'' dt'' \right\} x \exp \left\{ \frac{i}{\hbar} \int_{t_a}^t L' dt' \right\} \\ &= \int dx \langle x_b, t_b | \hat{x}(t) | x, t \rangle \langle x, t | x_a, t_a \rangle \\ &= \langle x_b, t_b | \hat{x}(t) | x_a, t_a \rangle. \end{aligned} \quad (2.171)$$

(Sometimes, for clarity, might add a subscript S for the action used.)

This is the *matrix element* of the operator $\hat{x}(t)$ between the states $|x_a, t_a\rangle$ and $|x_b, t_b\rangle$ in the Heisenberg picture. It is a non-trivial function of t .

This is an important result as it shows the connection between path integrals and operators.

Similarly we can show

$$\langle x_b, t_b | f(\hat{x}(t)) | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x f(x(t)) e^{\frac{i}{\hbar} S[x]}, \quad (2.172)$$

for any function of $x(t)$.

Time ordered products

Now consider correlations between two factors of x at different times t and t' .

- For $t > t'$

$$\begin{aligned}
\langle x(t)x(t') \rangle &\equiv \int_{x_a}^{x_b} \mathcal{D}x \ x(t)x(t')e^{\frac{i}{\hbar}S} \\
&= \int dx \int dx' \langle x_b, t_b | x, t \rangle x \langle x, t | x', t' \rangle x' \langle x', t' | x_a, t_a \rangle \\
&= \langle x_b, t_b | \hat{x}(t) \hat{x}(t') | x_a, t_a \rangle.
\end{aligned} \tag{2.173}$$

- For $t < t'$, we get the same result but with $t \leftrightarrow t'$

$$\langle x(t)x(t') \rangle = \langle x_b, t_b | \hat{x}(t') \hat{x}(t) | x_a, t_a \rangle. \tag{2.174}$$

These two results are not equivalent because the Heisenberg-picture operators $\hat{x}(t)$ and $\hat{x}(t')$ do not commute.

We combine the two results by writing

$$\langle x(t)x(t') \rangle = \langle x_b, t_b | T(\hat{x}(t) \hat{x}(t')) | x_a, t_a \rangle, \tag{2.175}$$

where we define the **time-ordered product** as

$$T(\hat{x}(t) \hat{x}(t')) \equiv \theta(t - t') \hat{x}(t) \hat{x}(t') + \theta(t' - t) \hat{x}(t') \hat{x}(t). \tag{2.176}$$

In each term, the operator at the earlier time appears on the right of the one at the later time.

This is easily generated to any number of local insertions:

$$\begin{aligned}
\langle f_1(x(t)) \dots f_n(x(t_n)) \rangle &= \int_{x_a}^{x_b} \mathcal{D}x \ f_1(\hat{x}(t_1)) \dots f_n(\hat{x}(t_n)) e^{\frac{i}{\hbar}S[x(t)]} \\
&= \langle x_b, t_b | T(f_1(\hat{x}(t_1)) \dots f_n(\hat{x}(t_n))) | x_a, t_a \rangle.
\end{aligned} \tag{2.177}$$

The difference between the two lines is that the quantities $f_i(x(t_i))$ on the first line are normal commuting functions, while the quantities $f_i(\hat{x}(t_i))$ on the right-hand side of the second line are non-commuting operators.

The time-ordering operator orders *all* of the operators in the product according to time (with the earliest at the right and latest at the left).

Time ordered products between general states

We may also consider the time-ordered product between more general states. For example,

$$\begin{aligned}
\langle \psi | T(\hat{x}(t_1) \dots \hat{x}(t_n)) | \phi \rangle &= \int dx_a \int dx_b \langle \psi | x_b, t_b \rangle \langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_n)) | x_a, t_a \rangle \langle x_a, t_a | \phi \rangle \\
&= \int dx_a \int dx_b \psi^*(x_b, t_b) \phi(x_a, t_a) \int_{x_a}^{x_b} \mathcal{D}x \ x(t_1) \dots x(t_n) e^{iS/\hbar}.
\end{aligned} \tag{2.178}$$

We can now recognise the integral on the right as a transition element, $\langle x(t_1) \dots x(t_n) \rangle$. These will play a central rôle in all that follows (they are also known as matrix elements or Green functions or correlation functions).

Including time derivatives

We will also want to consider transition elements with time derivatives of x .

We start by returning to our first definition of a path integral

$$\begin{aligned} & \langle x_b, t_b | x_a, t_a \rangle \\ &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{n=0}^N \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 - V(x_n, t_n) \right] \right\}, \end{aligned} \quad (2.179)$$

($x_0 = x_a$, $x_{N+1} = x_b$). The integral

$$\int_{-\infty}^{\infty} dx_k \frac{\partial}{\partial x_k} f(x_k) = 0, \quad (2.180)$$

for any function $f(x_k)$ which approaches zero sufficiently quickly as $|x_k| \rightarrow \infty$. We have, for any $k = 1, \dots, N$ and function F ,

$$\begin{aligned} 0 &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \times \\ &\quad \frac{\partial}{\partial x_k} \left[F(x_k) \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{n=0}^N \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 - V(x_n, t_n) \right] \right\} \right] \\ &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \times \\ &\quad \left[\frac{\partial F(x_k)}{\partial x_k} - \frac{i\epsilon}{\hbar} F(x_k) \left\{ \frac{m}{\epsilon^2} (x_{k+1} - 2x_k + x_{k-1}) + \frac{\partial V}{\partial x_k} \right\} \right] \exp \{ \dots \}. \end{aligned} \quad (2.181)$$

So we can write (slightly sloppily)

$$0 = \lim_{\epsilon \rightarrow 0} \left\langle \left[\frac{\partial F(x_k)}{\partial x_k} - \frac{i\epsilon}{\hbar} F(x_k) \left\{ \frac{m}{\epsilon} \left(\frac{x_{k+1} - x_k}{\epsilon} - \frac{x_k - x_{k-1}}{\epsilon} \right) + \frac{\partial V}{\partial x_k} \right\} \right] \right\rangle, \quad (2.182)$$

where the brackets mean, of course, the path integral

$$\langle O \rangle = \int_{x_a}^{x_b} Dx O e^{\frac{i}{\hbar} S}. \quad (2.183)$$

(Might also need to add a damping factor for convergence in the exponential.)

We will also need as $\epsilon \rightarrow 0$

$$\langle x_k \rangle \rightarrow \langle x(t) \rangle, \quad (2.184)$$

and

$$\begin{aligned} \left\langle \frac{1}{\epsilon}(x_{k+1} - x_k) \right\rangle &\rightarrow \langle \dot{x}(t + \epsilon/2) \rangle \rightarrow \langle \dot{x}(t) \rangle \\ \left\langle \frac{1}{\epsilon} \left(\frac{1}{\epsilon}(x_{k+1} - x_k) - \frac{1}{\epsilon}(x_k - x_{k-1}) \right) \right\rangle &\rightarrow \left\langle \frac{1}{\epsilon} (\dot{x}(t + \epsilon/2) - \dot{x}(t - \epsilon/2)) \right\rangle \rightarrow \langle \ddot{x}(t) \rangle. \end{aligned} \quad (2.185)$$

Ehrenfest's theorem

Now set $F = 1$, so in Eq. (2.182), then $\mathcal{O}(\epsilon)$ terms yield

$$\langle \ddot{x} \rangle = -\frac{1}{m} \left\langle \frac{\partial V}{\partial x} \right\rangle. \quad (2.186)$$

This is **Ehrenfest's Theorem**: the quantum version of Newton's classical equation of motion.

Operators from the path integral

Now take $F(x_k) = x_k$.

However, as we have $\dot{x} = p/m$ and now \hat{p} and \hat{x} do not commute, we will see that we must take care. From Eq. (2.182)

$$0 = \lim_{\epsilon \rightarrow 0} \left\langle 1 - \frac{i}{\hbar} \left\{ mx_k \left[\frac{x_{k+1} - x_k}{\epsilon} - \frac{x_k - x_{k-1}}{\epsilon} \right] + \epsilon x_k \frac{\partial V}{\partial x_k} \right\} \right\rangle. \quad (2.187)$$

As before ($m\dot{x} = p$)

$$0 = \left\langle 1 - \frac{i}{\hbar} x(t) [p(t + \epsilon/2) - p(t - \epsilon/2)] \right\rangle. \quad (2.188)$$

The explicit values of the time components make the operation unique and we finally derive

$$\langle x_b, t_b | \left\{ 1 - \frac{i}{\hbar} (\hat{p}(t) \hat{x}(t) - \hat{x}(t) \hat{p}(t)) \right\} | x_a, t_a \rangle = 0 \quad (t_a < t < t_b). \quad (2.189)$$

This immediately gives the usual equal-time commutation relation

$$[\hat{x}(t), \hat{p}(t)] = i\hbar. \quad (2.190)$$

In order to get this correct, we had to be careful with the ordering of \hat{x} and \hat{p} in time.

Zitterbewegung

However

$$\left\langle x_k \left(\frac{x_k - x_{k-1}}{\epsilon} \right) \right\rangle = \left\langle x_{k+1} \left(\frac{x_{k+1} - x_k}{\epsilon} \right) \right\rangle + \mathcal{O}(\epsilon). \quad (2.191)$$

(Everything just shifted by ϵ .) This means it is also valid to write Eq. (2.187) as

$$0 = \left\langle 1 - \frac{i}{\hbar} m \left[x_k \frac{x_{k+1} - x_k}{\epsilon} - x_{k+1} \frac{x_{k+1} - x_k}{\epsilon} \right] \right\rangle + \mathcal{O}(\epsilon). \quad (2.192)$$

This then leads to

$$\left\langle m \left(\frac{x_{k+1} - x_k}{\epsilon} \right)^2 \right\rangle = -\frac{\hbar}{i\epsilon} \langle 1 \rangle + \mathcal{O}(1). \quad (2.193)$$

Upon taking the limit $\epsilon \rightarrow 0$ in this expression, we find $\langle \dot{x}(t)^2 \rangle$ or $\langle p(t)^2 \rangle$ is infinite!

This means that the paths we integrate over are not smooth. The action is finite so from Eq. (2.179), we deduce $\epsilon(\delta x/\epsilon)^2$ is finite which gives

$$\delta x \sim \sqrt{\epsilon}, \quad \delta \dot{x} \sim 1/\sqrt{\epsilon}. \quad (2.194)$$

This means the paths are continuous, but jagged.

This phenomenon is called *Zitterbewegung* (“trembling motion”).

[See Feynman+Hibbs p177]

Defining the kinetic energy

This raises a problem for the definition of the kinetic energy.

- We can do this consistently by defining it as

$$\lim_{\epsilon \rightarrow 0} \frac{m}{2} \left\langle \left(\frac{x_{k+1} - x_k}{\epsilon} \right) \left(\frac{x_k - x_{k-1}}{\epsilon} \right) \right\rangle = \lim_{\epsilon \rightarrow 0} \frac{1}{2m} \langle p(t + \epsilon/2)p(t - \epsilon/2) \rangle, \quad (2.195)$$

i.e. taking the momentum functions slightly separated in time.

We can show that this *is* finite by taking $F(x_k) = x_{k+1} - x_k$ in the general result given below Eq. (2.182). This leads to

$$-\langle 1 \rangle = \frac{i\epsilon m}{\hbar} \left\langle \left(\frac{x_{k+1} - x_k}{\epsilon} \right) \left(\frac{x_{k+1} - x_k}{\epsilon} - \frac{x_k - x_{k-1}}{\epsilon} \right) + \underbrace{(x_{k+1} - x_k) \frac{\partial V}{\partial x_k}}_{O(\epsilon)} \right\rangle. \quad (2.196)$$

The potential term is subdominant in ϵ . Separating the other two terms gives

$$\begin{aligned} \frac{1}{2m} \langle p(t + \epsilon/2)p(t - \epsilon/2) \rangle &= \frac{m}{2} \left\langle \left(\frac{x_{k+1} - x_k}{\epsilon} \right)^2 \right\rangle + \frac{\hbar}{2i\epsilon} \langle 1 \rangle + \mathcal{O}(\epsilon) \\ &= -\frac{\hbar}{2i\epsilon} \langle 1 \rangle + \mathcal{O}(1) + \frac{\hbar}{2i\epsilon} \langle 1 \rangle + \mathcal{O}(\epsilon) \\ &= \mathcal{O}(1) + \mathcal{O}(\epsilon), \end{aligned} \quad (2.197)$$

upon using Eq. (2.193). The divergent terms in ϵ cancel each other and the limit $\epsilon \rightarrow 0$ exists.

This is an example of renormalisation in quantum mechanics.

The method of choosing different times for the factors $p(t)$ is known as *point-splitting regularisation*.

- Following for completeness only:

Alternatively use the *virial theorem* from classical dynamics,

$$\langle p \frac{\partial H}{\partial p} \rangle = \langle x \frac{\partial H}{\partial x} \rangle, \quad (2.198)$$

So here we have with $H = p^2/2m + V(x)$

$$\frac{1}{2m} \langle p^2 \rangle = \frac{1}{2} \langle x V'(x) \rangle. \quad (2.199)$$

and use the RHS instead of the LHS.

Key Concepts

1. The Feynman Path Integral for a transition amplitude between $|x_a, t_a\rangle$ and $|x_b, t_b\rangle$ is

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x e^{\frac{i}{\hbar} S[x(t)]}.$$

2. Normalisation factors can be evaluated directly or via the constraint from the completeness relation.
3. Actions derived from Lagrangians which are quadratic in x satisfy $S[\bar{x} + \eta] = S_{\text{cl}} + S[\eta]$, where $\bar{x}(t)$ is the classical path and $\eta(t)$ satisfies $\eta(t_{a,b}) = 0$. This can sometimes simplify the action, e.g. the forced harmonic oscillator.
4. It is possible to derive the Schrödinger equation from the expression for the amplitude in point (1) and vice versa.

5. There are two pictures to describe the evolution of a quantum system in time. In the Schrödinger picture, the time dependence appears in the states $|\psi, t\rangle$ while eigenstates (and hence operators) are time-independent, e.g. $|x\rangle$. In the Heisenberg picture, states are time-independent, $|\psi\rangle$, while eigenstates and operators evolve in time.
6. The transition element, $\langle x(t) \rangle = \langle x_b, t_b | \hat{x}(t) | x_a, t_a \rangle$. More generally,

$$\langle f(x(t_1)) \dots f(x(t_n)) \rangle = \langle x_b, t_b | T(f(\hat{x}(t_1)) \dots f(\hat{x}(t_n))) | x_a, t_a \rangle ,$$

where T is the time-ordering operator.

Chapter 3

Perturbation Theory

3.1 Perturbation Theory from Path Integrals

There are very few dynamical systems where we can find an exact solution.

However, we can often separate the action into a solvable part and a perturbation:

$$S[x(t)] = S_0[x(t)] + S_1[x(t)], \quad (3.1)$$

and then find meaningful results from there.

As an example, consider a particle in a slowly-varying potential, we may write:

$$S_0[x(t)] = \int_{t_a}^{t_b} dt \frac{1}{2} m \dot{x}^2 \quad \text{and} \quad S_1[x(t)] = - \int_{t_a}^{t_b} dt V(x(t), t). \quad (3.2)$$

Alternatively, we can split the potential as:

$$S_0[x(t)] = \int_{t_a}^{t_b} dt \left(\frac{1}{2} m \dot{x}^2 - U(x) \right) \quad \text{and} \quad S_1[x(t)] = - \int_{t_a}^{t_b} dt \tilde{V}(x(t), t). \quad (3.3)$$

where $\tilde{V}(x, t) = V(x, t) - U(x)$ so that the action in S_0 is time-independent. A popular choice is to take $U(x) = m\omega^2 x^2/2$, as this is a system we can solve.

Transition amplitude

The transition amplitude is

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} (S_0[x(t)] + S_1[x(t)]) \right\} \\ &= \int_{x_a}^{x_b} \mathcal{D}x e^{\frac{i}{\hbar} S_0[x(t)]} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar} S_1[x(t)] \right)^n \end{aligned} \quad (3.4)$$

or

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \langle x_b, t_b | x_a, t_a \rangle_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_a}^{t_b} dt_1 \cdots \int_{t_a}^{t_b} dt_n \\ &\quad \times \underbrace{\int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \cdots V(x(t_n), t_n) e^{\frac{i}{\hbar} S_0[x(t)]}}_{\langle x_b, t_b | T(V(\hat{x}(t_1), t_1) \cdots V(\hat{x}(t_n), t_n)) | x_a, t_a \rangle_0}. \end{aligned} \quad (3.5)$$

The subscript zero indicates that these transition amplitudes are evaluated with S_0 .

Each term in this sum is a transition element.

Now taking $t_a < t_1 < t_2 < \dots < t_n < t_b$, we may write

$$\begin{aligned} &\int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \cdots V(x(t_n), t_n) e^{\frac{i}{\hbar} S_0[x(t)]} \\ &= \int dx_1 \cdots \int dx_n \langle x_b, t_b | x_n, t_n \rangle_0 V(x_n, t_n) \\ &\quad \times \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle_0 \cdots V(x_1, t_1) \langle x_1, t_1 | x_a, t_a \rangle_0. \end{aligned} \quad (3.6)$$

We can therefore interpret the sum in Eq. (3.5) as the sum of “partial” amplitudes in which the particle is: not scattered + scattered once + scattered twice + ...

It is useful to represent this diagrammatically. We denote the transition amplitudes $\langle x_k, t_k | x_{k-1}, t_{k-1} \rangle_0$ by straight lines and insertions of the potential V by wavy lines. This gives:

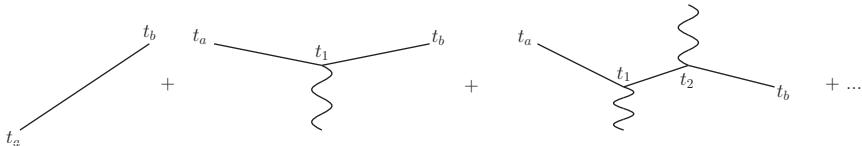


Figure 3.1: A diagrammatic representation of the sum in Eq. (3.5).

The integrals of x_k and t_k ensure we sum over all paths and the $1/n!$ ensures that paths with different time-orderings are not double-counted since we have the following identity

Identity

$$\begin{aligned} &\frac{1}{n!} \int_{t_a}^{t_b} dt_1 \int_{t_a}^{t_b} dt_2 \cdots \int_{t_a}^{t_b} dt_n V(t_1) \cdots V(t_n) \\ &= \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \cdots \int_{t_a}^{t_2} dt_1 V(t_1) \cdots V(t_n). \end{aligned} \quad (3.7)$$

For $n = 2$ we have

$$\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 V_1 V_2 = \int_{t_a}^{t_b} dt_2 \left(\int_{t_a}^{t_2} dt_1 V_1 V_2 + \int_{t_2}^{t_b} dt_1 V_1 V_2 \right). \quad (3.8)$$

For the second term swap order of indices (draw a diagram in the t_1-t_2 plane) which gives $\int_{t_a}^{t_b} dt_1 \int_{t_a}^{t_1} dt_2 V_1 V_2$ and then interchange indices $t_1 \leftrightarrow t_2$ to give the first term. So we have finally

$$\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 V_1 V_2 = 2! \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 V_1 V_2. \quad (3.9)$$

[See example sheet VII]

Series for transition amplitude

We therefore have from Eq. (3.5), (3.6)

$$\begin{aligned} & \langle x_b, t_b | x_a, t_a \rangle \\ &= \langle x_b, t_b | x_a, t_a \rangle_0 \\ &+ \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int dx_1 \dots \int dx_n \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \dots \int_{t_a}^{t_2} dt_1 \times \\ & \quad \langle x_b, t_b | x_n, t_n \rangle_0 V(x_n, t_n) \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle_0 \dots V(x_1, t_1) \langle x_1, t_1 | x_a, t_a \rangle_0. \end{aligned} \quad (3.10)$$

A rather ghastly looking result. This can be improved upon.

Formal sum of series

We will now start to expand the terms in the sum:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \langle x_b, t_b | x_a, t_a \rangle_0 \\ &- \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \int_{t_a}^{t_b} dt \langle x_b, t_b | x, t \rangle_0 V(x, t) \langle x, t | x_a, t_a \rangle_0 \\ &+ \left(-\frac{i}{\hbar} \right)^2 \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \int_{t_a}^{t_b} dt \int_{t_a}^t dt' \langle x_b, t_b | x, t \rangle_0 V(x, t) \\ &\quad \times \langle x, t | x', t' \rangle_0 V(x', t') \langle x', t' | x_a, t_a \rangle_0 + \dots . \end{aligned} \quad (3.11)$$

By relabelling $1 \leftrightarrow 2$ etc., we now factorise the integrals over x and t in the second and subsequent terms to get

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \langle x_b, t_b | x_a, t_a \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \int_{t_a}^{t_b} dt \langle x_b, t_b | x, t \rangle_0 V(x, t) \left[\langle x, t | x_a, t_a \rangle_0 \right. \\ &\quad \left. + \left(-\frac{i}{\hbar} \right) \int_{-\infty}^{\infty} dx' \int_{t_a}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \langle x', t' | x_a, t_a \rangle_0 + \dots \right]. \end{aligned} \quad (3.12)$$

The expression in square brackets, though, is just $\langle x, t | x_a, t_a \rangle$.

Therefore, we have shown

$$\langle x_b, t_b | x_a, t_a \rangle = \langle x_b, t_b | x_a, t_a \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \int_{t_a}^{t_b} dt \langle x_b, t_b | x, t \rangle_0 V(x, t) \langle x, t | x_a, t_a \rangle. \quad (3.13)$$

We interpret this pictorially as shown in Fig. 3.2.

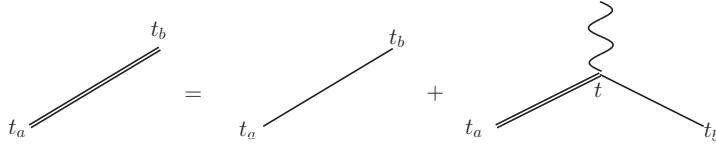


Figure 3.2: The full amplitude is the sum of the unscattered transition amplitude plus sum of all processes with the last scattering at time t .

Wavefunction

We can use this result to obtain a similar equation for wavefunctions:

$$\begin{aligned} \langle x, t | \psi \rangle &= \int_{-\infty}^{\infty} dx'' \langle x, t | x'', t_0 \rangle \langle x'', t_0 | \psi \rangle \\ &= \langle x, t | \psi \rangle|_{S_0} - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \langle x', t' | \psi \rangle. \end{aligned} \quad (3.14)$$

where the first term in Eq. (3.13) evolves from the initial time t_0 with the unperturbed action, S_0 , while the second term evolves with the full action, S . This gives

$$\psi(x, t) = \psi_0(x, t) - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \psi(x', t'), \quad (3.15)$$

Where $\psi_0(x, t)$ is the *unperturbed* wave function, which is a solution of the unperturbed Schrödinger equation:

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0(x, t) \right) \psi_0(x, t) = 0. \quad (3.16)$$

So again we have an integral equation, now for the wavefunction.

Schrödinger equation

Note that we can rewrite the last line of Eq. (3.15) as

$$\psi(x, t) = \psi_0(x, t) - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^{\infty} dt' \theta(t - t') \langle x, t | x', t' \rangle_0 V(x', t') \psi(x', t'). \quad (3.17)$$

(Can insert $\theta(t - t')$ as t' is less than t in the integral.) But recall that the Green's function, $G_0(x, x'; t, t') \equiv \theta(t - t')\langle x, t | x', t' \rangle$ satisfies

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0 \right) G_0(x, x'; t, t') = i\hbar\delta(t - t')\delta(x - x') . \quad (3.18)$$

Then

$$\begin{aligned} & \left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0 \right) \psi(x, t) \\ &= 0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^{\infty} dt' [i\hbar\delta(t - t')\delta(x - x')] V(x', t') \psi(x', t') \\ &= V(x, t)\psi(x, t), \end{aligned} \quad (3.19)$$

or

$$i\hbar \frac{\partial}{\partial t} \psi = (\hat{H}_0 + V)\psi = \hat{H}\psi , \quad (3.20)$$

and therefore shows that Eq. (3.15) is an integral equation for ψ which is equivalent to Schrödinger's equation.

3.2 Fixed Target Scattering – Time Independent The S-matrix

Consider elastic scattering of a particle of mass m in a fixed potential $V(\vec{r}, t)$. From section 2.11.1, Eq. (2.109), we can write

$$\lim_{\substack{t_b \rightarrow \infty \\ t_a \rightarrow -\infty}} \langle \vec{r}_b, t_b | \vec{r}_a, t_a \rangle = \lim_{\substack{t_b \rightarrow \infty \\ t_a \rightarrow -\infty}} \langle \vec{r}_b | \hat{U}(t_b, t_a) | \vec{r}_a \rangle \equiv \langle \vec{r}_b | \hat{S} | \vec{r}_a \rangle , \quad (3.21)$$

where the operator $\hat{S} \equiv \hat{U}(\infty, -\infty)$ is called the **Scattering Operator** or the **S-matrix**.

Since \hat{U} is unitary, \hat{S} is also unitary: $\hat{S}^\dagger \hat{S} = \hat{1}$. This is an expression of conservation: what goes in must come out!

We call $|\vec{r}_b, \infty\rangle$ the **out** state which represents a free particle in the far future.

Similarly $|\vec{r}_a, -\infty\rangle$ is the **in** state which represents a free particle in the far past.

This assumes that the potential $V(\vec{r}, t)$ is short-ranged: $V(\pm\infty, t) = 0$.

If the potential is time-independent, then time translation invariance implies

$$\lim_{\substack{t_b \rightarrow \infty \\ t_a \rightarrow -\infty}} \langle \vec{r}_b, t_b | \vec{r}_a, t_a \rangle = \lim_{T \rightarrow \infty} \langle \vec{r}_b, T/2 | \vec{r}_a, -T/2 \rangle = \lim_{T \rightarrow \infty} \langle \vec{r}_b, T | \vec{r}_a, 0 \rangle , \quad (3.22)$$

and we have the situation of Fig. 3.3.

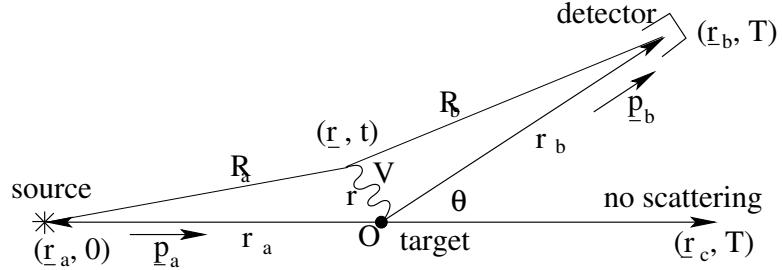


Figure 3.3: This illustrates the setup of a standard scattering experiment.

Lowest order scattering

We have, from Eq. (3.10 or Eq. (3.13)

$$\langle \vec{r}_b, T | \vec{r}_a, 0 \rangle = \langle \vec{r}_b, T | \vec{r}_a, 0 \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} d^3 r \int_0^T dt \langle \vec{r}_b, T | \vec{r}, t \rangle_0 V(\vec{r}) \langle \vec{r}, t | \vec{r}_a, 0 \rangle_0 + \mathcal{O}(V^2), \quad (3.23)$$

where again the first term represents the case of no scattering.

We are treating $V(\vec{r})$ as the perturbation so with $\vec{r} = (x_1, x_2, x_3)$

$$L_0(\vec{r}) = \frac{m}{2} (\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2). \quad (3.24)$$

In Cartesian coordinates, the path integral for the transition amplitude for a free particle factorises into three one-dimensional path integrals:

$$\langle \vec{r}', t' | \vec{r}, t \rangle_0 = \prod_{i=1}^3 \langle x'_i, t' | x_i, t \rangle_0. \quad (3.25)$$

At first (leading) order in perturbation theory, the transition amplitude, A_1 , is then

$$A_1 = -\frac{i}{\hbar} \int_{-\infty}^{\infty} d^3 r \int_0^T dt \left(\frac{m}{2\pi i \hbar(T-t)} \right)^{3/2} \exp \left(\frac{im|\vec{r}_b - \vec{r}|^2}{2\hbar(T-t)} \right) \times V(\vec{r}) \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \exp \left(\frac{im|\vec{r} - \vec{r}_a|^2}{2\hbar t} \right), \quad (3.26)$$

plugging in our previous expression for the free particle amplitude. We now use

$$\int_0^T \frac{dt}{[(T-t)t]^{3/2}} \exp \left\{ -\frac{\alpha}{T-t} - \frac{\beta}{t} \right\} = \frac{1}{T} \sqrt{\frac{\pi}{T}} \left(\frac{1}{\sqrt{\alpha}} + \frac{1}{\sqrt{\beta}} \right) \exp \left\{ -\frac{(\sqrt{\alpha} + \sqrt{\beta})^2}{T} \right\}. \quad (3.27)$$

Interlude: For interest, Feynman's integral for scattering

In Feynman's approach to scattering we need to evaluate the following integral:

$$F(\alpha, \beta) = \int_0^T \frac{dt}{(T-t)^{3/2} t^{3/2}} e^{-\alpha/(T-t)-\beta/t} \dots \quad (3.28)$$

We will start with the slightly simpler integral

$$I(a, b) = \int_0^\infty dx e^{-a/x^2 - bx^2}. \quad (3.29)$$

with a and b real and positive. Substituting $\xi = \sqrt{\frac{b}{a}}x$ gives

$$I(a, b) = \sqrt{\frac{a}{b}} \int_0^\infty d\xi e^{-b/\xi^2 - a\xi^2} = \sqrt{\frac{a}{b}} I(b, a). \quad (3.30)$$

However substituting $y = 1/x$ gives

$$I(a, b) = \int_0^\infty \frac{dy}{y^2} e^{-ay^2 - b/y^2} = -\frac{\partial}{\partial b} I(b, a). \quad (3.31)$$

It follows by combining Eqs. (3.30) and (3.31) that

$$\frac{\partial}{\partial b} I(b, a) = -\sqrt{\frac{a}{b}} I(b, a), \quad (3.32)$$

and therefore that $I(b, a) = I(0, a)e^{-2\sqrt{ab}}$. By Gaussian integration $I(0, a) = \frac{1}{2}\sqrt{\frac{\pi}{a}}$, so we find

$$I(a, b) = \frac{1}{2} \sqrt{\frac{\pi}{b}} e^{-2\sqrt{ab}}. \quad (3.33)$$

Now we can use this result for $I(a, b)$ to evaluate Feynman's integral $F(\alpha, \beta)$ when α and β are real and positive. First let $x = \sqrt{\frac{T-t}{t}}$, so that

$$\frac{a}{x^2} + bx^2 = a \frac{T}{(T-t)} + b \frac{T}{t} - a - b \quad \text{and} \quad \frac{dx}{dt} = -\frac{T}{2} \sqrt{\frac{T-t}{t}} \frac{1}{t(T-t)} \quad (3.34)$$

so that Eq. (3.29) becomes

$$I(a, b) = \frac{1}{2} T e^{a+b} \int_0^T \frac{dt}{(T-t)^{1/2} t^{3/2}} e^{-aT/(T-t)-bT/t}. \quad (3.35)$$

But then from the definition in Eq. (3.28):

$$F(\alpha, \beta) = -\frac{\partial}{\partial \alpha} \int_0^T \frac{dt}{(T-t)^{1/2} t^{3/2}} e^{-\alpha/(T-t)-\beta/t} = -\frac{\partial}{\partial \alpha} \left[\frac{2}{T} I\left(\frac{\alpha}{T}, \frac{\beta}{T}\right) e^{-\alpha/T-\beta/T} \right] \quad (3.36)$$

using Eq. (3.35), so using our result for $I(a, b)$, Eq. (3.33),

$$F(\alpha, \beta) = -\frac{\partial}{\partial \alpha} \sqrt{\frac{\pi}{\beta T}} e^{-(\sqrt{\alpha}+\sqrt{\beta})^2/T} = \frac{1}{T} \sqrt{\frac{\pi}{T}} \left(\frac{1}{\sqrt{\alpha}} + \frac{1}{\sqrt{\beta}} \right) e^{-(\sqrt{\alpha}+\sqrt{\beta})^2/T}. \quad (3.37)$$

Although the derivation above assumed that α and β are real and positive, the result also holds for complex α and β provided only that their real parts are positive, and then for pure imaginary α and β by analytic continuation, the cut of the square roots being taken along the negative real axis. (As for Fresnel integrals.)

End of Interlude

Set

$$R_a = |\vec{r}_a - \vec{r}|, \quad R_b = |\vec{r}_b - \vec{r}|, \quad (3.38)$$

and

$$\alpha = -\frac{im}{2\hbar}|\vec{r}_b - \vec{r}|^2 = -\frac{im}{2\hbar}R_a^2, \quad \beta = -\frac{im}{2\hbar}|\vec{r}_a - \vec{r}|^2 = -\frac{im}{2\hbar}R_b^2. \quad (3.39)$$

This gives

$$\begin{aligned} \frac{1}{\sqrt{\alpha}} + \frac{1}{\sqrt{\beta}} &= \left(\frac{2i\hbar}{m}\right)^{1/2} \left(\frac{1}{R_a} + \frac{1}{R_b}\right) \\ \left(\sqrt{\alpha} + \sqrt{\beta}\right)^2 &= -\frac{im}{2\hbar}(R_a + R_b)^2. \end{aligned} \quad (3.40)$$

Hence

$$\begin{aligned} A_1 &= -\frac{i}{\hbar} \left(\frac{m}{2\pi i\hbar}\right)^3 \frac{1}{T} \sqrt{\frac{\pi}{T}} \int_{-\infty}^{\infty} d^3 r \left(\frac{2i\hbar}{m}\right)^{1/2} \left(\frac{1}{R_a} + \frac{1}{R_b}\right) \\ &\quad \times V(\vec{r}) \times \exp\left\{\frac{im}{2\hbar T}(R_a + R_b)^2\right\}, \end{aligned} \quad (3.41)$$

or

$$A_1 = -\frac{i}{\hbar} \left(\frac{m}{2\pi i\hbar}\right)^{5/2} \frac{1}{T^{3/2}} \int_{-\infty}^{\infty} d^3 r \left(\frac{1}{R_a} + \frac{1}{R_b}\right) V(\vec{r}) \exp\left\{\frac{im}{2\hbar T}(R_a + R_b)^2\right\} \quad (3.42)$$

As we are taking the potential to be short-range, the values of \vec{r} which contribute to the integral will have $r \ll r_a, r_b$ so we may expand

$$R_a = |\vec{r}_a - \vec{r}| = r_a \left(1 - \frac{2\vec{r}_a \cdot \vec{r}}{r_a^2} + \frac{r^2}{r_a^2}\right)^{1/2} = r_a - \vec{n}_a \cdot \vec{r} + \mathcal{O}(1/r_a), \quad (3.43)$$

where $\vec{n}_a = \vec{r}_a/r_a$ is a unit vector in the direction of \vec{r}_a . Similarly $R_b = r_b - \vec{n}_b \cdot \vec{r} + \mathcal{O}(1/r_b)$ and

$$\begin{aligned} 1/R_a + 1/R_b &= 1/r_a + 1/r_b + \mathcal{O}(1/r_a^2, 1/r_b^2) \\ (R_a + R_b)^2 &= (r_a + r_b)^2 - 2(r_a + r_b)(\vec{n}_a + \vec{n}_b) \cdot \vec{r} + \mathcal{O}(1). \end{aligned} \quad (3.44)$$

To leading order then we have

$$\begin{aligned} A_1 &= -\frac{i}{\hbar} \left(\frac{m}{2\pi i\hbar}\right)^{5/2} \frac{1}{T^{3/2}} \left\{\frac{1}{r_a} + \frac{1}{r_b}\right\} \exp\left\{\frac{im}{2\hbar T}(r_a + r_b)^2\right\} \\ &\quad \times \int_{-\infty}^{\infty} d^3 r V(\vec{r}) \exp\left\{-\frac{im}{\hbar T}(r_a + r_b)(\vec{n}_a + \vec{n}_b) \cdot \vec{r}\right\}. \end{aligned} \quad (3.45)$$

The quantities r_a , r_b and T are known.

As the potential is short-range, the particle will behave like a free particle for most of the time. We therefore deduce the following quantities:

$$p = m \left(\frac{r_a + r_b}{T} \right), \quad E = \frac{1}{2}m \left(\frac{r_a + r_b}{T} \right)^2, \quad (3.46)$$

and hence have

$$\vec{p}_a = -p\vec{n}_a, \quad \vec{p}_b = p\vec{n}_b, \quad (3.47)$$

(energy conservation means that $|p_a| = |p_b| = p$). So *momentum transfer*

$$\vec{p}_a - \vec{p}_b = -m \frac{r_a + r_b}{T} (\vec{n}_a + \vec{n}_b) \equiv \hbar \vec{k}, \quad (3.48)$$

where \vec{k} is the *wave number transfer*. (Can also use notation \vec{q} .)

Substituting into Eq. (3.45) gives

$$A_1 = -\frac{i}{\hbar} \left(\frac{m}{2\pi i \hbar} \right)^{5/2} \frac{1}{T^{3/2}} \left(\frac{r_a + r_b}{r_a r_b} \right) \exp\left(\frac{i}{\hbar} ET\right) \times \tilde{V}(\vec{k}), \quad (3.49)$$

where

$$\tilde{V}(\vec{k}) = \int_{-\infty}^{\infty} d^3r V(\vec{r}) \exp\left(i\vec{k} \cdot \vec{r}\right). \quad (3.50)$$

Transition probability

We have that the *transition probability* per unit volume

$$P(a \rightarrow b) = |A_1|^2 = \frac{1}{\hbar^2} \left(\frac{m}{2\pi \hbar} \right)^5 \frac{1}{T^3} \left(\frac{r_a + r_b}{r_a r_b} \right)^2 |\tilde{V}(\vec{k})|^2 \quad (3.51)$$

Similarly, for no scattering (free particle and hence the final position \vec{r}_c) we have

$$\langle \vec{r}_c, T | \vec{r}_a, 0 \rangle_0 = \left(\frac{m}{2\pi i \hbar T} \right)^{3/2} e^{i \frac{m}{2\hbar T} (\vec{r}_c - \vec{r}_a)^2}, \quad (3.52)$$

giving

$$P(a \rightarrow c) = |A_0|^2 = |\langle \vec{r}_c, T | \vec{r}_a, 0 \rangle_0|^2 = \left(\frac{m}{2\pi \hbar} \right)^3 \frac{1}{T^3}. \quad (3.53)$$

The ratio of the scattering and no-scattering probabilities is then

$$\frac{P(a \rightarrow b)}{P(a \rightarrow c)} = \left(\frac{m}{2\pi \hbar^2} \right)^2 \left(\frac{r_a + r_b}{r_a r_b} \right)^2 |\tilde{V}(\vec{k})|^2. \quad (3.54)$$

Cross section

We describe the scattering process in terms of an effective target area known as the *scattering cross section*.

The region where the effect of the potential is felt is $d\sigma$ at distance r_a from the starting point, see Fig. 3.4.

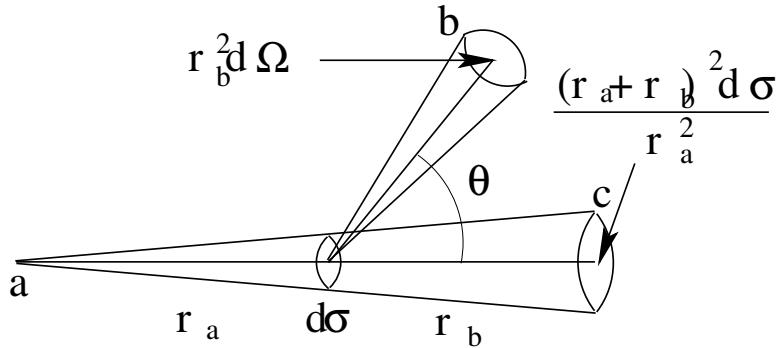


Figure 3.4: This illustrates the definition of a scattering cross section.

In the absence of the potential, paths through this area would go on to cover an area $((r_a + r_b)/r_a)^2 d\sigma$ at time T .

Instead, they are scattered into a small area of solid angle $d\Omega$ which has area $r_b^2 d\Omega$.

We therefore find:

$$P(a \rightarrow b) r_b^2 d\Omega = P(a \rightarrow c) \frac{(r_a + r_b)^2}{r_a^2} d\sigma. \quad (3.55)$$

This equation represents equality between the number of particles scattered into $d\Omega$ per unit time and $d\sigma$ times the number of incident particles crossing the scattering region per unit area per unit time.

Re-arranging this result gives

$$\frac{P(a \rightarrow b)}{P(a \rightarrow c)} = \left(\frac{r_a + r_b}{r_a r_b} \right)^2 \frac{d\sigma}{d\Omega}. \quad (3.56)$$

Comparing this to Eq. (3.54), gives

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2} \right)^2 |\tilde{V}(\vec{k})|^2. \quad (3.57)$$

This important result is the **differential cross section** in the **Born approximation**.

- Independent of T , r_a and r_b and therefore we are free to take these to infinity

- Born series, V^n if go to higher orders
- Total cross section

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega \equiv \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \frac{d\sigma}{d\Omega}.$$

θ – scattering angle.

ϕ – angle about ‘beam axis’ (line: $\vec{r}_a \rightarrow$ origin $\rightarrow \vec{r}_c$)

- Can obtain these result using time independent perturbation theory with plane wave states. Here took the other approach: initial/final states as particles with definite position.

This is Quantum Mechanics: wave–particle duality (!)

Central Potential

If we now assume that $V(\vec{r})$ is a *central potential* (i.e. one only depending on $|\vec{r}| = r$), we find

$$\begin{aligned} \tilde{V}(\vec{k}) &= \int_{-\infty}^{\infty} d^3r V(r) \exp(i\vec{k} \cdot \vec{r}) \\ &= 2\pi \int_0^{\infty} dr r^2 V(r) \int_0^{\pi} d\theta \sin \theta \exp(ikr \cos \theta) \\ &= \frac{4\pi}{k} \int_0^{\infty} dr r V(r) \sin(kr), \end{aligned} \quad (3.58)$$

We therefore find

$$\frac{d\sigma}{d\Omega} = \frac{4m^2}{\hbar^4 k^2} \left| \int_0^{\infty} dr r V(r) \sin(kr) \right|^2, \quad (3.59)$$

where, from the definitions before, $p_a^2 = p^2 = p_b^2$, $\vec{p}_a \cdot \vec{p}_b = p^2 \cos \theta$ so

$$k = \frac{1}{\hbar} |\vec{p}_a - \vec{p}_b| = \frac{2p}{\hbar} \sin \frac{1}{2}\theta,$$

with θ ($0 \leq \theta < \pi$) the scattering angle shown in Fig. 3.3 (or Fig. 3.4).

A particularly important example is the **Coulomb potential**,

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}, \quad (3.60)$$

(For compatibility with many standard texts, we use SI units; for Heaviside–Lorentz units simply remove the ϵ_0 .)

In order for the integral to converge, we multiply $V(r)$ by $\exp(-\mu r)$ and then take the limit $\mu \rightarrow 0$ in the final answer, see example sheet VII.

This gives

$$\int_0^\infty dr rV(r) \sin(kr) = -\frac{e^2}{4\pi\epsilon_0 k}, \quad (3.61)$$

and hence

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{16E^2} \frac{1}{\sin^4(\theta/2)}, \quad E = \frac{p^2}{2m}. \quad (3.62)$$

This is the same as the *classical* Rutherford cross section.

This correspondence between the classical and quantum results is unique to the $1/r$ potential – Rutherford was lucky!

3.3 Colliding Beams

We will now consider two particles of masses m_1 and m_2 interacting through a mutual potential so that the Lagrangian is

$$L = \frac{1}{2}m_1|\dot{\vec{r}}_1|^2 + \frac{1}{2}m_2|\dot{\vec{r}}_2|^2 - V(\vec{r}_1 - \vec{r}_2). \quad (3.63)$$

We will rewrite this in terms of coordinates representing centre-of-mass motion:

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}, \quad M = m_1 + m_2, \quad (3.64)$$

and coordinates representing relative motion:

$$\vec{r} = \vec{r}_1 - \vec{r}_2, \quad \mu = \frac{m_1m_2}{m_1 + m_2}. \quad (3.65)$$

We then find

$$L = \frac{1}{2}M|\dot{\vec{R}}|^2 + \frac{1}{2}\mu|\dot{\vec{r}}|^2 - V(\vec{r}). \quad (3.66)$$

If we work in the centre-of-mass frame, $\vec{R} = \vec{0}$ and the first term vanishes leaving $L = \frac{1}{2}\mu|\dot{\vec{r}}|^2 - V(\vec{r})$, which is the same Lagrangian as in fixed-particle scattering after the translation $m \rightarrow \mu$.

Therefore, for a colliding beam scattering experiment as shown in Fig 3.5, the differential cross section is simply

$$\frac{d\sigma}{d\Omega} = \left(\frac{\mu}{2\pi\hbar^2}\right)^2 |\tilde{V}(\vec{k})|^2 \equiv |f(\theta, \phi)|^2, \quad (3.67)$$

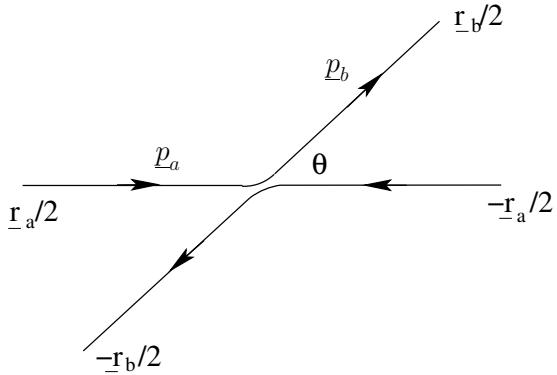


Figure 3.5: A standard colliding beam experiment.

where $\vec{k} = (\vec{p}_a - \vec{p}_b)/\hbar$ and we have defined a **scattering amplitude** $f(\theta, \phi)$.

For central potentials, we know that the scattering amplitude does not depend on ϕ and $f(\theta, \phi)$ is just a function of θ .

If we now consider the limit $m_2 \rightarrow \infty$, we recover the fixed target result. This is the Born-Oppenheimer approximation.

But for (non-identical) particles of the same mass, $m_1 = m_2 = m$, then we find $\mu = m/2$ and

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{4\pi\hbar^2} \right)^2 |\tilde{V}(\vec{k})|^2. \quad (3.68)$$

If the particles are identical, we have two indistinguishable possibilities, as shown in Fig. 3.6.

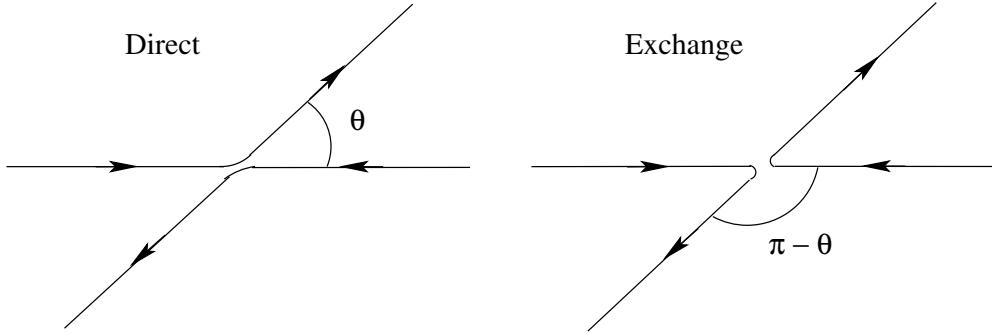


Figure 3.6: The two indistinguishable outcomes when identical particles scatter.

Classically we would add probabilities and would find

$$\frac{d\sigma_{Cl}}{d\Omega} = |f(\theta)|^2 + |f(\pi - \theta)|^2. \quad (3.69)$$

In quantum mechanics, we add the amplitudes as usual and find

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2. \quad (3.70)$$

For the Coulomb potential for example, this gives ($E = p^2/(2\mu)$)

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \left(\frac{1}{4\pi\epsilon_0} \right)^2 \frac{e^4}{16E^2} \left(\frac{1}{\sin^2(\theta/2)} + \frac{1}{\cos^2(\theta/2)} \right)^2 \\ &= \left(\frac{1}{4\pi\epsilon_0} \right)^2 \frac{e^4}{E^2} \frac{1}{\sin^4 \theta}. \end{aligned} \quad (3.71)$$

(As indistinguishable particles, then θ same as $\pi - \theta$ so for total cross section so just integrate over $0 \leq \theta \leq \pi/2$.)

For identical ‘spinless fermions’, the amplitudes have a relative minus sign and we instead find

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0} \right)^2 \frac{e^4}{E^2} \frac{\cos^2 \theta}{\sin^4 \theta}. \quad (3.72)$$

This vanishes at $\theta = \pi/2$ as it must. The shapes of the two distributions are shown in Fig. 3.7. This means that one can hope to tell whether particles are bosons or

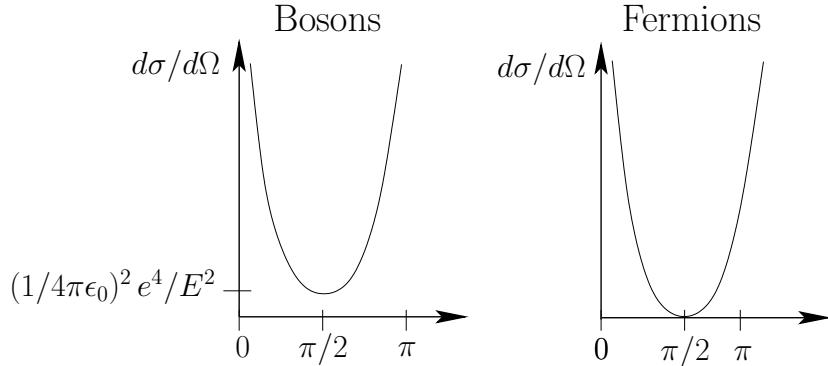


Figure 3.7: The shapes of the differential distributions $d\sigma/d\Omega$ for bosons (Eq. (3.71)) and fermions (Eq. (3.72)).

fermions by studying the *shape* of the differential cross section.

3.4 Perturbation Theory in the Operator Formalism

We now develop perturbation theory for the time evolution operator, \hat{U} .

Recall, Eq. (2.109), when we write the transition amplitude in the Heisenberg pic-

ture, we have

$$\langle x_b, t_b | x_a, t_a \rangle = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle. \quad (3.73)$$

The effect of the perturbation in the Lagrangian (and therefore action) will alter the operator from $\hat{U}_0(t_b, t_a)$ to $\hat{U}(t_b, t_a)$.

From Eq. (3.5) or Eq. (2.177), we have

$$\begin{aligned} & \int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \dots V(x(t_n), t_n) e^{\frac{i}{\hbar} S_0} \\ &= {}_0\langle x_b, t_b | T(V(\hat{x}_0(t_1), t_1) \dots V(\hat{x}_0(t_n), t_n)) | x_a, t_a \rangle_0, \end{aligned} \quad (3.74)$$

where the states $|x, t\rangle_0$, ${}_0\langle x, t\rangle$ and the operators $\hat{x}_0(t)$ are in the Heisenberg picture with respect to the unperturbed action S_0 rather than S .

These are defined by

$$\hat{x}_0(t) = \hat{U}_0^\dagger(t, t_0) \hat{x} \hat{U}_0(t, t_0), \quad (3.75)$$

where \hat{x} is the Schrödinger picture operator.

Furthermore recall

$$i\hbar \frac{\partial}{\partial t} \hat{U}_0 = \hat{H}_0 \hat{U}_0. \quad (3.76)$$

(For a time independent \hat{H}_0 , the usual situation, then $\hat{U}_0(t, t_0) = \exp(i/\hbar(t - t_0)\hat{H}_0)$.)

Evolving with the unperturbed action is known as the **Dirac** or **interaction** picture for time dependence in quantum mechanics (denoted by subscript 0 or D).

Analogous equations to Eq. (3.75) hold for all other operators and so the potential in the Dirac picture can be written as

$$V(\hat{x}_0(t), t) = \hat{U}_0^\dagger(t, t_0) V(\hat{x}, t) \hat{U}_0(t, t_0). \quad (3.77)$$

This is studied further in example sheet VIII.

Dyson series

Using Eq. (3.5) and Eq. (3.12) gives

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= {}_0\langle x_b, t_b | x_a, t_a \rangle_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{t_a}^{t_b} dt_1 \dots \int_{t_a}^{t_b} dt_n \times \\ &\quad {}_0\langle x_b, t_b | T(V(\hat{x}_0(t_1), t_1) \dots V(\hat{x}_0(t_n), t_n)) | x_a, t_a \rangle_0 \\ &= {}_0\langle x_b, t_b | x_a, t_a \rangle_0 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \dots \int_{t_a}^{t_2} dt_1 \times \\ &\quad {}_0\langle x_b, t_b | V(\hat{x}_0(t_n), t_n) \dots V(\hat{x}_0(t_1), t_1) | x_a, t_a \rangle_0. \end{aligned} \quad (3.78)$$

The time dependence in this picture is governed by S_0 and so the interaction picture states are related to the Schrödinger picture states through

$$|x_a, t_a\rangle_0 = \hat{U}_0^\dagger(t_a, t_0)|x_a\rangle \quad \text{and} \quad {}_0\langle x_b, t_b| = \langle x_b, t_b| = \langle x_b|\hat{U}_0(t_b, t_0). \quad (3.79)$$

We also have

$$\hat{U}_0(t_k, t_0)\hat{U}_0^\dagger(t_{k-1}, t_0) = \hat{U}_0(t_k, t_0)\hat{U}_0(t_0, t_{k-1}) = \hat{U}_0(t_k, t_{k-1}), \quad (3.80)$$

so using this many times gives

$$\begin{aligned} \langle x_b|\hat{U}(t_b, t_a)|x_a\rangle &= \langle x_b|\hat{U}_0(t_b, t_a)|x_a\rangle \\ &+ \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_a}^{t_b} dt_n \dots \int_{t_a}^{t_2} dt_1 \langle x_b|\hat{U}_0(t_b, t_n)V(\hat{x}, t_n)\hat{U}_0(t_n, t_{n-1})V(\hat{x}, t_{n-1})\dots \\ &\quad \times V(\hat{x}, t_1)\hat{U}_0(t_1, t_a)|x_a\rangle. \end{aligned} \quad (3.81)$$

This equation is true for all states $|x_a\rangle$ and $|x_b\rangle$ so we can therefore derive the following operator equation

$$\begin{aligned} \hat{U}(t_b, t_a) &= \hat{U}_0(t_b, t_a) + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_a}^{t_b} dt_n \dots \int_{t_a}^{t_2} dt_1 \\ &\quad \hat{U}_0(t_b, t_n)V(\hat{x}, t_n)\hat{U}_0(t_n, t_{n-1})\dots V(\hat{x}, t_1)\hat{U}_0(t_1, t_a). \end{aligned} \quad (3.82)$$

This expression is known as the **Dyson series**.

We can then sum this formally to get the operator equivalent of Eq. (3.13)

$$\hat{U}(t_b, t_a) = \hat{U}_0(t_b, t_a) - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{U}_0(t_b, t)V(\hat{x}, t)\hat{U}(t, t_a). \quad (3.83)$$

This equation (or equivalently the Dyson series) can be derived directly from the Schrödinger Equation (see example sheet VIII). Note that here $V(\hat{x}, t)$ is in the Schrödinger picture.

3.5 Time-dependent Transitions

Common situation is the case where the perturbation in S_1 is time-dependent.

The two most common choices for S_0 are then either the free particle case or the harmonic oscillator which both have a spectrum of energy eigenvalues E_n corresponding to bound states and corresponding energy eigenstates $|n\rangle$, so that

$$\hat{H}_0|n\rangle = E_n|n\rangle, \quad (3.84)$$

or equivalently $\hat{H}_0|n, t\rangle = E_n|n, t\rangle$ in the Heisenberg picture.

We will work in this basis (as opposed to the position basis) because the unperturbed transition amplitude is diagonal in this basis:

$$\begin{aligned}\langle m, t | n, t' \rangle &= \langle m | \hat{U}_0(t, t') | n \rangle = \langle m | e^{-\frac{i}{\hbar}(t-t')\hat{H}_0} | n \rangle \\ &= e^{-\frac{i}{\hbar}(t-t')E_n} \delta_{mn}.\end{aligned}\quad (3.85)$$

Using $|a, t_a\rangle$ and $|b, t_b\rangle$ as the initial and final energy eigenstates, the operator equation in Eq. (3.83) gives

$$\begin{aligned}\langle b, t_b | a, t_a \rangle &= \langle b | \hat{U}(t_b, t_a) | a \rangle \\ &= \langle b | \hat{U}_0(t_b, t_a) | a \rangle - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \langle b | \hat{U}_0(t_b, t) V(\hat{x}, t) \hat{U}_0(t, t_a) | a \rangle + \dots \\ &= \langle b | \hat{U}_0(t_b, t_a) | a \rangle - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \sum_{m,n} \langle b | \hat{U}_0(t_b, t) | m \rangle \langle m | V(\hat{x}, t) | n \rangle \langle n | \hat{U}_0(t, t_a) | a \rangle + \dots \\ &= e^{-\frac{i}{\hbar}(t_b-t_a)E_a} \delta_{ab} - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \sum_{m,n} e^{-\frac{i}{\hbar}(t_b-t)E_b} \delta_{mb} V_{mn}(t) e^{-\frac{i}{\hbar}(t-t_a)E_a} \delta_{na} + \dots \\ &= e^{-\frac{i}{\hbar}(t_b-t_a)E_a} \delta_{ab} - \frac{i}{\hbar} e^{-\frac{i}{\hbar}(E_b t_b - E_a t_a)} \int_{t_a}^{t_b} dt e^{\frac{i}{\hbar}t(E_b - E_a)} V_{ba}(t) + \dots\end{aligned}\quad (3.86)$$

where we have introduced the notation $V_{mn}(t)$ for the matrix element of the potential

$$\begin{aligned}V_{mn}(t) &\equiv \langle m | V(\hat{x}, t) | n \rangle = \int_{-\infty}^{\infty} dx \langle m | V(\hat{x}, t) | x \rangle \langle x | n \rangle \\ &= \int_{-\infty}^{\infty} dx u_m^*(x) V(x, t) u_n(x).\end{aligned}\quad (3.87)$$

The same steps yield the following second term

$$\left(-\frac{i}{\hbar}\right)^2 \sum_n \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 e^{-\frac{i}{\hbar}(t_b-t_2)E_b} V_{bn}(t_2) e^{-\frac{i}{\hbar}(t_2-t_1)E_n} V_{na}(t_1) e^{-\frac{i}{\hbar}(t_1-t_a)E_a}, \quad (3.88)$$

and similar expressions for higher orders.

We represent this diagrammatically as shown in Fig. 3.8. All intermediate “virtual” states are summed over and the “interaction times” $t_1 < t_2 < \dots < t_n$ are integrated over.

Unless $a = b$, the first (trivial) term vanishes and the transition probability becomes

$$P(a \rightarrow b) = |\langle b, t_b | a, t_a \rangle|^2 = \frac{1}{\hbar^2} \left| \int_{t_a}^{t_b} dt e^{i\omega_{ba}t} V_{ba}(t) + \mathcal{O}(V^2) \right|^2 \quad (3.89)$$

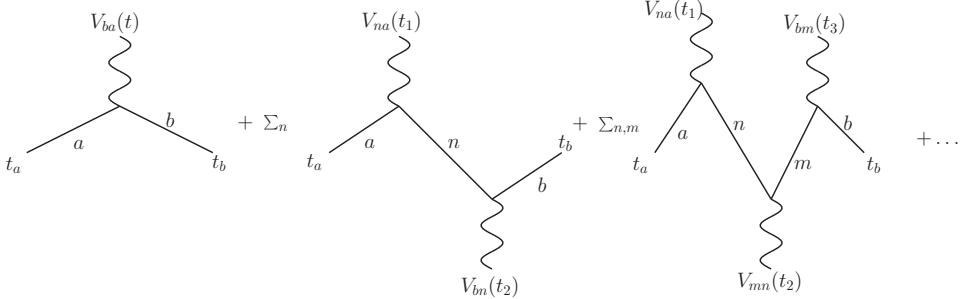


Figure 3.8: Diagrammatic representation of Eq. (3.86).

where ω_{ba} is the *transition frequency*. There is interference between terms of higher orders so the next correction to the probability is $\mathcal{O}(V^3)$ and not $\mathcal{O}((V^2)^2)$.

If we now define

$$\tilde{V}_{ba} = \int_{t_a}^{t_b} dt e^{i\omega_{ba}t} V_{ba}(t), \quad (3.90)$$

we find

$$P(a \rightarrow b) = \frac{1}{\hbar^2} |\tilde{V}_{ba}|^2. \quad (3.91)$$

Fermi's golden rule

In the case where the perturbation is time-independent, we can perform the integrals over t and find

$$\langle b, t_b | a, t_a \rangle = e^{\frac{i}{\hbar} E_a T} \delta_{ab} + \frac{e^{-\frac{i}{\hbar} E_b T} - e^{-\frac{i}{\hbar} T E_a}}{E_b - E_a} V_{ba} + O(V^2), \quad (3.92)$$

where $T = t_b - t_a$ as usual.

Therefore, to first-order the transition probability for the time-independent case and $a \neq b$ is

$$\begin{aligned} P(a \rightarrow b) &= \frac{\left| e^{-\frac{i}{\hbar} E_a T} (e^{-iT\omega_{ba}} - 1) \right|^2}{\hbar^2 \omega_{ba}^2} |V_{ba}|^2 \\ &\equiv \frac{f(T, \omega_{ba})}{\hbar^2} |V_{ba}|^2. \end{aligned} \quad (3.93)$$

The function

$$f(t, \omega) = \frac{\sin^2(\omega t/2)}{(\omega t/2)^2} t^2 \quad (3.94)$$

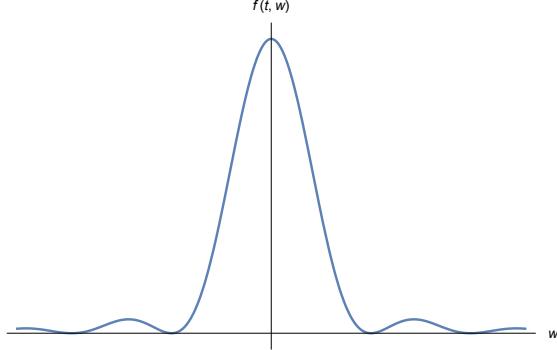


Figure 3.9: The function, $f(t, \omega)$, which multiplies $|V_{ba}|^2/\hbar^2$ in the probability of the transition, corresponding to Eq. (3.94).

consists of a large peak centred on $\omega = 0$ with height t^2 . It has zeroes at $\omega = 2n\pi/t$, so width $\sim 2\pi/t$ with other smaller oscillations symmetrically on either side. This is plotted in Fig. 3.9.

This means that the only significant transition probability is to those states whose energy lies in a band of width $\delta E \simeq 2\pi\hbar/t$ about the initial energy, E_a .

Now for an arbitrary function $h(\omega)$ consider for large t

$$\begin{aligned} \int_{-\infty}^{+\infty} d\omega f(t, \omega) h(\omega) d\omega &= 2t \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2} h(2x/t) \\ &= 2t \int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2} [h(0) + O(1/t)] = 2\pi t h(0) + O(1), \end{aligned} \quad (3.95)$$

upon using the standard integral

$$\int_{-\infty}^{+\infty} dx \frac{\sin^2 x}{x^2} = \pi. \quad (3.96)$$

Thus for large t , $f(t, \omega)$ acts like a delta function,

$$\lim_{t \rightarrow \infty} f(t, \omega) = 2\pi t \delta(\omega). \quad (3.97)$$

We may also consider a case of a transition not to a final state but to a range \mathcal{R} of final states around E_b . We then find

$$P(a \rightarrow \mathcal{R}) = \int_{\mathcal{R}} P(a \rightarrow E) \rho(E) dE, \quad (3.98)$$

where $\rho(E)$ is the *density of final states* which is the number of states with energy in the range $E \rightarrow E + dE$.

If we take the range \mathcal{R} to be sufficiently small, then we can consider $\rho(E)$ and V_{ba} to be roughly constant in that region. As $f(t, \omega)$ behaves like a delta-function for

large T , we can extend the limits on the integral without changing its value. We therefore find

$$\begin{aligned} P(a \rightarrow \mathcal{R}) &= \frac{1}{\hbar^2} |V_{ba}|^2 \rho(E_b) \int_{-\infty}^{\infty} dE 2\pi T [\delta(E/\hbar) + O(1/T)] \\ &= \frac{2\pi}{\hbar} |V_{ba}|^2 \rho(E_b) T. \end{aligned} \quad (3.99)$$

The resulting transition rate is therefore

$$R = \frac{2\pi}{\hbar} |V_{ba}|^2 \rho(E_b). \quad (3.100)$$

This result is **Fermi's Golden Rule**.

3.6 Feynman's Perturbation Theory

3.6.1 Classical mechanics

The perturbation theory considered so far is intrinsically quantum mechanical: the unperturbed amplitude is a Green function for the Schrödinger equation, which describes quantum propagation. We can also do perturbation theory in classical mechanics.

As an example, consider a forced anharmonic oscillator, with action $S = S_0[x, J] + S_1[x]$, and Lagrangian

$$L = L_0 + L_1 = \underbrace{\frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2 + Jx}_{\text{forced SHO}} - \underbrace{\frac{\lambda}{4} x^4}_{\text{anharmonic}} \quad (3.101)$$

where $J = J(t)$ is an arbitrary function of t . The classical equation of motion is:

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) x = \frac{J}{m} - \frac{\lambda}{m} x^3. \quad (3.102)$$

Homogeneous equation

The homogeneous equation

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) x = 0, \quad (3.103)$$

is that of a simple harmonic oscillator. Let the solution of this equation be $\bar{x}_0(t)$, with boundary conditions $\bar{x}_0(t_a) = x_a$ and $\bar{x}_0(t_b) = x_b$.

To solve the full inhomogeneous equation, we construct a Green function $\Delta(t, t')$ such that

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) \Delta(t, t') = -\delta(t - t'), \quad (3.104)$$

which satisfies the boundary conditions $\Delta(t_b, t') = \Delta(t_a, t') = 0$.

It is straightforward (example sheet IX) to show that

$$\begin{aligned}\Delta(t, t') &= \frac{1}{\omega \sin \omega T} [\theta(t - t') \sin \omega(t_b - t) \sin \omega(t' - t_a) \\ &\quad + \theta(t' - t) \sin \omega(t - t_a) \sin \omega(t_b - t')] ,\end{aligned}\quad (3.105)$$

where $T = t_b - t_a$ as usual.

Note that this Green function is *not* causal, because of the boundary conditions. We have both *retarded* ($t' < t$) and *advanced* ($t' > t$) pieces.

We call $\Delta(t, t')$ the **Feynman Green function** or the **Feynman propagator**. Note also that $\Delta(t, t') = \Delta(t', t)$.

Full solution

The full solution of Eq. (3.102) with the correct boundary conditions is then

$$\bar{x}(t) = \bar{x}_0(t) + \frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') (-J(t') + \lambda \bar{x}(t')^3) \quad (3.106)$$

The second term on the RHS is the solution of the full inhomogeneous equation with trivial (zero) boundary conditions (check this explicitly), whilst the first term “fixes up” the boundary conditions.

More precisely, Eq. (3.106) is an integral equation for $\bar{x}(t)$ which we can solve iterately:

$$\begin{aligned}\bar{x}(t) &= \bar{x}_0(t) - \frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') J(t') \\ &\quad + \frac{\lambda}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') \left(\bar{x}_0(t') - \frac{1}{m} \int_{t_a}^{t_b} dt'' \Delta(t', t'') J(t'') \right)^3 + \dots\end{aligned}\quad (3.107)$$

We may simplify the problem (and hence this expression) by choosing $x_a = x_b = 0$, so $\bar{x}_0(t) = 0$.

Iterating further, we may represent Eq. (3.107) diagrammatically: In these diagrams, each line corresponds to $(1/m) \Delta(t, t')$ (with appropriate times for t and t'), each cross to $-\int dt J(t)$, each vertex to $\lambda \int dt$, and the diagrams at $O(\lambda^2)$ (and higher) include some combinatorial factors from the expansion of Eq. (3.107) that must be evaluated explicitly.

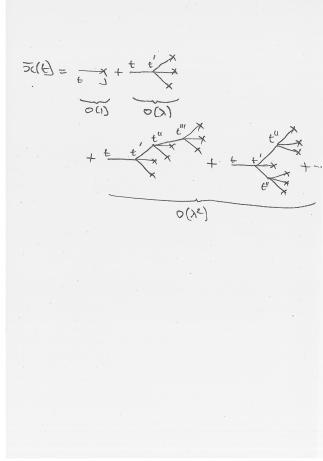


Figure 3.10: A diagrammatic representation of the sum.

1. $\Delta(t, t')$ “propagates” us from t' to t .
2. $J(t)$ acts as a “source” (and a “sink”) for motion.
3. The $(\lambda/4)x^4$ anharmonic term looks like a 4-point “interaction”.
4. We integrate over *all* intermediate times – time ordering is taken care of by the retarded and advanced pieces of $\Delta(t, t')$.
5. Finally, we sum over all possible (tree) graphs.

This looks rather like the *quantum* perturbation theory we studied in the preceding sections...

3.6.2 Quantum mechanics

We will now consider the forced anharmonic oscillator where we take S_0 to be the action for the forced harmonic oscillator we can solve and then add a higher order correction as the perturbation to form $S[x, J] = S_0[x, J] + S_1[x]$ with:

$$S_0[x, J] = \int_{t_a}^{t_b} dt \left(\frac{m}{2}(\dot{x}^2 - \omega^2 x^2) + Jx \right) \quad \text{and} \quad S_1[x] = -\frac{\lambda}{4} \int_{t_a}^{t_b} d\tau x^4. \quad (3.108)$$

We first consider the transition element

$$\langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | x_a, t_a \rangle_J = \int \mathcal{D}x \ x(t_1) \dots x(t_m) \exp \left\{ \frac{i}{\hbar} S[x, J] \right\}, \quad (3.109)$$

where the subscript J is to emphasise that this includes the force term $J(t)$.

Functional differentiation

To proceed, we need to define a functional derivative because we are working on the action which is a functional of continuous functions $x(t)$ and $J(t)$. We need a generalisation for a finite set of

$$\frac{\partial}{\partial J_i} \sum_j J_j x_j = x_i, \quad \text{or} \quad \frac{\partial}{\partial J_i} J_j = \delta_{ij}. \quad (3.110)$$

Generalise so that

$$\frac{\partial}{\partial J(t)} J(t') = \delta(t - t'), \quad (3.111)$$

giving

$$\begin{aligned} \frac{\delta}{\delta J(t)} \int_{t_a}^{t_b} J(t') x(t') dt' &= \int_{t_a}^{t_b} \delta(t - t') x(t') dt' \\ &= x(t) \quad t_a < t' < t_b \quad (0 \text{ otherwise}). \end{aligned} \quad (3.112)$$

Returning to Eq. (3.109), we now have

$$\begin{aligned} &\langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | x_a, t_a \rangle_J \\ &= \int \mathcal{D}x \ x(t_1) \dots x(t_m) \exp \frac{i}{\hbar} \left\{ S[x, 0] + \int_{t_a}^{t_b} dt J(t) x(t) \right\} \\ &= \int_{x_a}^{x_b} \mathcal{D}x \left(\frac{\hbar}{i} \frac{\delta}{\delta J(t_1)} \right) \dots \left(\frac{\hbar}{i} \frac{\delta}{\delta J(t_m)} \right) \exp \frac{i}{\hbar} \left\{ S[x, 0] + \int_{t_a}^{t_b} J(t) x(t) dt \right\} \\ &= \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \langle x_b, t_b | x_a, t_a \rangle_J. \end{aligned} \quad (3.113)$$

We therefore find that the m -point transition element can be expressed as a functional derivative of the exact transition amplitude where both amplitudes are valid for non-zero $J(t)$.

However, if we set $J = 0$ after the differentiation, we recover the results for the amplitudes with $J = 0$:

$$\langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | x_a, t_a \rangle = \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \langle x_b, t_b | x_a, t_a \rangle_J \Big|_{J=0} \quad (3.114)$$

Perturbation expansion

In order to obtain a perturbative expansion, we first expand $\exp(iS_1/\hbar)$ as a power series in λ , as we've done in the previous sections. This gives

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle_J &= \int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} (S_0[x, J] + S_1[x]) \right\} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\lambda}{4\hbar} \right)^n \int_{t_a}^{t_b} d\tau_1 \dots \int_{t_a}^{t_b} d\tau_n \int_{x_a}^{x_b} \mathcal{D}x \ x(\tau_1)^4 \dots x(\tau_n)^4 \\ &\quad \times \exp \frac{i}{\hbar} \left\{ S_0[x, 0] + \int_{t_a}^{t_b} J(t) x(t) dt \right\}. \end{aligned} \quad (3.115)$$

Secondly we now replace all the factors of $x(\tau_i)^4$ by functional derivatives with respect to $J(\tau_i)$

$$\begin{aligned} &\langle x_b, t_b | x_a, t_a \rangle_J \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\lambda}{4\hbar} \right)^n \left[\prod_{k=1}^n \int_{t_a}^{t_b} d\tau_k \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau_k)} \right)^4 \right] \int_{x_a}^{x_b} \mathcal{D}x \ \exp \left\{ \frac{i}{\hbar} S_0[x, J] \right\}, \end{aligned} \quad (3.116)$$

or

$$\begin{aligned} &\langle x_b, t_b | x_a, t_a \rangle_J \\ &= \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \int_{x_a}^{x_b} \mathcal{D}x \ \exp \left\{ \frac{i}{\hbar} S_0[x, J] \right\} \\ &= \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \times F_\omega(T) \exp \left\{ \frac{i}{\hbar} S_0[\bar{x}, J] \right\}, \end{aligned} \quad (3.117)$$

where the final path integral in the final line is now just the path integral for the forced harmonic oscillator solved in Eq. (2.77).

Alternatively this result combined with Eq. (3.113) gives the expression for *all* transition amplitudes to *all* orders in perturbation theory, all in terms of the transition amplitude for the forced harmonic oscillator:

$$\begin{aligned} &\langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | x_a, t_a \rangle_J \\ &= \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \\ &\quad \times F_\omega(T) \exp \left\{ \frac{i}{\hbar} S_0[\bar{x}, J] \right\}. \end{aligned} \quad (3.118)$$

Further evaluation

Here we will simplify things by taking homogeneous boundary conditions: $x_a = 0$ and $x_b = 0$. Then the classical path satisfies

$$\ddot{\bar{x}} + \omega^2 \bar{x} = \frac{J}{m}, \quad (3.119)$$

with $\bar{x}(t_a) = 0 = \bar{x}(t_b)$. This has the solution

$$\bar{x}(t) = -\frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') J(t') \quad (3.120)$$

where $\Delta(t, t')$ is the corresponding Green function defined previously such that

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) \Delta(t, t') = -\delta(t - t'), \quad \Delta(t_b, t') = 0, \quad \Delta(t_a, t') = 0. \quad (3.121)$$

Using our standard integration by parts, we now find

$$\begin{aligned} S_0[\bar{x}, J] &= \int_{t_a}^{t_b} dt \left(\frac{m}{2} (\dot{\bar{x}}^2 - \omega^2 \bar{x}^2) + J \bar{x} \right) \\ &= \frac{1}{2} \int_{t_a}^{t_b} dt J(t) \bar{x}(t) \\ &= -\frac{1}{2m} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t'). \end{aligned} \quad (3.122)$$

[Evaluating this further (a little work) we find $S_0[\bar{x}, J]$ to agree with the result of example sheet II.]

Substituting this into Eq. (3.118), then gives

$$\begin{aligned} &\frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | 0, t_a \rangle_J \\ &= \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \\ &\quad \times \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}. \end{aligned} \quad (3.123)$$

3.7 Examples

3.7.1 The Harmonic Oscillator

Two-point correlation function

As a first example we will set $\lambda = 0$ and evaluate the *two-point correlation function*.

We have

$$\begin{aligned}
& \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2)) | 0, t_a \rangle_{J=0} \\
&= \left[\left(-\frac{\hbar}{i} \right)^2 \frac{\delta^2}{\delta J(t_1) \delta J(t_2)} \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \\
&= \left[\left(-\frac{\hbar}{i} \right)^2 \frac{\delta^2}{\delta J(t_1) \delta J(t_2)} \left\{ 1 - \frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') + \mathcal{O}(J^4) \right\} \right]_{J=0} \\
&= \frac{i\hbar}{2m} \frac{\delta}{\delta J(t_1)} 2 \int_{t_a}^{t_b} dt J(t) \Delta(t, t_2) \\
&= \frac{i\hbar}{m} \Delta(t_1, t_2), \tag{3.124}
\end{aligned}$$

where we have used $\Delta(t, t') = \Delta(t', t)$.

Note that the terms which contain four or more occurrences of J do not contribute because they vanish when we take $J = 0$ at the end.

Four-point correlation function

We can repeat a similar exercise to find the *four-point* function:

$$\begin{aligned}
& \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2) \hat{x}(t_3) \hat{x}(t_4)) | 0, t_a \rangle_{J=0} \\
&= \left[\frac{\hbar^4 \delta^4}{\delta J(t_1) \delta J(t_2) \delta J(t_3) \delta J(t_4)} \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \\
&= \frac{\hbar^4 \delta^4}{\delta J(t_1) \delta J(t_2) \delta J(t_3) \delta J(t_4)} \frac{1}{2!} \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}^2 \\
&= -\frac{\hbar^2}{m^2} [\Delta(t_1, t_2) \Delta(t_3, t_4) + \Delta(t_1, t_3) \Delta(t_2, t_4) + \Delta(t_1, t_4) \Delta(t_2, t_3)]. \tag{3.125}
\end{aligned}$$

We also use a diagrammatic representation of this, where each time is represented by a point and each occurrence of $\Delta(t_i, t_j)$ is represented by a line between those points, see Fig. 3.11.

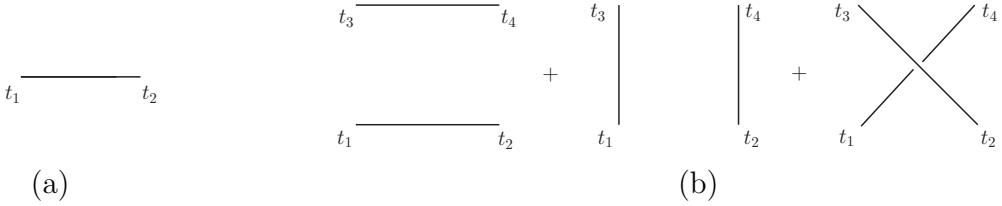


Figure 3.11: Diagrammatic representations of (a) the two-point function (Eq. (3.124)) and (b) the four-point function (Eq. (3.125)). Each straight line connecting t_i and t_j represents a factor of $\Delta(t_i, t_j)$.

Again there is only one term in the exponential which contributes. The J^2 -term vanishes when you perform four derivatives and the terms with more than four J s vanish when J is set to zero at the end.

The final result is symmetric with respect to swapping any pair of $\{t_1, t_2, t_3, t_4\}$ because of the symmetry of the differentiation. This is a general property. Indeed, the general result when $\lambda = 0$ is

$$\begin{aligned} & \frac{1}{F_\omega(T)} \langle 0, t_b | \hat{x}(t_1) \dots \hat{x}(t_m) | 0, t_a \rangle_{J=0} \\ &= \left(\frac{i\hbar}{m} \right)^{m/2} \sum_{\text{all pairings}} \Delta(t_{i_1}, t_{i_2}) \dots \Delta(t_{i_{m-1}}, t_{i_m}), \end{aligned} \quad (3.126)$$

where m is even and is zero when m is odd (because every term in the exponential has an even number of J s). The sum runs over all distinct ways of forming $m/2$ pairs from the set.

This result is known as **Wick's Theorem**.

3.7.2 The Anharmonic Oscillator

We will now consider $\lambda \neq 0$ and evaluate the four-point function again, to first order in λ . We have

$$\begin{aligned} & \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2) \hat{x}(t_3) \hat{x}(t_4)) | 0, t_a \rangle_{J=0} \\ &= \left[\frac{\hbar^4 \delta^4}{\delta J(t_1) \delta J(t_2) \delta J(t_3) \delta J(t_4)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar \delta}{i\delta J(\tau)} \right)^4 \right\} \right. \\ & \quad \times \left. \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \end{aligned} \quad (3.127)$$

The first-order (order λ) contribution is obtained from the first term in the expansion of the first exponential. This gives eight derivatives in total, so the only term to contribute in the second exponential is the term to the fourth power. We therefore get

$$\begin{aligned} & \frac{\hbar^4 \delta^4}{\delta J(t_1) \delta J(t_2) \delta J(t_3) \delta J(t_4)} \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar \delta}{i\delta J(\tau)} \right)^4 \right\} \\ & \times \frac{1}{4!} \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}^4. \end{aligned} \quad (3.128)$$

We will first perform the derivatives with respect to $J(\tau)$ and keep only the terms where each derivative acts on a different term in the second bracket.

This gives

$$\begin{aligned} & \frac{\hbar^4 \delta^4}{\delta J(t_1) \delta J(t_2) \delta J(t_3) \delta J(t_4)} \left(-\frac{i\lambda}{4\hbar} \right) \left(\frac{\hbar}{i} \right)^4 \\ & \times \frac{8.6.4.2}{4!} \int_{t_a}^{t_b} d\tau \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt' \Delta(\tau, t') J(t') \right\}^4 \\ & = -i \frac{3!\lambda}{\hbar} \int_{t_a}^{t_b} dt \prod_{i=1}^4 \left(\frac{i\hbar}{m} \Delta(t, t_i) \right). \end{aligned} \quad (3.129)$$

The Feynman diagram for this is shown in Fig. 3.12.

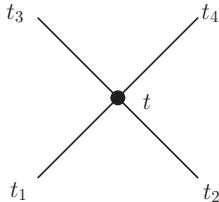


Figure 3.12: The Feynman diagram for the leading order term for the anharmonic oscillator, Eq. (3.129).

The terms which we did not calculate are those where two derivatives with respect to $J(\tau)$ act on J s from the same $J(t)\Delta(t, t')J(t')$ term, giving a term proportional to $\Delta(\tau, \tau)$.

One can check explicitly that these lead to disconnected diagrams. We are in general only interested in connected contributions and hence we do not consider them further here.

A summary of the Feynman rules for the anharmonic oscillator is given in Fig. 3.13. One can check that these agree with the expressions in Eqs. (3.124), (3.125) and (3.129).

$$\bullet \quad t \quad -i\frac{3!\lambda}{\hbar} \int_{t_a}^{t_b} dt$$

$$t \xrightarrow{\hspace{1cm}} t' \quad \frac{i\hbar}{m} \Delta(t, t')$$

Figure 3.13: The Feynman rules for interpreting diagrams for the anharmonic oscillator.

3.7.3 Taking the $t_a \rightarrow -\infty, t_b \rightarrow +\infty$ limits

Want to pick out a definite state, but $\Delta(t, t')$ oscillates wildly for large times.

- The ground state in a ground state problem (as here)
- Definite ‘in’ and ‘out’ states in a scattering problem

To make well defined (all equivalent):

1. Take $t = -i\tau$ as in Statistical mechanics, see section 2.15
2. Rotate t slightly, $t \rightarrow t - i\epsilon$, see section 2.14 (‘Retarded Green function’)
3. Equivalently dampen path integral (also mentioned in section 2.14)

The last two are called the **$i\epsilon$ prescription**. We now briefly consider point 3.

The trick is to take

$$\omega' = \omega - i\epsilon, \quad (3.130)$$

where ϵ is infinitesimal but non-zero and > 0 , ie 0^+ , in the action, so

$$S' = S + i\epsilon \int_{-\infty}^{\infty} x^2 dt \quad \Rightarrow \quad e^{\frac{i}{\hbar} S'} = e^{\frac{i}{\hbar} S - \epsilon \int x^2 dt}. \quad (3.131)$$

So states with $x \neq 0$ as $t_{b,a} \rightarrow \pm\infty$ are exponentially suppressed. Now consider the propagator.

Propagator

In the limit $t_{b,a} \rightarrow \pm\infty$ the first term in $\Delta(t, t')$ in Eq. (3.105) becomes

$$\begin{aligned} & \lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \frac{\sin \omega'(t_b - t) \sin \omega'(t' - t_a)}{\sin \omega' T} \\ &= \lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \frac{\frac{1}{2i} e^{i\omega'(t_b - t)} \frac{1}{2i} e^{i\omega'(t' - t_a)}}{\frac{1}{2i} e^{i\omega' T}} = \frac{1}{2i} e^{-i\omega'(t - t')}, \end{aligned} \quad (3.132)$$

because, eg

$$\sin \omega'(t_b - t) = \frac{1}{2i} [e^{i\omega'(t_b - t)} - e^{-i\omega'(t_b - t)}] \rightarrow \frac{1}{2i} e^{i\omega'(t_b - t)}, \quad (3.133)$$

as $e^{-i\omega'(t_b - t)} = e^{-i(\omega - i\epsilon')(t_b - t)} \rightarrow 0$. This, together with a similar analysis for the second term in Eq. (3.105) gives

$$\begin{aligned} \lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \Delta(t, t') &= \frac{1}{2i\omega'} (e^{-i\omega'(t-t')} \theta(t-t') + e^{i\omega'(t-t')} \theta(t'-t)) \\ &\equiv \Delta_F(t-t'), \end{aligned} \quad (3.134)$$

which is the ‘standard’ Feynman propagator. We can now drop the prime on ω' .

Since ‘in’ and ‘out’ states are suppressed, the in and out states are just ground or ‘vacuum’ states of the SHO.

Formalism

Formalism used in (eg):

- Bound state problems (but rarely)
- Coupled oscillators, anharmonic term gives phonon–phonon scattering
- Quantum Field Theory (QFT)

Key Concepts

1. For a general action, $S = S_0[x] + S_1[x]$, where $S_1[x] = - \int dt V(x(t), t)$, we find

$$\langle x_b, t_b | x_a, t_a \rangle = \langle x_b, t_b | x_a, t_a \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \int_{t_a}^{t_b} \langle x_b, t_b | x, t \rangle_0 V(x, t) \langle x, t | x_a, t_a \rangle_0 \quad (3.135)$$

Substituting recursively for the last amplitude in the integral gives an expansion in powers of $V(x, t)$.

2. The Born approximation for the differential cross section in fixed target scattering is

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2} \right)^2 |\tilde{V}(\vec{q})|^2. \quad (3.136)$$

The total cross section is obtained by integrating this over angular phase space.

3. The analogue of Eq. (3.135) for operators is

$$\hat{U}(t_b, t_a) = \hat{U}_0(t_b, t_a) - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{U}_0(t_b, t) V(\hat{x}, t) \hat{U}(t, t_a). \quad (3.137)$$

4. For time-dependent perturbations in the energy eigenstate basis of the unperturbed system, we find

$$\langle b, t_b | a, t_a \rangle = e^{iT E_a / \hbar} \delta_{ab} + \frac{e^{-iT E_b / \hbar} - e^{-iT E_a / \hbar}}{E_b - E_a} V_{ba} + \dots, \quad (3.138)$$

where $V_{ij}(t) = \langle i | V(\hat{x}, t) | j \rangle$. This leads to Fermi's golden rule

$$R = \frac{2\pi}{\hbar} |V_{ba}|^2 \rho(E_b). \quad (3.139)$$

5. We may write m -point functions as functional derivatives of transition amplitudes as follows:

$$\langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | x_a, t_a \rangle_J = \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \langle x_b, t_b | x_a, t_a \rangle_J, \quad (3.140)$$

where we may choose to set $J = 0$ afterwards. For the forced unharmonic oscillator, we may rewrite this as

$$\begin{aligned} & \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_m)) | 0, t_a \rangle_J \\ &= \left(\frac{\hbar}{i} \right)^m \frac{\delta^m}{\delta J(t_1) \dots \delta J(t_m)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar \delta}{i\delta J(\tau)} \right)^4 \right\} \\ & \quad \times \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}. \end{aligned} \quad (3.141)$$

For a given order of m and λ , there will usually only be one term in the last exponential which gives a non-zero contribution after taking $J = 0$.

Chapter 4

Relativistic Quantum Mechanics

4.1 4-Vector Notation and Lorentz Transformations

4.1.1 4-Vector Notation

The coordinates of an object or ‘event’ in four-dimensional space-time, Minkowski space, are in a **non-orthogonal basis** so we need to introduce *contravariant* and *covariant* components of a four vector.

Contravariant/covariant four-vectors

Contravariant four-vector components have ‘upper’ indices

$$x^\mu \equiv (x^0, x^1, x^2, x^3) \equiv (ct, \vec{x}). \quad (4.1)$$

Similarly, we define a covariant four-vector whose components have ‘lower’ indices:

$$x_\mu \equiv (x_0, x_1, x_2, x_3) \equiv (ct, -\vec{x}). \quad (4.2)$$

A general four-vector a^μ is defined in the same way

$$\begin{aligned} a^\mu &\equiv (a^0, a^1, a^2, a^3) \equiv (a^0, \vec{a}) \\ a_\mu &\equiv (a_0, a_1, a_2, a_3) \equiv (a^0, -\vec{a}) \end{aligned} \quad (4.3)$$

so that $a^0 = a_0$ and $a^i = -a_i$, $i = 1, 2, 3$. Upper and lower indices are related by the *metric tensor* $\eta^{\mu\nu}$ (or $g^{\mu\nu}$)

$$a^\mu = \eta^{\mu\nu} a_\nu \quad a_\mu = \eta_{\mu\nu} a^\nu \quad (4.4)$$

where

$$\eta^{\mu\nu} = \eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (4.5)$$

and we use the Einstein summation convention where there is an implicit sum over the *repeated index*: $\nu = 0, 1, 2, 3$.

The *scalar product* in Minkowski space is defined, for general 4-vectors a^μ and b^μ by

$$\begin{aligned} a \cdot b \equiv a^\mu b_\mu &= a_\mu b^\mu = \eta^{\mu\nu} a_\mu b_\nu = \eta_{\mu\nu} a^\mu b^\nu \\ &= a^0 b^0 - \vec{a} \cdot \vec{b}, \end{aligned} \quad (4.6)$$

where \vec{a} and \vec{b} are ordinary 3-vectors.

We **do not underline** 4-vectors: every pair of repeated indices is implicitly summed over and each pair consists of one upper and one lower index. An expression with two identical upper (or lower) indices (e.g. $a^\mu b^\mu$) is simply wrong.

Differential operators

$$\begin{aligned} \partial_\mu &\equiv \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c} \frac{\partial}{\partial t}, \vec{\nabla} \right) \\ \partial^\mu &\equiv \frac{\partial}{\partial x_\mu} = \left(\frac{1}{c} \frac{\partial}{\partial t}, -\vec{\nabla} \right) \\ \text{d'Alembertian: } \partial_\mu \partial^\mu &= \partial^\mu \partial_\mu = \partial^2 = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2. \end{aligned} \quad (4.7)$$

Momentum and energy

The conserved 4-momentum is denoted by:

$$p^\mu \equiv \left(\frac{E}{c}, \vec{p} \right), \quad (4.8)$$

with

$$p^2 = \frac{E^2}{c^2} - \vec{p} \cdot \vec{p} = m^2 c^2 \quad \text{for a free particle,} \quad (4.9)$$

or

$$E^2 = \vec{p}^2 c^2 + m^2 c^4. \quad (4.10)$$

where m is the mass of the particle.

4.1.2 Lorentz transformations

Lorentz transformations are linear transformations on the components of 4-vectors which leave invariant the scalar product

$$a'^\mu = \Lambda^\mu_\nu a^\nu \quad \text{with} \quad \Lambda^\mu_\alpha \Lambda^\nu_\beta \eta_{\mu\nu} = \eta_{\alpha\beta}. \quad (4.11)$$

Strictly, these are *homogeneous* Lorentz transformations – translations are not included.

The ‘standard’ Lorentz transformation is a ‘boost’ along the x direction

$$\Lambda^\mu{}_\nu = \begin{pmatrix} \cosh \omega & -\sinh \omega & 0 & 0 \\ -\sinh \omega & \cosh \omega & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4.12)$$

where the ‘rapidity’ ω satisfies

$$\begin{aligned} \tanh \omega &\equiv \beta \equiv v/c \\ \cosh \omega &\equiv \gamma = (1 - \beta^2)^{-1/2} = (1 - (v/c)^2)^{-1/2} \\ \sinh \omega &= \gamma \beta. \end{aligned} \quad (4.13)$$

Hence $ct' = \gamma (ct - (v/c)x)$ and $x' = \gamma (x - vt)$ as usual, relating the time and space co-ordinates of a given event in two inertial frames in relative motion.

The group of homogeneous Lorentz transformations includes ordinary 3-dimensional rotations. In fact, such rotations form a subgroup known as the *rotation group*. A familiar example is the rotation of Cartesian co-ordinates about the z -axis, corresponding to the Lorentz transformation

$$\Lambda^\mu{}_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \phi & \sin \phi & 0 \\ 0 & -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4.14)$$

It is clear that in order to describe particles in high-energy collisions we must be able to combine descriptions at the smallest scales, i.e. quantum mechanics, with the description of particles moving close to the speed of light, i.e. special relativity.

To do this we must develop equations which are relativistically invariant (i.e. invariant under Lorentz transformations).

4.2 The relativistic generalisation of the Schrödinger equation

Recall that the Schrödinger equation for a free particle

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t), \quad (4.15)$$

can be obtained from the (non-relativistic) classical total energy

$$E = H = \frac{\vec{p}^2}{2m}, \quad (4.16)$$

by means of the operator substitution prescriptions

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad \vec{p} \rightarrow -i\hbar \vec{\nabla}. \quad (4.17)$$

Using the relativistic expression for the total energy of a free particle $E^2 = \vec{p}^2 c^2 + m^2 c^4$, Schrödinger (and Klein, Gordon and Fock) suggested this as a starting point, thus obtaining

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \phi(\vec{r}, t) = -\hbar^2 c^2 \nabla^2 \phi(\vec{r}, t) + m^2 c^4 \phi(\vec{r}, t), \quad (4.18)$$

or

$$(\hbar^2 \partial^2 + m^2 c^2) \phi(x) = 0. \quad (4.19)$$

which is called the *Klein Gordon (KG) equation* for the wavefunction $\phi(\vec{r}, t)$ of a free relativistic particle.

So the operator prescription in covariant form is

$$p^\mu \rightarrow \hat{p}^\mu = i\hbar \left(\frac{1}{c} \frac{\partial}{\partial t}, -\vec{\nabla} \right) = i\hbar \frac{\partial}{\partial x_\mu} = i\hbar \partial^\mu. \quad (4.20)$$

4.2.1 Free particle solutions and a problem

By substitution into the KG equation (4.18) we see it has plane-wave solutions

$$\phi(\vec{r}, t) = \exp\{i\vec{k} \cdot \vec{r} - i\omega t\}, \quad (4.21)$$

provided that ω , \vec{k} and m are related by

$$\hbar^2 \omega^2 = \hbar^2 c^2 \vec{k}^2 + m^2 c^4. \quad (4.22)$$

Taking the square-root, we get $\hbar\omega = \pm(\hbar^2 c^2 \vec{k}^2 + m^2 c^4)^{1/2}$.

Such solutions are readily seen to be eigenfunctions of the momentum and energy operators, with eigenvalues $\vec{p} \equiv \hbar\vec{k}$ and $E \equiv \hbar\omega$, respectively.

Thus, if we interpret $\hbar\omega$ as an allowed total energy of the free particle solution, there is an ambiguity in the **sign** of the total energy: there are both +ve and -ve energy solutions, and these have energy

$$E = \pm \sqrt{\vec{p}^2 c^2 + m^2 c^4}. \quad (4.23)$$

The positive-energy eigenvalues are in agreement with the classical relativistic relation between energy, mass, and momentum, but what should we make of particles with negative total energy?

If we define the four-vector $k^\mu \equiv (\omega/c, \vec{k})$, so $p^\mu = \hbar k^\mu$ we can write the solution in covariant form

$$\phi(x) \equiv \exp(-ik \cdot x) \equiv \exp(-ip \cdot x/\hbar). \quad (4.24)$$

4.2.2 A further problem – continuity equation and probability interpretation

Denote the Schrödinger equation by (SE) and its complex-conjugate by (SE)^{*}. Considering $0 = \psi^*(\text{SE}) - \psi(\text{SE})^*$ gives a continuity equation

$$\frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} = 0, \quad (4.25)$$

where

$$\rho = \psi^* \psi \quad \text{and} \quad \vec{j} = -\frac{i\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*), \quad (4.26)$$

are the probability density and probability current density, respectively.

If we repeat this for the Klein Gordon equation (see problem sheet X), we obtain the quantities

$$\rho = \frac{i\hbar}{2mc^2} \left(\phi^* \frac{\partial \phi}{\partial t} - \phi \frac{\partial \phi^*}{\partial t} \right) \quad \text{and} \quad \vec{j} = -\frac{i\hbar}{2m} \left(\phi^* \vec{\nabla} \phi - \phi \vec{\nabla} \phi^* \right). \quad (4.27)$$

Note

- \vec{j} is identical in form to the non-relativistic Schrödinger current density (we have chosen to normalise \vec{j} so that this is the case).
- The candidate for the probability density, $\rho(x)$, is no longer positive definite – negative energy solutions for eg plane wave (free particle) have $\rho < 0$, (see problem sheet X). Therefore there is a further difficulty, there is no obvious probability-density interpretation.
- ρ can be shown to reduce to $\psi^* \psi$ in the non-relativistic limit.

4.3 The Dirac Equation

Dirac tried to avoid the twin difficulties of negative energy and negative probability by proposing a relativistic wave equation which, like the Schrödinger equation, is

linear in $\partial/\partial t$, hoping to avoid the sign ambiguity in the square-root of E^2 , and also the presence of time derivatives in the ‘probability density’.

Relativity then dictates that the equation should also be linear in the spatial derivatives in order to treat space and time on an equal footing.

Following Dirac, we start with a Hamiltonian equation of the form

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \hat{H} \psi(\vec{r}, t), \quad (4.28)$$

and write

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left\{ c \vec{\alpha} \cdot \vec{p} + \beta mc^2 \right\} \psi(\vec{r}, t) = \hat{H} \psi(\vec{r}, t) \quad (4.29)$$

where

$$\vec{\alpha} \cdot \vec{p} = -i\hbar \alpha^i \frac{\partial}{\partial x^i}. \quad (4.30)$$

By assumption, the quantities α^i and β are independent of derivatives, therefore α^i and β commute with \vec{r} , t , \vec{p} and E but not necessarily with each other.

Since relativistic invariance must be maintained, *ie* $E^2 = \vec{p}^2 c^2 + m^2 c^4$, Dirac demanded that

$$\hat{H}^2 \psi(\vec{r}, t) = \left(c^2 \vec{p}^2 + m^2 c^4 \right) \psi(\vec{r}, t). \quad (4.31)$$

From Eq. (4.29) we have

$$\begin{aligned} \hat{H}^2 \psi(\vec{r}, t) &= \left(c \vec{\alpha} \cdot \vec{p} + \beta mc^2 \right)^2 \psi(\vec{r}, t) \\ &= \left(c^2 (\vec{\alpha} \cdot \vec{p})^2 + \beta^2 m^2 c^4 + mc^3 (\alpha \cdot \vec{p} \beta + \beta \alpha \cdot \vec{p}) \right) \psi(\vec{r}, t) \\ &\equiv \left(c^2 \vec{p}^2 + m^2 c^4 \right) \psi(\vec{r}, t). \end{aligned} \quad (4.32)$$

The $\vec{\alpha}$ and β objects

We thus need them to obey

$$\{\alpha^i, \alpha^j\} = 2\delta^{ij} \quad \text{the anticommutator of } \alpha^i \text{ and } \alpha^j \quad (4.33)$$

$$\{\alpha^i, \beta\} = 0, \quad \beta^2 = 1 \quad (4.34)$$

1. From these relations it’s clear that the α^i and β cannot be ordinary numbers. If we assume they’re *matrices*, then since \hat{H} is hermitian, α^i and β must also be hermitian (and therefore *square*) $n \times n$ matrices.

2. The matrices α^i and β are hermitian so their eigenvalues are all real. Therefore, since $(\alpha^i)^2 = \beta^2 = I$ (the unit matrix), all the eigenvalues must be ± 1 .
3. $\text{Tr}(\alpha^i) = \text{Tr}(\beta) = 0$.

Proof:

$$\begin{aligned}\text{Tr}(\alpha^i) &= \text{Tr}(\beta^2 \alpha^i) = \text{Tr}(\beta \alpha^i \beta) \quad [\text{using } \text{Tr}(AB) = \text{Tr}(BA)] \\ &= -\text{Tr}(\alpha^i \beta^2) \quad [\text{using } \alpha^i \beta = -\beta \alpha^i] \\ &= -\text{Tr}(\alpha^i) = 0\end{aligned}$$

4. Since the eigenvalues are ± 1 , and the trace is the sum of the eigenvalues ($= 0$), n must be *even*.

It is not possible to find a set of 4 traceless hermitian 2×2 matrices which satisfy the anti-commutation relations; the 3 Pauli matrices σ^i satisfy $\{\sigma^i, \sigma^j\} = 2\delta^{ij}$, but there is no 4th matrix.

The smallest representation of α^i and β is 4×4 , and may be constructed using the Pauli matrices σ^i as sub-matrices. The *standard representation* has β diagonal:

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad (4.35)$$

where each element is a 2×2 submatrix, and $\vec{\alpha}$ is shorthand for a ‘three vector’ of 4×4 matrices α^i .

The 2×2 sigma matrices are defined as

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.36)$$

Since the Hamiltonian is a 4×4 matrix, the wave-function $\psi(\vec{r}, t)$ it acts on is naturally a *4-component column matrix* or *4-component spinor*

$$\psi(\vec{r}, t) = \begin{pmatrix} \psi_1(\vec{r}, t) \\ \psi_2(\vec{r}, t) \\ \psi_3(\vec{r}, t) \\ \psi_4(\vec{r}, t) \end{pmatrix}. \quad (4.37)$$

Probability Density

The Dirac equation for a free particle is

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left(-i\hbar c \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi(\vec{r}, t). \quad (4.38)$$

Construction of the probability density is straightforward.

Take the Hermitian conjugate of Eq. (4.38) (*i.e.* complex conjugate and transpose)

$$-i\hbar \frac{\partial}{\partial t} \psi^\dagger(\vec{r}, t) = \psi^\dagger(\vec{r}, t) \left(i\hbar c \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right). \quad (4.39)$$

Note that ψ^\dagger is a row vector whose components are the complex conjugates of the components of ψ . Then $0 = \psi^\dagger(DE) - (DE)^\dagger \psi$ gives the continuity equation

$$\frac{\partial}{\partial(ct)} \rho + \vec{\nabla} \cdot \vec{j} = 0, \quad (4.40)$$

with

$$\rho = \psi^\dagger \psi \quad \text{and} \quad \vec{j} = \psi^\dagger \vec{\alpha} \psi, \quad (4.41)$$

where $\rho = \psi^\dagger \psi \equiv |\psi|^2$ is a positive definite quantity as required of a probability density.

We can write the continuity equation in covariant form as

$$\partial_\mu j^\mu = 0 \quad \text{with} \quad j^\mu = (\rho, \vec{j}). \quad (4.42)$$

This is usually known as *probability-current density conservation* and it implies that $\psi^\dagger \psi$ transforms like the time-like component of a 4-vector, with $\psi^\dagger \vec{\alpha} \psi$ the corresponding space part, which we identify as the usual probability-current density.

4.3.1 Free Particle Solutions

Let's look for plane-wave solutions of the form

$$\begin{aligned} \psi(\vec{r}, t) &= \exp(-ik \cdot x) w(p) = \exp(-ip \cdot x/\hbar) w(p) \\ &= \exp \left\{ -\frac{i}{\hbar} (cp^0 t - \vec{p} \cdot \vec{r}) \right\} w(p), \end{aligned} \quad (4.43)$$

where $w(p)$ is a 4-component column matrix or **spinor**.

Substituting into the Dirac equation (4.38) and dividing out by $c \exp(-ip \cdot x/\hbar)$, yields

$$p^0 w(p) = (\vec{\alpha} \cdot \vec{p} + \beta mc) w(p), \quad (4.44)$$

which is sometimes called the momentum-space or ‘ p -space’ Dirac equation. The trial solution presumably represents a particle of energy cp^0 and momentum \vec{p} .