

The University of Edinburgh
School of Physics and Astronomy



Lecture Notes

Quantum Theory

September 2015

Abstract

Historically quantum mechanics began with two quite different mathematical formulations: the wave equation of Schrödinger, and the matrix algebra of Heisenberg, Born and Jordan. While these approaches are well suited to the time-independent non-relativistic bound state problems of atomic and molecular physics, many problems in condensed matter, statistical physics and particle physics are better suited to a more intuitive formulation of quantum mechanics based on the ideas of Dirac and Feynman, namely the *path integral* or *sum over histories* approach. In this course we begin with a review of the fundamental ideas of quantum mechanics; we introduce the path integral for a non-relativistic point particle, and we use it to derive time-dependent perturbation theory, the Born series for nonrelativistic scattering, and Feynman perturbation theory. The course concludes with an introduction to relativistic quantum mechanics and some of the basic ideas of quantum field theory.

Preamble

Formulations of Quantum Mechanics

Quantum Mechanics started with two ostensibly-different formulations, both based on the Hamiltonian:

(1925) Heisenberg, Born and Jordan: *Matrix Mechanics*

(1925) Schrödinger: *Wave Mechanics*

These were shown to be equivalent by Dirac and Schrödinger (and Born?) in 1926, and later generalised by Dirac's *transformation theory*.

Wave Mechanics and *Matrix Mechanics* are well-suited to the study of non-relativistic bound states and other time-independent systems, and also to scattering and time-dependent problems.

(1942) Feynman: *Path Integral* or *Sum over Histories*

Feynman's formulation is based on the Lagrangian and is ideal for scattering and time-dependent problems, and (especially) for relativistic and many-particle systems. Unfortunately, bound-state problems are generally harder to solve using path integrals, as we shall see.

Structure of the course:

- (1) Elements of quantum mechanics;
- (2) Path integrals for single particles;
- (3) Perturbation theory and scattering;
- (4) Relativistic quantum theory – mostly wave mechanics, plus a hint of field theory.

Acknowledgements

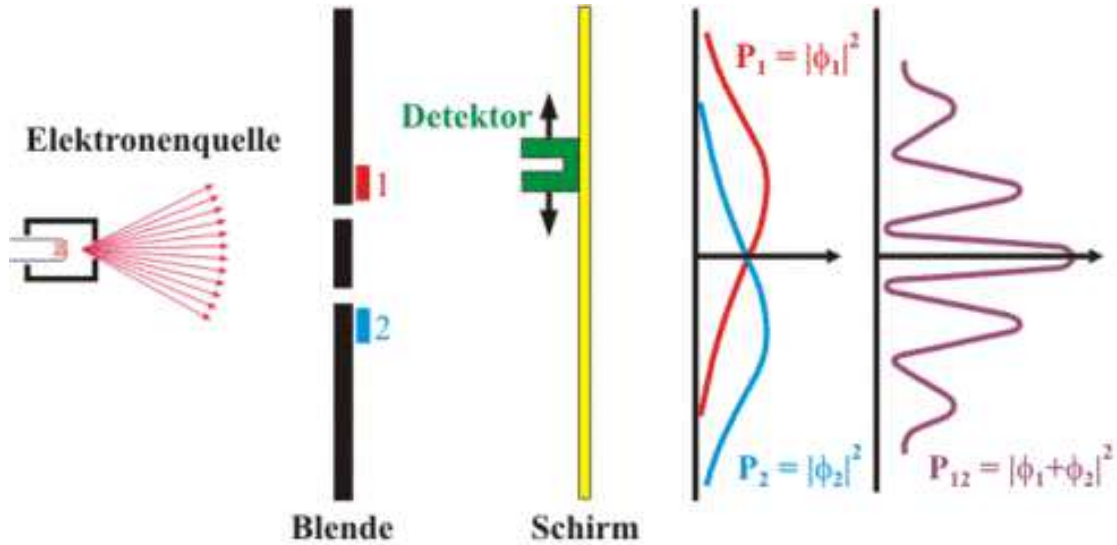
These notes are based on the Quantum Theory lectures written by Richard Ball and typeset by Friedmar Schütze. Many thanks to both for providing copies of their work. Any mistakes are of course my responsibility - please send error reports to bjp@ph.ed.ac.uk

Brian Pendleton

Edinburgh, September 2015

1. Quantum Kinematics

We begin by revisiting one of the classic experiments that led to quantum theory. The setup of the two-slit experiment is summarised in the diagram.



Particles (electrons, photons, ...) are fired from a source towards a screen or “grating” which contains two slits, 1 and 2. They are then detected, or “observed”, on a second screen.

The classical *expectation* is a count profile $P_1 + P_2$, which is the sum of the count profiles P_1 and P_2 for the individual slits (red and blue curves).

However, the observed *interference pattern* in the count profile P_{12} of particles (purple curve) suggests that such particles behave like waves, so we must add *amplitudes* (called ϕ_1 and ϕ_2 in the figure); the number of particles (intensity) at any point is given by $|\sum \text{amplitude}|^2$. Interference means that we observe no particles at all in some places - entirely contrary to classical expectation! Furthermore, there is no way to predict where any given particle will be detected - we deal only in probabilities. The results of this experiment (and many, many more!) are encoded in the basic axioms of Quantum Mechanics.

1.1. Fundamental principles (or postulates, axioms)

States and linearity: In quantum mechanics, every possible physical state of a given system is in one-to-one correspondence with a one-dimensional subspace of a complex linear vector space, \mathcal{H} , with a complex inner product - a Hilbert space.

So, if $|\psi\rangle \in \mathcal{H}$, the physical state corresponds to all vectors $c|\psi\rangle$ with $c \in \mathbb{C} \setminus \{0\}$. There is no physical state corresponding to zero.

Since the vector space is linear, given two states $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$, we can construct a third state

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

This is called *linear superposition* of states.

Dual space: To every $|\psi\rangle \in \mathcal{H}$ we associate a *dual* or *adjoint* vector $\langle\psi| \in \mathcal{H}^*$. The duality is *antilinear*:

$$\langle\psi_3| = c_1^* \langle\psi_1| + c_2^* \langle\psi_2|$$

We then have an inner product mapping $\mathcal{H} \otimes \mathcal{H}^* \rightarrow \mathbb{C}$. If $|\psi\rangle \in \mathcal{H}$ and $\langle\phi| \in \mathcal{H}^*$, then

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \in \mathbb{C}. \quad (1.2)$$

(This is like the usual dot-product $\underline{a} \cdot \underline{b}$ for real vectors $\underline{a}, \underline{b}$, but the result is in general complex.)

Since $|\psi\rangle$ and $c|\psi\rangle$ correspond to the same physical state, we usually normalise $|\psi\rangle$ to unity: we *choose*:

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

This fixes $|c|^2 = 1$, so $c = e^{i\alpha}$. The phase α is often ignored: we say “the system is in the state $|\psi\rangle$ ”.

Example: In the two-slit experiment, the Hilbert space has two states:

- |1⟩ (the particle goes through slit 1)
- |2⟩ (the particle goes through slit 2)

The state $|f\rangle$ observed in the detector will in general be some linear combination of these:

$$|f\rangle = c_1 |1\rangle + c_2 |2\rangle$$

Examples of two-state systems in nature: electron spin, double-well potential, neutral-kaon mixing. . .

Probability: the probability that a system observed initially in state $|\psi\rangle$ will be observed finally in state $|\phi\rangle$ is

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

The complex numbers $\langle \phi | \psi \rangle$ are called *probability amplitudes* because they add and multiply just like classical probabilities. For example:

- The amplitude for $\psi \rightarrow \phi$ and then $\phi \rightarrow \chi$ is $\langle \chi | \phi \rangle \langle \phi | \psi \rangle$.
- The amplitude for $\psi \rightarrow \phi$ or χ is $\langle \phi | \psi \rangle + \langle \chi | \psi \rangle$; (indistinguishable ϕ, χ)
- This means that

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

but

$$P(\psi \rightarrow \phi \text{ or } \chi) \neq P(\psi \rightarrow \phi) + P(\psi \rightarrow \chi)$$

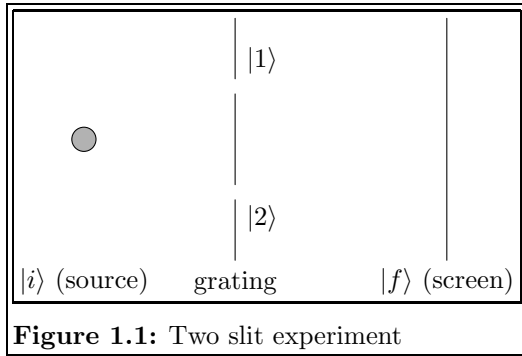
because

$$|\langle \phi | \psi \rangle + \langle \chi | \psi \rangle|^2 = |\langle \phi | \psi \rangle|^2 + |\langle \chi | \psi \rangle|^2 + 2\text{Re} \langle \phi | \psi \rangle^* \langle \chi | \psi \rangle$$

The last term is the *interference term*. In particular, $P(\psi \rightarrow \phi \text{ or } \chi)$ can be zero even if $P(\psi \rightarrow \phi)$ and $P(\psi \rightarrow \chi)$ are both non-zero.

In general amplitudes can *interfere!*

An excellent example is the two slit experiment. A theorist's sketch of the experimental setup of this experiment is shown in figure 1.1.



The probability amplitude for a particle (electron) initially in the state $|i\rangle$ (at the source) to pass through slit 1, and be detected in the final state $|f\rangle$ (on the second screen) is:

$$\phi_1 = \langle f | 1 \rangle \langle 1 | i \rangle$$

Similarly, the amplitude for the electron initially in the state $|i\rangle$ to pass through slit 2, and be detected in the state $|f\rangle$ is:

$$\phi_2 = \langle f | 2 \rangle \langle 2 | i \rangle$$

The probability amplitude for a particle (electron) initially in the state $|i\rangle$ (at the source) to be detected in the final state $|f\rangle$ (on the second screen) is obtained by *adding the amplitudes to pass through through the individual slits*:

$$\langle f | i \rangle = \phi_1 + \phi_2 = \langle f | 1 \rangle \langle 1 | i \rangle + \langle f | 2 \rangle \langle 2 | i \rangle$$

For the probability, we have:

$$\begin{aligned} P(i \rightarrow f) &= |\langle f | i \rangle|^2 = |\phi_1 + \phi_2|^2 \\ &= |\langle f | 1 \rangle \langle 1 | i \rangle + \langle f | 2 \rangle \langle 2 | i \rangle|^2 \\ &= |\langle f | 1 \rangle \langle 1 | i \rangle|^2 + |\langle f | 2 \rangle \langle 2 | i \rangle|^2 + 2\text{Re} \{ \langle f | 1 \rangle \langle 1 | i \rangle \langle f | 2 \rangle^* \langle 2 | i \rangle^* \} \\ &\neq |\langle f | 1 \rangle \langle 1 | i \rangle|^2 + |\langle f | 2 \rangle \langle 2 | i \rangle|^2 \end{aligned} \tag{1.4}$$

Question: Why?

Answer: The probability $P(i \rightarrow f) \neq P(i \rightarrow f \text{ via } 1) + P(i \rightarrow f \text{ via } 2)$ because $P(i \rightarrow f)$ can *vanish* if the amplitudes for the different paths cancel. The last term in the second-last line of equation (1.4) is the *interference term*.

Question: For a given $i \rightarrow f$, which way does the electron go? Through slit 1 or slit 2?

Answer: We don't know – if we don't look...

If we do look, this changes the experiment – if we find the particle goes through slit 1, then

$$P(i \rightarrow f) \rightarrow P(i \rightarrow f \text{ via } 1) = |\langle f|1\rangle \langle 1|i\rangle|^2$$

and there is no interference.

In quantum mechanics, electrons can go through slit 1, or slit 2, or “both” - provided we don't check!

Distinguishability: In the two-slit experiment, we don't know whether the particle we detected at some point on the screen passed through slit 1 or slit 2 – the two outcomes are *indistinguishable*. In this case, we add amplitudes

$$P(\psi \rightarrow \xi \text{ or } \chi) = |\langle \xi|\psi\rangle + \langle \chi|\psi\rangle|^2 \neq P(\psi \rightarrow \xi) + P(\psi \rightarrow \chi)$$

If we have two final states $|\xi\rangle$ and $|\chi\rangle$, which are *distinguishable*, the probability for $\psi \rightarrow \xi$ or χ is

$$P(\psi \rightarrow \xi \text{ or } \chi) = |\langle \xi|\psi\rangle|^2 + |\langle \chi|\psi\rangle|^2 = P(\psi \rightarrow \xi) + P(\psi \rightarrow \chi)$$

i.e. we add probabilities – just as in classical probability.

1.2. Basis states

Within our assumption for the space of states to be a Hilbert space we implicitly assumed the linear space to be *complete*. This means that there exists a set of basis states $\{|n\rangle\}$ (assumed for the moment to be countable) such that for any $|\psi\rangle \in \mathcal{H}$:

$$|\psi\rangle = \sum_n \psi_n |n\rangle \quad (1.5)$$

for some complex numbers ψ_n – the *components* of $|\psi\rangle$ in the basis $\{|n\rangle\}$. The basis vectors may be chosen to be *orthonormal*:

$$\langle m|n\rangle = \delta_{mn}. \quad (1.6)$$

Then the following equation holds:

$$\langle m|\psi\rangle = \sum_n \psi_n \langle m|n\rangle = \psi_m. \quad (1.7)$$

So ψ_m is the probability amplitude for $|\psi\rangle$ to go to $|m\rangle$, and we have

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle \quad (1.8)$$

Since this is true for all $|\psi\rangle \in \mathcal{H}$, we often write

$$\sum_n |n\rangle \langle n| = \hat{1} \quad (1.9)$$

where $\hat{1}$ is the unit or identity operator, and the sum is over a complete set of states $\{|n\rangle\}$. This is an *extremely* useful result and we shall use it many, many times in what follows.

Equation (1.9) expresses the completeness of the basis states: at any moment a state must be in some linear superposition of them. Note that completeness is necessary for the probability interpretation to work:

$$1 = \langle \psi|\psi\rangle = \sum_n \langle \psi|n\rangle \langle n|\psi\rangle = \sum_n |\langle n|\psi\rangle|^2 = \sum_n P(\psi \rightarrow n) \quad (1.10)$$

Example: In the two-slit experiment we have a two-component basis, we can represent the states $|1\rangle$ and $|2\rangle$ as

$$|1\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |2\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and

$$\langle f|i\rangle = \sum_{n=1,2} \langle f|n\rangle \langle n|i\rangle$$

simply expresses the fact that the electron must follow a path through *either* slit-1 or slit-2. The states $|i\rangle$ and $|f\rangle$ will in general be linear superpositions of $|1\rangle$ and $|2\rangle$.

1.3. Operators and Observables

Consider an observable which takes real values ξ_n in basis states $|n\rangle$. Then we can construct an operator:

$$\hat{\xi} \equiv \sum_n \xi_n |n\rangle \langle n| \quad (1.11)$$

corresponding to the observable. Equation (1.11) is called the *spectral representation* of the operator.

It is easy to see that:

- (a) $\hat{\xi}$ is a linear operator: $\hat{\xi}(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle) = c_1 \hat{\xi} |\psi_1\rangle + c_2 \hat{\xi} |\psi_2\rangle$
 (b) $\hat{\xi}$ is hermitian:

$$\begin{aligned} \langle \psi | \hat{\xi} | \phi \rangle &= \sum_n \xi_n \langle \psi | n \rangle \langle n | \phi \rangle = \left(\sum_n \xi_n \langle \phi | n \rangle \langle n | \psi \rangle \right)^* \quad (\text{because } \xi_n^* = \xi_n) \\ &= \langle \phi | \hat{\xi} | \psi \rangle^* \equiv \langle \psi | \hat{\xi}^\dagger | \phi \rangle \quad (\text{by definition of the Hermitian conjugate}) \end{aligned}$$

More succinctly, we may write simply: $\hat{\xi}^\dagger = \hat{\xi}$.

- (c) $|n\rangle$ are eigenstates of $\hat{\xi}$, with eigenvalues ξ_n :

$$\hat{\xi} |n\rangle = \sum_m \xi_m |m\rangle \langle m | n \rangle = \xi_n |n\rangle \quad (1.12)$$

- (d) If we have a second observable which takes values η_n on $|n\rangle$, then $\hat{\xi}$ and $\hat{\eta}$ commute:

$$\hat{\xi} \hat{\eta} |n\rangle = \xi_n \eta_n |n\rangle = \eta_n \xi_n |n\rangle = \hat{\eta} \hat{\xi} |n\rangle \quad \forall n, \quad \text{so } [\hat{\xi}, \hat{\eta}] = 0.$$

Measurement: When we make a measurement, the state $|\psi\rangle$ of the system just before the measurement *collapses* into some eigenstate $|n\rangle$ of $\hat{\xi}$: the probability that we measure ξ_n is $|\langle n | \psi \rangle|^2$. The average result over many measurements is thus:

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

which is often called the *expectation value* of $\hat{\xi}$ in the state $|\psi\rangle$. We can think of the measurement process as *projecting* $|\psi\rangle$ onto $|n\rangle$:

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

is the appropriate projection operator, with properties $\hat{P}_n^2 = \hat{P}_n$ and $\sum_n \hat{P}_n = \hat{1}$.

When we make a measurement the state changes:

$$|\psi\rangle \mapsto \hat{P}_n |\psi\rangle = |n\rangle \langle n | \psi \rangle$$

with a probability:

$$\|\hat{P}_n |\psi\rangle\|^2 = \langle \psi | n \rangle \langle n | n \rangle \langle n | \psi \rangle = |\langle n | \psi \rangle|^2.$$

Degeneracy: Often a given operator $\hat{\xi}$ will have degeneracies:

$$\hat{\xi} |n, m\rangle = \xi_n |n, m\rangle$$

for all $m \in M_n$ where M_n is a certain set. Measuring ξ_n then projects onto a degenerate subspace:

$$|\psi\rangle \mapsto \hat{P}_n |\psi\rangle = \sum_m |n, m\rangle \langle n, m | \psi \rangle.$$

To project onto a definite eigenstate requires that we measure further observables which commute with $\hat{\xi}$. This leads to the notion of a *maximally commuting set of observables* – see *Quantum Physics*. (The basis states may be organised into irreducible representations of discrete or continuous symmetries of the system: the observables then correspond to generators of these symmetries – see *Symmetries of Quantum Mechanics*.)

1.4. Change of basis

Consider a change of basis $\{|n\rangle\} \mapsto \{|\bar{n}\rangle\}$. We may express the new basis states in terms of the old ones:

$$|\bar{n}\rangle = \sum_m |m\rangle \langle m|\bar{n}\rangle \equiv \sum_m |m\rangle U_{mn} \quad (1.13)$$

The U_{mn} are sometimes called transformation coefficients (Dirac). Orthonormality of the new basis then implies that

$$\delta_{n'n} = \langle \bar{n}'|\bar{n}\rangle = \sum_m \langle \bar{n}'|m\rangle \langle m|\bar{n}\rangle = \sum_m U_{nm}^\dagger U_{mn} \quad (1.14)$$

where we used $\langle \bar{n}'|m\rangle = \langle m|\bar{n}'\rangle^* = U_{nm}^* \equiv U_{nm}^\dagger$. So U_{mn} is the mn element of a *unitary* matrix. In operator notation we define

$$|\bar{n}\rangle \equiv \hat{U}|n\rangle \quad \text{which gives} \quad U_{mn} = \langle m|\hat{U}|n\rangle \quad (\text{exercise for the student})$$

From (1.14), \hat{U} is a *unitary operator*: $\hat{U}^\dagger \hat{U} = \hat{1}$. Unitary operators are not in general observables because they don't have real eigenvalues.

1.5. Space as a continuum – position and wavenumber

Consider again the two slit experiment shown in figure 1.1, and let us generalise to an N -slit experiment. Then

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

Position basis: If we let $N \rightarrow \infty$, we will need a *continuous* label x . We get the usual transition from discrete to continuous variables

$$|n\rangle \mapsto |x\rangle \quad ; \quad \sum_n \mapsto \int dx \quad ; \quad \delta_{nm} \mapsto \delta(x - x').$$

The component of $|\psi\rangle$ in the basis $|x\rangle$ is now a *function* of the continuous variable x , let's call it $\psi(x)$. We have

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

If we normalise our states so that

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

then

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

so

$$\psi(x) = \langle x|\psi\rangle \quad \text{and} \quad \psi^*(x) = \langle \psi|x\rangle.$$

We may then write

$$|\psi\rangle = \int_a^b dx |x\rangle \langle x|\psi\rangle \quad \text{and thus} \quad \hat{1} = \int_a^b dx |x\rangle \langle x| \quad (1.15)$$

which is the completeness relation (the particle must be somewhere).

Squares of probability amplitudes are now interpreted as *probability densities*:

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

so $|\psi(x)|^2 dx$ is the probability that the particle is between x and $x + dx$, and hence $\psi(x)$ is the usual spatial wavefunction of wave mechanics.

In the continuous version of (1.11) we may define the position operator as

$$\hat{x} = \int_a^b dx x |x\rangle \langle x| \quad (1.16)$$

and verify that

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

From equation (1.16), the *expectation value* of x in the state $|\psi\rangle$ is

$$\langle \psi | \hat{x} | \psi \rangle = \int_a^b dx \langle \psi | x \rangle x \langle x | \psi \rangle = \int_a^b dx \psi^*(x) x \psi(x) \quad (1.17)$$

There is of course no need to restrict ourselves to a finite interval (a, b) . We can let $a \rightarrow -\infty$ and $b \rightarrow \infty$ and take $x \in (-\infty, \infty)$, in which case the transition amplitude for the continuously-infinite-slit experiment may be written

$$\langle f | i \rangle = \int_{-\infty}^{\infty} dx \langle f | x \rangle \langle x | i \rangle$$

Fourier transform basis: We do not have to stay in the position basis. For example consider the Fourier transform basis:

$$|k\rangle \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{+ikx} |x\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x | k \rangle , \quad (1.18)$$

from which we may read off:

$$\langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \quad \text{and hence} \quad \langle k | x \rangle = \frac{1}{\sqrt{2\pi}} e^{-ikx} . \quad (1.19)$$

Then we obtain the following relation:

$$\langle k' | k \rangle = \int_{-\infty}^{\infty} dx \langle k' | x \rangle \langle x | k \rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{i(-k'+k)x} = \delta(k' - k), \quad (1.20)$$

so the transformation is unitary. We can construct a hermitian operator \hat{k} such that:

$$\hat{k} = \int dk k |k\rangle \langle k| \quad \Rightarrow \quad \hat{k} |k\rangle = k |k\rangle \quad (\text{exercise})$$

It follows that

$$\begin{aligned} \hat{k} |x\rangle &= \int dk k |k\rangle \langle k | x \rangle = i \frac{\partial}{\partial x} \int dk |k\rangle \langle k | x \rangle \\ &= i \frac{\partial}{\partial x} |x\rangle . \end{aligned} \quad (1.21)$$

where we used (1.19) to write

$$k \langle k | x \rangle = i \frac{\partial}{\partial x} \left(\frac{1}{\sqrt{2\pi}} e^{-ikx} \right),$$

and hence the last expression on the first line of (1.21).

An immediate consequence of (1.21) is $\langle \psi | \hat{k} | x \rangle = i \frac{\partial}{\partial x} \langle \psi | x \rangle$. Taking the complex conjugate and recalling that \hat{k} is hermitian gives

$$\langle x | \hat{k} | \psi \rangle = -i \frac{\partial}{\partial x} \psi(x). \quad (1.22)$$

Finally

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

which should look familiar from wave mechanics.

Similarly, if we define

$$\tilde{\psi}(k) = \langle k | \psi \rangle = \int dx \langle k | x \rangle \langle x | \psi \rangle = \int \frac{dx}{\sqrt{2\pi}} e^{-ikx} \psi(x) \quad (1.23)$$

we easily find (exercise)

$$\langle k | \hat{k} | \psi \rangle = k \tilde{\psi}(k) \quad \text{and} \quad \langle \phi | \hat{k} | \psi \rangle = \int dk \tilde{\phi}^*(k) k \tilde{\psi}(k), \quad (1.24)$$

while (exercise)

$$\langle k | \hat{x} | \psi \rangle = i \frac{\partial}{\partial k} \tilde{\psi}(k). \quad (1.25)$$

and hence

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

A summary is given in table 1.1. In either basis we get the commutator:

basis	\hat{x}	\hat{k}
position: $ x\rangle$	x	$-i \frac{\partial}{\partial x}$
wavenumber: $ k\rangle$	$i \frac{\partial}{\partial k}$	k

Table 1.1: Operators in different bases

$$[\hat{x}, \hat{k}] = i \quad (1.26)$$

This tells us that the two operators do not correspond to simultaneous observables (as expected). The Heisenberg uncertainty principle can be deduced:

$$\Delta x \Delta k \geq \frac{1}{2}. \quad (1.27)$$

Later we will show that momentum $p = \hbar k$.

Historical note: The commutator (1.26) was deduced independently by Born and Dirac, and the uncertainty principle was formulated independently by each of Heisenberg, Dirac and Jordan.

Three dimensions: All of the above can be generalised to three space dimensions rather easily. For position states and operators:

$$\langle \underline{x}' | \underline{x} \rangle = \delta^{(3)}(\underline{x} - \underline{x}') \quad \hat{1} = \int_{-\infty}^{\infty} d^3x |\underline{x}\rangle \langle \underline{x}| \quad \hat{x} = \int_{-\infty}^{\infty} d^3x \underline{x} |\underline{x}\rangle \langle \underline{x}| \quad \hat{x} |\underline{x}\rangle = \underline{x} |\underline{x}\rangle$$

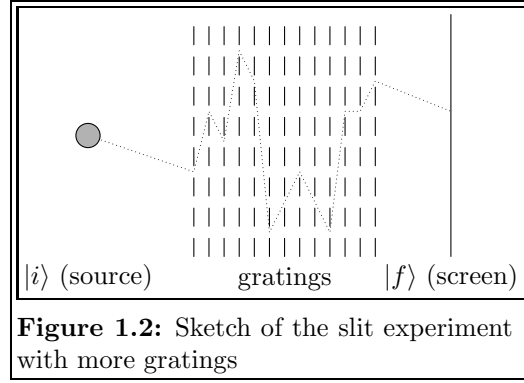
Similarly for the wavevector basis $\{|k\rangle\}$. The wavefunctions in the two bases are related by (exercise)

$$\tilde{\psi}(\underline{k}) = \langle \underline{k} | \psi \rangle = \int d^3x \langle \underline{k} | \underline{x} \rangle \langle \underline{x} | \psi \rangle = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\underline{k}\cdot\underline{x}} \psi(\underline{x})$$

1.6. Time as a continuum

We now add more gratings to the slit experiment. Let the n^{th} grating be passed at position x_n at time t_n , and call this state $|x_n, t_n\rangle$. If we have N gratings the transition amplitude becomes

$$\begin{aligned} \langle f|i\rangle &= \int dx_1 \langle f|x_1, t_1\rangle \langle x_1, t_1|i\rangle \\ &= \int dx_1 \int dx_2 \\ &\quad \langle f|x_2, t_2\rangle \langle x_2, t_2|x_1, t_1\rangle \langle x_1, t_1|i\rangle \\ &= \int dx_1 \cdots \int dx_N \langle f|x_N, t_N\rangle \cdots \langle x_1, t_1|i\rangle \end{aligned} \quad (1.28)$$



where $t_1 < t_2 < \dots < t_N$. By adding more and more gratings the time intervals get smaller and smaller and we fix each path between $|i\rangle$ and $|f\rangle$ more and more precisely. But we also get more and more integrals in order to integrate over all the paths!

For simplicity (and notational convenience) we take $|i\rangle = |x_a, t_a\rangle$ and $|f\rangle = |x_b, t_b\rangle$ and let

$$t_n = t_a + n\varepsilon \quad ; \quad \varepsilon = \frac{t_b - t_a}{N + 1}, \quad (1.29)$$

so that $t_0 = t_a$ and $t_{N+1} = t_b$. Then we obtain for the transition amplitude:

$$\langle x_b, t_b|x_a, t_a\rangle = \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=1}^{N+1} \langle x_n, t_n|x_{n-1}, t_{n-1}\rangle \right). \quad (1.30)$$

The expression in the first pair of parentheses tells us to “integrate over all paths”, and the expression in the second pair is the amplitude for each path.

For $N \rightarrow \infty$ (i.e. $\varepsilon \rightarrow 0$) this becomes:

$$\langle x_b, t_b|x_a, t_a\rangle = \int_{x_a}^{x_b} \mathcal{D}x \langle x_b, t_b|x_a, t_a\rangle |_{x(t)} \quad (1.31)$$

where the continuous path $x(t)$ is such that $x(t_a) = x_a$ and $x(t_b) = x_b$. So, to find the transition amplitude we take the amplitude for *each* path $x(t)$, and then sum (i.e. integrate) over *all* paths between x_a and x_b . This is easy to understand physically but much harder to understand mathematically!

In fact, the limit only exists if we take care to normalise each integral carefully (see later).

What is the amplitude for each path $x(t)$? Intuitively, for a path which is infinitesimal ($t_n = t_{n-1} + \varepsilon$):

$$\langle x_n, t_n|x_{n-1}, t_{n-1}\rangle \sim \exp[i\varepsilon\phi(x_n, x_{n-1}, t_n, t_{n-1})], \quad (1.32)$$

where ϕ is real. This is because:

- (a) in the limit $\varepsilon \rightarrow 0$, the amplitude should be constant (continuity), this is just a normalisation constant;
- (b) the phase should depend only on $x_n, x_{n-1}, t_n, t_{n-1}$ (locality)
- (c) The transition $|x_{n-1}, t_{n-1}\rangle \mapsto |x_n, t_n\rangle$ is just a change of basis, so we expect (up to a constant) $|\langle x_n, t_n|x_{n-1}, t_{n-1}\rangle| \sim 1$, i.e. the amplitude is just a phase (unitarity).

Using (1.30) and (1.32) we can write *the transition amplitude along the path $x(t)$* as:

$$\begin{aligned} \langle x_b, t_b|x_a, t_a\rangle |_{x(t)} &\sim \lim_{N \rightarrow \infty} \prod_{n=1}^{N+1} \exp\{i\varepsilon\phi(x_n, x_{n-1}, t_n, t_{n-1})\} \\ &\sim \exp\left\{i \lim_{N \rightarrow \infty} \sum_{n=1}^{N+1} (t_n - t_{n-1})\phi(x_n, x_{n-1}, t_n, t_{n-1})\right\} \\ &\sim \exp\left\{i \int_{t_a}^{t_b} dt \phi(x(t), \dot{x}(t), t)\right\} \end{aligned} \quad (1.33)$$

To say more (about ϕ) we need to revise and develop some classical mechanics...

2. Quantum Dynamics

2.1. 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. For a non-relativistic point particle in a potential V in one dimension this is:

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

Classical dynamics is based upon the principle of least action: the classical path $\bar{x}(t)$ is an extremum of the functional S . Formally

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

where $\delta S/\delta x$ is the *functional derivative*. For a small variation of the path: $x(t) \mapsto x(t) + \delta x(t)$:

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

where, as usual, we integrated by parts in the last step. If the end-points of the path are fixed, i.e. $\delta x(t_a) = \delta x(t_b) = 0$, then the first term in the last line of (2.4) vanishes, and we obtain Lagrange's equation for the classical path

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

Consider now the *value* of the action S on the classical path: $S_{\text{cl}} \equiv S[\bar{x}(t)]$. S_{cl} will be a function of the end points, i.e. of x_a, t_a, x_b , and t_b .

Let us now vary the endpoint $(x_b, t_b) \mapsto (x_b, t_b) + (\delta x_b, \delta t_b)$, but keep (x_a, t_a) fixed. Lagrange's equation (2.5) holds for the classical path so, from (2.4), we get (choosing $\delta t_b = 0$ for now)

$$\delta S_{\text{cl}} = \left[\frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_a}^{t_b} = [p \delta x]_{t_a}^{t_b} = p(t_b) \delta x_b - p(t_a) \delta x_a = p(t_b) \delta x_b$$

Hence

$$\frac{\partial S_{\text{cl}}}{\partial x_b} = p_b \quad (2.6)$$

where we used the usual definition of the canonical momentum p conjugate to x : $p = \frac{\partial L}{\partial \dot{x}}$.

Now consider $\frac{dS_{\text{cl}}}{dt_b}$. From (2.1) we may write:

$$\frac{dS_{\text{cl}}}{dt_b} = L(x_b, \dot{x}_b, t_b) = \frac{\partial S_{\text{cl}}}{\partial t_b} + \frac{\partial S_{\text{cl}}}{\partial x_b} \dot{x}_b$$

This gives

$$\frac{\partial S_{\text{cl}}}{\partial t_b} = L - p_b \dot{x}_b = -E_b \quad \Rightarrow \quad E_b = -\frac{\partial S_{\text{cl}}}{\partial t_b} \quad (2.7)$$

where E_b is the energy (or, more precisely, the Energy Function or Hamiltonian) at b .

Equations (2.6) and (2.7) are known as the Hamilton-Jacobi equations.

Example 1: The free particle. The Lagrangian L , and the Lagrange equation of motion (EoM) for the classical path $\bar{x}(t)$ are

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

Integrating twice, and imposing the boundary conditions $\bar{x}(t_a) = x_a$ and $\bar{x}(t_b) = x_b$, the solution is (exercise):

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

so v is the (constant) velocity of the particle. The classical action is

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

and, using the Hamilton-Jacobi equations, we get

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

Example 2: The simple harmonic oscillator. The Lagrangian and Lagrange EoM are

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

The solution which satisfies the boundary conditions $\bar{x}(t_a) = x_a$ and $\bar{x}(t_b) = x_b$, with $T \equiv t_b - t_a$, is

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

This is important - check it carefully! Then we have, using integration by parts and the fact that $\bar{x}(t)$ satisfies the classical equation of motion to simplify the calculation,

$$\begin{aligned} S[\bar{x}] &= \int_{t_a}^{t_b} \frac{m}{2} (\dot{\bar{x}}^2 - \omega^2 \bar{x}^2) dt = \frac{m}{2} [\bar{x}\dot{\bar{x}}]_{t_a}^{t_b} - \frac{m}{2} \int_{t_a}^{t_b} \bar{x} (\ddot{\bar{x}} + \omega^2 \bar{x}) dt = \frac{m}{2} [\bar{x}\dot{\bar{x}}]_{t_a}^{t_b} + 0 \\ &= \frac{m\omega}{2 \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right] \end{aligned}$$

You should verify this very important result, and use the Hamilton-Jacobi equations to check that

$$p_b = m\dot{\bar{x}}|_{t=t_b} \quad \text{and} \quad E_b = \frac{m}{2} (\dot{\bar{x}}^2 + \omega^2 \bar{x}^2) |_{t=t_b}.$$

2.2. The Amplitude for a Path

We saw already in (1.33) that we expect the amplitude for the path $x(t)$ to be:

$$\langle x_b, t_b | x_a, t_a \rangle |_{x(t)} \sim \exp \left\{ i \int_{t_a}^{t_b} dt \phi(x, \dot{x}, t) \right\}. \quad (2.8)$$

Furthermore, we expect some sort of classical \leftrightarrow quantum correspondence, and we want the classical limit to be included in the quantum description. Classically, we have:

$$S[x(t)] = \int_{t_a}^{t_b} dt L(x, \dot{x}, t) \quad (2.9)$$

So we guess that $\phi \propto L$. Now we need to fix up the units: we have $[S] = [t][E] = [x][p]$. So if we introduce a dimensionful constant \hbar , with units $[S]$ (action), then we can take $\int \phi dt = S/\hbar$, i.e. we assume:

$$\langle x_b, t_b | x_a, t_a \rangle |_{x(t)} = e^{iS[x(t)]/\hbar}. \quad (\text{Dirac}) \quad (2.10)$$

Equation (2.10) is our basic dynamical assumption, just as Schrödinger's wave mechanics assumes the Schrödinger equation to be the equation of motion for quantum systems. The overall (as yet undetermined) normalisation constant will be (implicitly) absorbed into $\mathcal{D}x$.

Note that:

- (1) If $S \rightarrow S + c$ (where c is a constant), all amplitudes change by $e^{ic/\hbar}$, so physics is unchanged.
- (2) If $\delta S \sim \mathcal{O}(2\pi\hbar) \sim \mathcal{O}(h)$, the phase changes by $\mathcal{O}(1)$, this sets the size of quantum fluctuations.

2.3. The Feynman Path Integral

With the assumption (2.10) the transition amplitude becomes:

$$\langle x_b, t_b | x_a, t_a \rangle = \underbrace{\int_{x_a}^{x_b} \mathcal{D}x}_{\substack{\text{sum over all paths} \\ \text{suitably normalised}}} \underbrace{e^{iS[x(t)]/\hbar}}_{\substack{\text{amplitude for} \\ \text{each path}}} \quad (2.11)$$

Though the notation in (2.11) is very neat, to do calculations we will have to use the limiting procedure as given above in (1.30) and (1.33):

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

where $A_N = (\nu(\varepsilon))^{N+1}$, i.e. a normalising factor $\nu(\varepsilon)$ for each discrete interval.

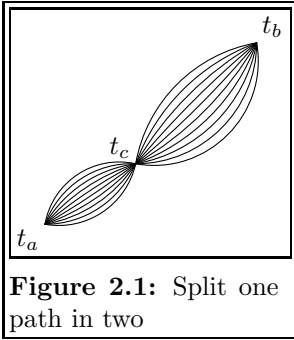


Figure 2.1: Split one path in two

Note the fundamental property: if we insert a complete set of states into the LHS of (2.11), we can split the path in two:

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

This is shown pictorially in figure 2.1. It is very useful for determining the normalisation factor ν (see below).

2.4. The classical limit (heuristic)

For ‘quantum situations’, t_b & t_a and x_b & x_a are “close”, $S[x(t)] = \mathcal{O}(\hbar)$, so the phase fluctuations are of $\mathcal{O}(1)$, and paths far from the classical path may be important.

For ‘classical situations’, t_b, t_a, x_b and x_a are “far apart” and $S[x(t)] \gg \hbar$ in general. (Formally, the classical limit is obtained by taking $\hbar \rightarrow 0$.) Now consider paths “very close” to a given path $x(t)$. Even though $\delta x(t)$ is small, δS will in general be large compared with \hbar , because S is so large. So $e^{i\delta S/\hbar} = \cos(\delta S/\hbar) + i \sin(\delta S/\hbar)$ will oscillate violently and contributions from nearby paths will *cancel*. However, the *classical* path $\bar{x}(t)$ is special: δS is of order $\mathcal{O}(\delta x^2)$, so nearby paths can add constructively. So, as $\hbar \rightarrow 0$ the classical path gives the dominant contribution (i.e. we derive the principle of least action and hence classical mechanics) and therefore

$$\langle x_b, t_b | x_a, t_a \rangle \sim e^{iS_{\text{cl}}/\hbar} \quad (\text{this is the ‘semiclassical approximation’})$$

2.5. Momentum and Energy

Let us try to make the statements for the phase variations in the previous section a bit more rigorous. As we have seen, in classical situations $S_{\text{cl}} \gg \hbar$ and the amplitude oscillates very rapidly. To see just how rapidly, consider a small change in the endpoint: $x_b \rightarrow x_b + \delta x_b$, keeping t_b fixed. Then:

$$S_{\text{cl}} \rightarrow S_{\text{cl}} + \frac{\partial S_{\text{cl}}}{\partial x_b} \delta x_b.$$

So the change in phase, $\delta S/\hbar$, is $k_b \delta x_b$, where the wavenumber

$$k_b \equiv \frac{1}{\hbar} \frac{\partial S_{\text{cl}}}{\partial x_b} = \frac{p_b}{\hbar} \quad (\text{by Hamilton–Jacobi.}) \quad (2.12)$$

Here, p_b is the classical momentum at the endpoint (cf. (2.6)). So $p = \hbar k$, or in operator language $\hat{p} = \hbar \hat{k}$, and thus from (1.26):

$$[\hat{x}, \hat{p}] = i\hbar. \quad (2.13)$$

Similarly, if we change the time at the endpoint and keep x_b fixed, i.e. $t_b \rightarrow t_b + \delta t_b$, we get

$$S_{\text{cl}} \rightarrow S_{\text{cl}} + \frac{\partial S_{\text{cl}}}{\partial t_b} \delta t_b.$$

The change in phase is now $-\omega_b \delta t_b$, where the frequency is (cf. (2.7)):

$$\omega_b \equiv -\frac{1}{\hbar} \frac{\partial S_{\text{cl}}}{\partial t_b} = \frac{E_b}{\hbar} \quad (\text{by Hamilton–Jacobi}) \quad (2.14)$$

and we have $E = \hbar\omega$.

2.6. The Free Particle

Let us evaluate the path integral explicitly for a free particle. The “continuum” expression for the Feynman path integral in (2.11) is elegant and succinct but we shall evaluate it here using a limiting procedure. We shall make use of a range of Gaussian integrals – see separate handout. We use the following discrete approximation to the free particle Lagrangian $L = T = 1/2 m \dot{x}^2 \approx 1/2 m((x_n - x_{n-1})/\varepsilon)^2$, so that

$$\langle x_b, t_b | x_a, t_a \rangle = \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \exp \left\{ \frac{i\varepsilon m}{\hbar} \sum_{n=1}^{N+1} \left(\frac{x_n - x_{n-1}}{\varepsilon} \right)^2 \right\} \quad (2.15)$$

where A_N is a normalisation constant to be fixed. In (2.15) we have a sequence of nested Gaussian integrals. Doing these integrals is straightforward but tedious. Each of the integrals is of the form

$$\begin{aligned} \text{I} &= \int_{-\infty}^{\infty} e^{i(x-u)^2/a} e^{i(u-y)^2/b} du \\ &= \int_{-\infty}^{\infty} \exp \left\{ i \left(\frac{1}{a} + \frac{1}{b} \right) u^2 - 2i \left(\frac{x}{a} + \frac{y}{b} \right) u + i \left(\frac{x^2}{a} + \frac{y^2}{b} \right) \right\} du \\ &= \int_{-\infty}^{\infty} \exp \left\{ i \left(\frac{1}{a} + \frac{1}{b} \right) \left(u - \frac{x/a + y/b}{1/a + 1/b} \right)^2 \right\} \exp \left\{ -i \frac{(x/a + y/b)^2}{1/a + 1/b} + i \left(\frac{x^2}{a} + \frac{y^2}{b} \right) \right\} du \end{aligned} \quad (2.16)$$

where we completed the square in the second line. For brevity, we make the following substitutions:

$$\alpha \equiv -i \left(\frac{1}{a} + \frac{1}{b} \right) = -i \frac{a+b}{ab} ; \quad v \equiv u + \frac{i}{\alpha} \left(\frac{x}{a} + \frac{y}{b} \right) \quad (2.17)$$

and note that

$$\begin{aligned} \left(\frac{x^2}{a} + \frac{y^2}{b} \right) - \frac{ab}{a+b} \left(\frac{x}{a} + \frac{y}{b} \right)^2 &= \frac{1}{a+b} \left[x^2 + \frac{bx^2}{a} + y^2 + \frac{ay^2}{b} - ab \left(\frac{x}{a} + \frac{y}{b} \right)^2 \right] \\ &= \frac{1}{a+b} \left[x^2 + \frac{bx^2}{a} + y^2 + \frac{ay^2}{b} - 2xy - \frac{bx^2}{a} - \frac{ay^2}{b} \right] \\ &= \frac{(x-y)^2}{a+b}. \end{aligned} \quad (2.18)$$

We now plug (2.17) and (2.18) into (2.16) and use equation (1) (or (7)) from the sheet of Gaussian integrals:

$$\begin{aligned} \text{I} &= \int_{-\infty}^{\infty} e^{-\alpha v^2} \exp \left\{ i \frac{(x-y)^2}{a+b} \right\} dv = \sqrt{\frac{\pi}{\alpha}} \exp \left\{ i \frac{(x-y)^2}{a+b} \right\} \\ &= \sqrt{i \frac{\pi ab}{a+b}} \exp \left\{ i \frac{(x-y)^2}{a+b} \right\}. \end{aligned} \quad (2.19)$$

We can now evaluate the integrals in (2.15) one at a time using (2.19), starting with the integral over x_1 :

$$\int dx_1 \exp \left\{ i \frac{m}{2\varepsilon\hbar} \left((x_2 - x_1)^2 + (x_1 - x_0)^2 \right) \right\}$$

This is of the form of (2.16) with $a = b = 2\varepsilon\hbar/m$, so $ab/(a+b) = \varepsilon\hbar/m$ and $a+b = 4\varepsilon\hbar/m$. Hence

$$\begin{aligned} &\langle x_b, t_b | x_a, t_a \rangle \\ &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=1}^{N+1} \exp \left\{ i \frac{m}{2\varepsilon\hbar} (x_n - x_{n-1})^2 \right\} \right) \\ &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=2}^N \int dx_n \right) \left(\prod_{n=3}^{N+1} \exp \left\{ i \frac{m(x_n - x_{n-1})^2}{2\varepsilon\hbar} \right\} \right) \sqrt{\frac{i\pi\varepsilon\hbar}{m}} \exp \left\{ i \frac{m(x_2 - x_0)^2}{4\varepsilon\hbar} \right\} \\ &= \dots = \lim_{N \rightarrow \infty} A_N \left(\frac{i\pi\varepsilon\hbar}{m} \right)^{\frac{N}{2}} \sqrt{\frac{2 \cdot 2^N}{2(N+1)}} \exp \left\{ i \frac{m(x_{N+1} - x_0)^2}{2\hbar(N+1)\varepsilon} \right\} \\ &= \lim_{N \rightarrow \infty} A_N \left(\frac{2\pi i\hbar\varepsilon}{m} \right)^{\frac{N+1}{2}} \sqrt{\frac{m}{2\pi i\hbar(N+1)\varepsilon}} \exp \left\{ i \frac{m(x_{N+1} - x_0)^2}{2\hbar(N+1)\varepsilon} \right\} \end{aligned}$$

Exercise: check this explicitly (a slightly laborious exercise, but worth the effort.)

Since $x_0 = x_a$, $x_{N+1} = x_b$, and $(N+1)\varepsilon = t_b - t_a \equiv T$, if we choose

$$A_N = (\nu(\varepsilon))^{N+1} = \left(\frac{m}{2\pi i \hbar \varepsilon} \right)^{\frac{N+1}{2}}, \quad \text{i.e. } \nu(\varepsilon) = \sqrt{\frac{m}{2\pi i \hbar \varepsilon}}$$

then, since the limit $N \rightarrow \infty$ is trivial,

$$\langle x_b, t_b | x_a, t_a \rangle = \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left\{ i \frac{m}{2\hbar} \frac{(x_b - x_a)^2}{T} \right\} \equiv F_0(T) e^{iS_{\text{cl}}/\hbar}, \quad (2.20)$$

since, as we showed above for the free particle,

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

Note that our choice for $\nu(\varepsilon)$ renders the *normalisation factor* or *pre-factor* $F_0(T)$ independent of x_a and x_b - see also below for discussion.

Notes:

- (1) At large times (where $S_{\text{cl}} \gg 1$), letting $x = x_b + \Delta x$, $t = t_b + \Delta t$ and expanding the exponent in a Taylor series we find (exercise)

$$\langle x, t | x_a, t_a \rangle \simeq \langle x_b, t_b | x_a, t_a \rangle e^{(i/\hbar)(p_b \Delta x - E_b \Delta t)},$$

i.e. a plane wave with momentum p_b and energy $E_b = p_b^2/2m$, as expected from Hamilton-Jacobi.

- (2) The free particle amplitude is a very useful object: we often call it the *free-particle Green function* (see later), and write

$$G_0(x_b - x_a, t_b - t_a) \equiv \langle x_b, t_b | x_a, t_a \rangle \quad (t_b > t_a) \quad (2.21)$$

which makes explicit its translational invariance: G_0 depends only on the *difference* between the initial and final positions and times. In momentum space (exercise)

$$\begin{aligned} \tilde{G}_0(p, t) &\equiv \int_{-\infty}^{\infty} dx e^{ixp/\hbar} G_0(x, t) = \sqrt{\frac{m}{2\pi i \hbar t}} \int_{-\infty}^{\infty} dx \exp \left\{ \frac{ixp}{\hbar} + \frac{imx^2}{2\hbar t} \right\} \\ &= \exp \left(-i \frac{p^2 t}{2m\hbar} \right) = \exp \left(-i \frac{Et}{\hbar} \right) \end{aligned} \quad (2.22)$$

where $E = p^2/2m$, i.e. a plane wave with classical energy E as expected.

- (3) **Normalisation:** choosing $\nu(\varepsilon) = \sqrt{\frac{m}{2\pi i \hbar \varepsilon}}$ seems strange at first, since $\nu(\varepsilon) \rightarrow \infty$ as $\varepsilon \rightarrow 0$, so the amplitude diverges for infinitesimal time intervals. This is not an accident: if the amplitude for finite times is to be finite, then

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

must be finite, and we *must* choose $\nu(\varepsilon) = \sqrt{\frac{m}{2\pi i \hbar \varepsilon}}(1 + O(\varepsilon))$, (so that the $O(\varepsilon)$ term goes to zero as $\varepsilon \rightarrow 0$). Moreover, since $\langle x_b, t_b | x_a, t_a \rangle$ is a Gaussian in $(x_b - x_a)$ with width $\hbar(t_b - t_a)/m$ and (with this normalisation) unit area, as $t_b \rightarrow t_a$

$$\langle x_b, t_b | x_a, t_a \rangle \rightarrow \delta(x_b - x_a) = \langle x_b, t_a | x_a, t_a \rangle$$

as required by orthonormality.

Finally, it is straightforward to verify that with this normalisation

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{-\infty}^{\infty} dx \langle x_b, t_b | x, t \rangle \langle x, t | x_a, t_a \rangle \quad (2.23)$$

for any $t_a < t < t_b$ (tutorial exercise).

(4) The result $\langle x_b, t_b | x_a, t_a \rangle = F_0(T) e^{iS_{cl}/\hbar}$ is also not accidental.

To see this, we consider an alternative method of calculation. Write an arbitrary path $x(t)$ as $x(t) = \bar{x}(t) + \eta(t)$, where $\bar{x}(t)$ is the classical path with boundary conditions $x(t_a) = x_a$ and $x(t_b) = x_b$. Then $\eta(t_a) = \eta(t_b) = 0$, and $\eta(t)$ describes the ‘quantum fluctuations’ about the classical path. Furthermore, since $\frac{\delta S}{\delta x}|_{x=\bar{x}} = 0$ there will be no terms linear in η in the action, and, since the Lagrangian is quadratic, we find $S[x] = S[\bar{x} + \eta] = S[\bar{x}] + S[\eta]$. Explicitly

$$\begin{aligned} S[x] = S[\bar{x} + \eta] &= \frac{m}{2} \int_{t_a}^{t_b} (\dot{\bar{x}} + \dot{\eta})^2 dt = \frac{m}{2} \left\{ \int_{t_a}^{t_b} (\dot{\bar{x}}^2 + \dot{\eta}^2) dt + 2 \int_{t_a}^{t_b} \dot{\bar{x}} \dot{\eta} dt \right\} \\ &= \frac{m}{2} \left\{ \int_{t_a}^{t_b} (\dot{\bar{x}}^2 + \dot{\eta}^2) dt + 2[\eta \dot{\bar{x}}]_{t_a}^{t_b} - 2 \int_{t_a}^{t_b} \eta \ddot{\bar{x}} dt \right\} \end{aligned} \quad (2.24)$$

The last two terms vanish because $\eta(t_a) = \eta(t_b) = 0$, and $\ddot{\bar{x}} = 0$ by the equation of motion.

But $S[\bar{x}] = S_{cl}$, and $\int_{x_a}^{x_b} \mathcal{D}x = \int_0^0 \mathcal{D}\eta$ (since \bar{x} is fixed, hence $dx_n = d\eta_n \forall n$), therefore

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x e^{iS[x(t)]/\hbar} = e^{iS_{cl}/\hbar} \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} \equiv F_0(T) e^{iS_{cl}/\hbar}, \quad (2.25)$$

where $T = t_b - t_a$ as before, and the path integral is over all paths $\eta(t)$ with $\eta(t_a) = \eta(t_b) = 0$. The normalisation factor $F_0(T)$ is independent of x_a and x_b :

$$F_0(T) = \langle 0, t_b | 0, t_a \rangle = \langle 0, T | 0, 0 \rangle \quad (2.26)$$

by translational invariance (in time). We can compute $F_0(T)$ by evaluating the path integral over $\eta(t)$ explicitly (tutorial).

Alternatively, using (2.23)

$$\begin{aligned} \langle 0, T | 0, 0 \rangle &= \int_{-\infty}^{\infty} dx \langle 0, T | x, t \rangle \langle x, t | 0, 0 \rangle \\ \text{so } F_0(T) &= \int_{-\infty}^{\infty} dx F_0(T-t) \exp\left(\frac{imx^2}{2\hbar(T-t)}\right) F_0(t) \exp\left(\frac{imx^2}{2\hbar t}\right) \\ &= \sqrt{\frac{2\pi i \hbar (T-t)t}{mT}} F_0(T-t) F_0(t) \end{aligned} \quad (2.27)$$

Now let $T \gg t$ so that $(T-t) \simeq T$ and $F_0(T-t) \simeq F_0(T)$, and we find

$$F_0(t) = \sqrt{\frac{m}{2\pi i \hbar t}} \quad (2.28)$$

as before. Note that in this argument no discretisation of the path integral is required.

2.7. The Harmonic Oscillator

The Lagrangian is:

$$L = \frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2. \quad (2.29)$$

We use the same trick as for the free particle: we write $x = \bar{x} + \eta$, then

$$S[\bar{x} + \eta] = S[\bar{x}] + S[\eta] \quad (2.30)$$

because the cross term vanishes:

$$\int_{t_a}^{t_b} dt (\dot{\bar{x}} \dot{\eta} - \omega^2 \bar{x} \eta) = [\eta \dot{\bar{x}}]_{t_a}^{t_b} - \int_{t_a}^{t_b} dt \eta (\ddot{\bar{x}} + \omega^2 \bar{x}) = 0 \quad (2.31)$$

The first term on the RHS is zero because $\eta(t_b) = \eta(t_a) = 0$, and the second vanishes because \bar{x} satisfies the equation of motion. (This ‘trick’ works for any Lagrangian quadratic in x .)

Again $\mathcal{D}x = \mathcal{D}\eta$, and hence

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x e^{iS[x(t)]/\hbar} = e^{iS_{\text{cl}}/\hbar} \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} = F_\omega(t_b - t_a) e^{iS_{\text{cl}}/\hbar}, \quad (2.32)$$

where S_{cl} is the classical action

$$S_{\text{cl}} = \frac{m\omega}{2 \sin \omega T} \left((x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right) \quad (2.33)$$

and the normalisation factor is

$$F_\omega(T) = \int_0^0 \mathcal{D}\eta e^{iS[\eta]/\hbar} = \langle 0, T | 0, 0 \rangle \quad (2.34)$$

which is again independent of the boundary conditions on x . As before for the free particle the explicit evaluation of the normalisation factor is tedious. It can be computed by expanding $\eta(t)$ in a Fourier series (see Feynman & Hibbs, 3.11), by matrix methods, or implicitly – using the same method as for the free particle:

$$\begin{aligned} \langle 0, T | 0, 0 \rangle &= \int_{-\infty}^{\infty} dx \langle 0, T | x, t \rangle \langle x, t | 0, 0 \rangle \\ \text{so } F_\omega(T) &= \int_{-\infty}^{\infty} dx F_\omega(T-t) \exp\left(\frac{im\omega x^2}{2\hbar} \frac{\cos \omega(T-t)}{\sin \omega(T-t)}\right) F_\omega(t) \exp\left(\frac{im\omega x^2}{2\hbar} \frac{\cos \omega t}{\sin \omega t}\right) \\ &= F_\omega(T-t) F_\omega(t) \sqrt{\frac{2\pi i \hbar \sin \omega(T-t) \sin \omega t}{m\omega \sin \omega T}} \end{aligned} \quad (2.35)$$

As before, let $T \gg t$ so that $F_\omega(T-t) \simeq F_\omega(T)$, hence

$$\begin{aligned} F_\omega(T) &= F_\omega(T) F_\omega(t) \sqrt{\frac{2\pi i \hbar \sin \omega T \sin \omega t}{m\omega \sin \omega T}} \left(1 + O(t/T)\right) \\ \text{hence } F_\omega(t) &= \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega t}} \end{aligned} \quad (2.36)$$

This result holds for all t , as can be checked by direct substitution into equation (2.35). Note that as $\omega \rightarrow 0$, $F_\omega(t) \rightarrow F_0(t)$, as it must.

2.8. The Forced Harmonic Oscillator

Consider the forced harmonic oscillator with Lagrangian

$$L = \frac{m}{2}(\dot{x}^2 - \omega^2 x^2) + Jx \quad (2.37)$$

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

$$\ddot{x} + \omega^2 x = \frac{J}{m}. \quad (2.38)$$

The action depends on both $x(t)$ and $J(t)$, but since it is still quadratic it again splits into two independent parts:

$$\begin{aligned} S[x, J] &= S[\bar{x} + \eta, J] = \frac{m}{2} \int dt \left((\dot{\bar{x}} + \dot{\eta})^2 - \omega^2 (\bar{x} + \eta)^2 + \frac{2J}{m} (\bar{x} + \eta) \right) \\ &= S[\bar{x}, J] + S[\eta, 0] + m \int dt \left(\dot{\bar{x}}\dot{\eta} - \omega^2 \eta \bar{x} + \frac{J}{m} \eta \right) \\ &= S[\bar{x}, J] + S[\eta, 0] + m [\dot{\bar{x}}\eta]_{t_a}^{t_b} - m \int dt [\eta(\ddot{\bar{x}} + \omega^2 \bar{x} - (J/m))] \\ &= S[\bar{x}, J] + S[\eta, 0] \end{aligned} \quad (2.39)$$

The *fluctuation term* $S[\eta, 0]$ is independent of J because the coupling of J to x (and hence to η) is linear. A minor modification of the steps in equation (2.32) gives (exercise)

$$\langle x_b, t_b | x_a, t_a \rangle = F_\omega(T) e^{iS_{\text{cl}}/\hbar} \quad (2.40)$$

where now $S_{\text{cl}} = S[\bar{x}, J]$, and the normalisation factor is the *same* as for the unforced harmonic oscillator.

2.9. Schrödinger's Equation

To complete the picture, we derive the Schrödinger equation for a particle in an external potential:

$$L = \frac{m}{2} \dot{x}^2 - V(x, t). \quad (2.41)$$

Recalling that momentum $p = \hbar k$, we introduce the momentum basis following equations (1.18) through (1.20):

$$|p\rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{+ipx/\hbar} |x\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x|p\rangle, \quad (2.42)$$

from which we may read off

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad ; \quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}. \quad (2.43)$$

The $1/\sqrt{2\pi\hbar}$ is to ensure that the states $|p\rangle$ are correctly normalised:

$$\langle p'|p\rangle = \int_{-\infty}^{\infty} dx \langle p'|x\rangle \langle x|p\rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi\hbar} e^{i(-p'+p)x/\hbar} = \delta(p' - p) \quad \text{and} \quad \hat{1} = \int_{-\infty}^{\infty} dp |p\rangle \langle p| \quad (2.44)$$

Now consider the infinitesimal amplitude

$$\begin{aligned} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \sqrt{\frac{m}{2\pi i \hbar \varepsilon}} \exp \left\{ \frac{i\varepsilon}{\hbar} \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\varepsilon} \right)^2 - V(x_n, t_n) \right] \right\} \\ &= \sqrt{\frac{m}{2\pi i \hbar \varepsilon}} \exp \left\{ \frac{im}{2\hbar\varepsilon} (x_{n+1} - x_n)^2 - \frac{i\varepsilon}{\hbar} V(x_n, t_n) \right\} \\ &= \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \exp \left\{ \frac{ip_n}{\hbar} (x_{n+1} - x_n) \right\} \exp \left\{ -\frac{i\varepsilon}{2m\hbar} p_n^2 \right\} \exp \left\{ -\frac{i\varepsilon}{\hbar} V(x_n, t_n) \right\}, \end{aligned} \quad (2.45)$$

where the second line may be recovered from the third using equation (8) on the sheet of gaussian integrals (exercise.)

If we introduce a basis of (time-independent) momentum eigenstates satisfying $\hat{p}|p_n\rangle = p_n|p_n\rangle$, and recall that $\hat{x}|x_n\rangle = x_n|x_n\rangle$, we may use (2.43) to rewrite (2.45) as

$$\begin{aligned} \langle x_{n+1}, t_{n+1} | x_n, t_n \rangle &= \int_{-\infty}^{\infty} dp_n \exp \left\{ -\frac{i\varepsilon}{\hbar} \frac{p_n^2}{2m} \right\} \langle x_{n+1} | p_n \rangle \exp \left\{ -\frac{i\varepsilon}{\hbar} V(x_n, t_n) \right\} \langle p_n | x_n \rangle \\ &= \int_{-\infty}^{\infty} dp_n \langle x_{n+1} | \exp \left\{ -\frac{i\varepsilon}{\hbar} \frac{\hat{p}^2}{2m} \right\} | p_n \rangle \langle p_n | \exp \left\{ -\frac{i\varepsilon}{\hbar} V(\hat{x}, t_n) \right\} | x_n \rangle \\ &= \langle x_{n+1} | \exp \left\{ -\frac{i\varepsilon}{\hbar} \frac{\hat{p}^2}{2m} \right\} \exp \left\{ -\frac{i\varepsilon}{\hbar} V(\hat{x}, t_n) \right\} | x_n \rangle, \end{aligned} \quad (2.46)$$

To get the last line we used the completeness of the momentum basis $\int dp_n |p_n\rangle \langle p_n| = \hat{1}$.

Finally, we use the Baker-Campbell-Hausdorff formula

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + (1/2)[\hat{A}, \hat{B}] + \dots} \quad (2.47)$$

to combine the exponentials. All terms beyond the first two on the RHS are of order $\mathcal{O}(\varepsilon^2)$, so

$$\langle x_{n+1}, t_{n+1} | x_n, t_n \rangle = \langle x_{n+1} | \exp \left\{ -\frac{i\varepsilon}{\hbar} H(\hat{x}, \hat{p}, t_n) \right\} | x_n \rangle, \quad (2.48)$$

where

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

is the quantum-mechanical analogue of the classical Hamiltonian.

Remembering that $\varepsilon = t_{n+1} - t_n$, we can rewrite (2.48) as

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

which we can use to write $|x, t\rangle$ in terms of $|x\rangle$

$$|x, t\rangle = \exp \left\{ \frac{i}{\hbar} (t - t_0) \hat{H}(t_0) \right\} |x\rangle \quad (2.49)$$

for some t_0 such that $t - t_0$ is infinitesimal.

If we differentiate (2.49) with respect to t , and then let $t - t_0 \rightarrow 0$, we obtain

$$\frac{\partial}{\partial t} |x, t\rangle = \frac{i}{\hbar} \hat{H}(t) |x, t\rangle \quad \Rightarrow \quad \hat{H}(t) |x, t\rangle = -i\hbar \frac{\partial}{\partial t} |x, t\rangle.$$

where we used $\hat{H}(t_0) \rightarrow \hat{H}(t)$ as $t - t_0 \rightarrow 0$.

Following (1.21) we have $\hat{p} |x, t\rangle = i\hbar \frac{\partial}{\partial x} |x, t\rangle$. Now define $\psi(x, t) = \langle x, t | \psi \rangle$, so $\langle \psi | x, t \rangle = \psi^*(x, t)$, then (exercise)

$$\hat{H}\psi(x, t) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t). \quad (2.50)$$

Equation (2.50) is of course *Schrödinger's equation*.

Notes:

1. The argument is reversible: starting from the Schrödinger equation, we can derive Feynman's path integral representation. Indeed, this is the route followed by most text books.
2. We can use the expression in the third line of (2.45) to construct an alternative representation of the path integral, called the phase space path integral:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \lim_{N \rightarrow \infty} \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=1}^{N+1} \int \frac{dp_n}{2\pi\hbar} \right) \\ &\quad \exp \left\{ \frac{i\varepsilon}{\hbar} \sum_{n=1}^{N+1} \left[p_n \frac{(x_n - x_{n-1})}{(t_n - t_{n-1})} - \frac{p_n^2}{2m} - V(x_n, t_n) \right] \right\} \\ &\equiv \int \mathcal{D}x \int \mathcal{D}p \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt (p\dot{x} - H(x, p, t)) \right\} \end{aligned} \quad (2.51)$$

where H is the classical Hamiltonian. This has the advantage of a natural measure – there are no normalisation factors (because of Liouville's theorem) – and it is particularly useful in statistical mechanics.

3. We can use (2.51) to give yet another derivation of the free particle amplitude:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \lim_{N \rightarrow \infty} \left(\prod_{n=1}^N \int dx_n \right) \left(\prod_{n=1}^{N+1} \int \frac{dp_n}{2\pi\hbar} \right) \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left(p_n(x_n - x_{n-1}) - \frac{\varepsilon p_n^2}{2m} \right) \right\} \\ &= \lim_{N \rightarrow \infty} \frac{1}{2\pi\hbar} \left(\prod_{n=1}^{N+1} \int dp_n \right) \prod_{n=1}^N \delta(p_{n+1} - p_n) \exp \left\{ \frac{i}{\hbar} \left(p_{N+1}x_b - p_1x_a - \frac{\varepsilon}{2m} \sum_{n=1}^{N+1} p_n^2 \right) \right\} \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} p(x_b - x_a) - \frac{i}{2m\hbar} (N+1)\varepsilon p^2 \right\} \\ &= \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}} \exp \left\{ \frac{im}{2\hbar} \frac{(x_b - x_a)^2}{t_b - t_a} \right\} \end{aligned}$$

where we rewrote the sum in the first line

$$\sum_{n=1}^{N+1} p_n(x_n - x_{n-1}) = p_{N+1}x_b - p_1x_a - \sum_{n=1}^N x_n(p_{n+1} - p_n).$$

in order to perform the N integrals over the x_n . We then used the resulting delta functions to perform the integrals over the first N momenta p_i , leaving just one momentum integral (over $p_{N+1} \equiv p$) which may be done using integral (8) on the sheet of Gaussian Integrals.

4. Equation (2.49) may be regarded as the solution of the Schrödinger equation for infinitesimal $t - t_0$. If the Hamiltonian were *time-independent*, i.e. $\hat{H}(t) = \hat{H}$, then (2.49) would hold for all t and t_0 ,

$$|x, t\rangle = \exp\left\{\frac{i}{\hbar}(t - t_0)\hat{H}\right\}|x\rangle \equiv \hat{U}^\dagger(t, t_0)|x\rangle \quad \forall t$$

For a general time-dependent Hamiltonian, we must define:

$$|x, t\rangle = \hat{U}^\dagger(t, t_0)|x\rangle \quad (2.52)$$

where, from (2.49) and the equation below it, the *time evolution operator* $\hat{U}(t, t_0)$ satisfies the Schrödinger-like equation (exercise):

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t, t_0) = \hat{H}(t)\hat{U}(t, t_0) \quad (2.53)$$

with the boundary condition $\hat{U}(t_0, t_0) = \hat{1}$.

Clearly, \hat{U} must be unitary, since it changes bases $|x\rangle \mapsto |x, t\rangle$:

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

5. The Schrödinger and Heisenberg pictures

We may write

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

where we have defined the time-dependent state vector $|\psi, t\rangle \equiv \hat{U}(t, t_0)|\psi\rangle$, which from (2.53) satisfies the Schrödinger equation

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

We say that $|\psi, t\rangle$ and $|x\rangle$ are the state vector and the position eigenstate in the *Schrödinger picture* for time dependence in quantum mechanics. Similarly, $|\psi\rangle$ and $|x, t\rangle$ are the equivalent quantities in the *Heisenberg picture*. These two “pictures” for describing time dependence in the operator formulation of quantum mechanics are of course equivalent in that they give the same physical predictions for all observables.

The wave-function $\psi(x, t) = \langle x|\psi, t\rangle = \langle x, t|\psi\rangle$ is (by definition) the same in both pictures.

Clearly, Schrödinger-picture operators such as $\hat{x} = \int dx x|x\rangle\langle x|$ are time-independent while in the Heisenberg picture $\hat{x}(t) \equiv \int dx x|x, t\rangle\langle x, t|$ is time-dependent. So we write $\hat{x}|x\rangle = x|x\rangle$ and $\hat{x}(t)|x, t\rangle = x|x, t\rangle$.

What is the relation between \hat{x} and $\hat{x}(t)$? Inverting (2.52) gives $|x\rangle = \hat{U}(t, t_0)|x, t\rangle$, hence

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

This must hold $\forall |x, t\rangle$. Hence, for the two pictures to be equivalent, we must have

$$\hat{x}(t) = \hat{U}^\dagger(t, t_0)\hat{x}\hat{U}(t, t_0) \quad (2.54)$$

Similarly for other operators. Note that $[\hat{x}(t), \hat{x}(t')] \neq 0$ unless $t = t'$.

However, since

$$i\hbar\frac{\partial}{\partial t}\langle x, t|\psi\rangle = \langle x, t|\hat{H}|\psi\rangle = \langle x|\hat{U}\hat{H}|\psi\rangle$$

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi, t\rangle = \langle x|\hat{H}|\psi, t\rangle = \langle x|\hat{H}\hat{U}|\psi\rangle$$

we must have $\hat{U}\hat{H} = \hat{H}\hat{U} \Rightarrow \hat{H} = \hat{U}^\dagger\hat{H}\hat{U}$, so the Hamiltonian is the *same* in both pictures at all times.

Note that *all* Heisenberg-picture states and operators coincide with their Schrödinger-picture equivalents at time $t = t_0$.

We can derive an equation of motion for the position operator in the Heisenberg picture:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{x}(t) &= \left(i\hbar\frac{\partial\hat{U}^\dagger}{\partial t}\right)\hat{x}\hat{U} + \hat{U}^\dagger\hat{x}\left(i\hbar\frac{\partial\hat{U}}{\partial t}\right) = -\hat{U}^\dagger\hat{H}\hat{x}\hat{U} + \hat{U}^\dagger\hat{x}\hat{H}\hat{U} \\ &= -\hat{U}^\dagger\hat{H}\hat{U}\hat{U}^\dagger\hat{x}\hat{U} + \hat{U}^\dagger\hat{x}\hat{U}\hat{U}^\dagger\hat{H}\hat{U} \\ &= [\hat{x}(t), \hat{H}] \end{aligned} \quad (2.55)$$

This is the *Heisenberg Equation of motion* for the time-evolution of the position operator in the Heisenberg picture. Since the state vector $|\psi\rangle$ is time-independent in the Heisenberg picture, it doesn't have an equation of motion.

The same argument can be used for any operator $\hat{O}(t)$. We say $\hat{O}(t)$ is *conserved* if $\partial\hat{O}(t)/\partial t = 0$, whence $[\hat{O}(t), \hat{H}] = 0$. For example, momentum is conserved if and only if $[\hat{p}(t), \hat{H}] = 0$.

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

6. For $t > t'$, the transition amplitude $\langle x, t | x', t' \rangle$ is the *retarded Green function* for the Schrödinger equation. Since

$$\psi(x, t) = \langle x, t | \psi \rangle = \int dx' \langle x, t | x', t' \rangle \langle x', t' | \psi \rangle \quad \forall t, t'$$

if we define

$$G(x, x'; t, t') = \begin{cases} \langle x, t | x', t' \rangle & t > t' \\ 0 & t < t' \end{cases} \quad (2.56)$$

$$\text{then} \quad \theta(t - t') \psi(x, t) = \int dx' G(x, x'; t, t') \psi(x', t') \quad \forall t, t'$$

Now, since $\psi(x, t)$ satisfies the time-dependent Schrödinger equation, we find

$$\begin{aligned} & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) - i\hbar \frac{\partial}{\partial t} \right) \theta(t - t') \psi(x, t) = -i\hbar \delta(t - t') \psi(x, t) \\ \text{which implies} \quad & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) - i\hbar \frac{\partial}{\partial t} \right) G(x, x'; t, t') = -i\hbar \delta(t - t') \delta(x - x') \quad \forall t, t' \end{aligned}$$

To recover the first equation from the second, multiply the latter by $\psi(x', t')$, integrate with respect to x' , and then compare with the last line of (2.56)

Note: We choose $G(x, x'; t, t') = 0$ for $t < t'$ because in non-relativistic quantum mechanics we only consider paths in which the particle moves forwards in time.

7. For time-independent Hamiltonians, it is useful to expand in a basis of energy eigenstates $|n\rangle$ with $n = 0, 1, 2, 3, \dots$

$$\hat{H} |n\rangle = E_n |n\rangle \quad ; \quad u_n(x) \equiv \langle x | n \rangle. \quad (2.57)$$

So for $t > 0$ the Green function is:

$$\begin{aligned} G(x, y; t) & \equiv \langle x, t | y, 0 \rangle = \langle x | e^{-it\hat{H}/\hbar} | y \rangle = \sum_n \langle x | e^{-it\hat{H}/\hbar} | n \rangle \langle n | y \rangle \\ & = \sum_n e^{-itE_n/\hbar} u_n(x) u_n^*(y) \end{aligned} \quad (2.58)$$

Define the Fourier transform of $G(x, y; t)$ wrt t as $\tilde{G}(x, y; E) = \int_{-\infty}^{\infty} dt e^{itE/\hbar} G(x, y; t) e^{i\epsilon t/\hbar}$, so

$$\tilde{G}(x, y; E) = \sum_n \int_0^{\infty} dt e^{it(E-E_n)/\hbar} u_n(x) u_n^*(y) e^{i\epsilon t/\hbar} = i\hbar \sum_n \frac{u_n(x) u_n^*(y)}{E - E_n + i\epsilon} \quad (2.59)$$

The $i\epsilon$ ($\epsilon > 0$, infinitesimal) is introduced to ensure that for positive real energies the integral converges at the upper limit. Evidently, bound states correspond to poles in $\tilde{G}(x, y; E)$ which lie just below the real axis in the complex E plane. *i.e.* at $E_n - i\epsilon$, ensuring that when we do the inverse transform we recover the retarded (or causal) Green function (*i.e.* $G(x, y; t) = 0$ for $t < 0$.)

[Technical note: An $i\epsilon$ is also necessary for the convergence of the path integral, e.g. for the harmonic oscillator, $E_n \rightarrow E_n - i\epsilon$ if $\omega \rightarrow \omega - i\epsilon, \omega > 0$, *i.e.* $\omega^2 \rightarrow \omega^2 - i\epsilon$, so

$$S[x] \rightarrow S[x] + i\epsilon m \int dt x^2, \quad \text{and} \quad \exp\{iS/\hbar\} \rightarrow \exp\{iS/\hbar\} \exp\left\{-\epsilon(m/\hbar) \int dt x^2\right\}$$

The last term is a convergence factor which damps paths with very large x^2 , it ensures that the path integral gives causal propagation in non-relativistic quantum mechanics.]

Setting $x = y$ and integrating over x in (2.58) (*i.e.* taking the trace) gives (for $t > 0$):

$$\int_{-\infty}^{\infty} dx \langle x, t | x, 0 \rangle = \int dx G(x, x; t) = \sum_n e^{-itE_n/\hbar} \int dx |u_n(x)|^2 = \sum_n e^{-itE_n/\hbar} \quad (2.60)$$

for orthonormal energy eigenfunctions $u_n(x)$.

Hence, if we know $G(x, y; t)$, we can use this expression to deduce the energy eigenvalues. For example let us consider the harmonic oscillator:

$$\begin{aligned} \int_{-\infty}^{\infty} dx \langle x, t | x, 0 \rangle &= \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega t}} \exp \left\{ \underbrace{\frac{im\omega}{2\hbar \sin \omega t} 2x^2 (\cos \omega t - 1)}_{iS_{cl}/\hbar} \right\} \\ &= \frac{1}{2i} \frac{1}{\sin \frac{\omega t}{2}} \quad (\text{gaussian integral}) \\ &= \frac{e^{-i\omega t/2}}{1 - e^{-i\omega t}} = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} = \sum_n e^{-itE_n/\hbar} \quad (\text{using (2.60)}) \end{aligned} \quad (2.61)$$

It follows that

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

The eigenfunctions may also be deduced in this way (tutorial.)

2.10. Single particle in an Electromagnetic Field

The Lagrangian for a particle of charge e in an electromagnetic field is (in Heaviside-Lorentz units)

$$L(\underline{x}, \dot{\underline{x}}, t) = \frac{1}{2} m |\dot{\underline{x}}|^2 - e\phi + \frac{e}{c} \dot{\underline{x}} \cdot \underline{A} \quad (2.62)$$

where $\phi(\underline{x}, t)$ is the electric potential (also known as the “scalar” or “electrostatic” potential) and $\underline{A}(\underline{x}, t)$ is the magnetic vector potential with

$$\underline{E} = -\nabla\phi - \frac{1}{c} \frac{\partial \underline{A}}{\partial t} \quad \text{and} \quad \underline{B} = \nabla \times \underline{A} \quad (2.63)$$

The classical Hamiltonian is

$$H(\underline{x}, \underline{p}, t) = \frac{1}{2m} \left| \underline{p} - \frac{e}{c} \underline{A} \right|^2 + e\phi \quad (2.64)$$

Exercise: verify explicitly that the Lagrangian (2.62) gives the Lorentz force $\underline{F} = e\underline{E} + (e/c) \dot{\underline{x}} \times \underline{B}$ and the classical Hamiltonian above. (See Junior Honours *Lagrangian Dynamics* notes & tutorials.)

One can then derive the quantum Hamiltonian $H(\hat{\underline{x}}, \hat{\underline{p}}, t)$ and the corresponding Schrödinger equation. This requires a little care because $[\hat{\underline{p}}, \underline{A}(\hat{\underline{x}}, t)] \neq 0$ (tutorial).

Gauge invariance: Classically, the \underline{E} and \underline{B} fields (and thus the Lorentz force, and hence the classical path) are unchanged under the *gauge transformation*

$$\underline{A} \rightarrow \underline{A} + \nabla\chi \quad \text{and} \quad \phi \rightarrow \phi - \frac{1}{c} \frac{\partial \chi}{\partial t} \quad (\text{exercise}) \quad (2.66)$$

for any function $\chi(\underline{x}, t)$. However, the Lagrangian does change:

$$L \rightarrow L + \frac{e}{c} \dot{\underline{x}} \cdot \nabla\chi + \frac{e}{c} \frac{\partial \chi}{\partial t} = L + \frac{e}{c} \frac{d\chi}{dt} \quad (2.67)$$

where we used $\dot{\underline{x}} \cdot \nabla\chi + \frac{\partial \chi}{\partial t} = \frac{d\chi}{dt}$, the total derivative with respect to t . But adding a total derivative to the Lagrangian doesn't change the classical Lagrange equations of motion (see *Lagrangian Dynamics* notes), so our previous claim that classical physics is *gauge invariant* remains valid.

The action also changes:

$$S = \int_{t_a}^{t_b} dt L \rightarrow S + \frac{e}{c} \int_{t_a}^{t_b} dt \frac{d\chi}{dt} = S + \frac{e}{c} (\chi(\underline{x}_b, t_b) - \chi(\underline{x}_a, t_a)) \quad (2.68)$$

so the quantum mechanical transition *amplitude* changes:

$$\langle \underline{x}_b, t_b | \underline{x}_a, t_a \rangle = \int_{\underline{x}_a}^{\underline{x}_b} \mathcal{D}\underline{x} e^{iS/\hbar} \rightarrow \left(\int_{\underline{x}_a}^{\underline{x}_b} \mathcal{D}\underline{x} e^{iS/\hbar} \right) \exp \left\{ \frac{ie}{\hbar c} (\chi(\underline{x}_b, t_b) - \chi(\underline{x}_a, t_a)) \right\} \quad (2.69)$$

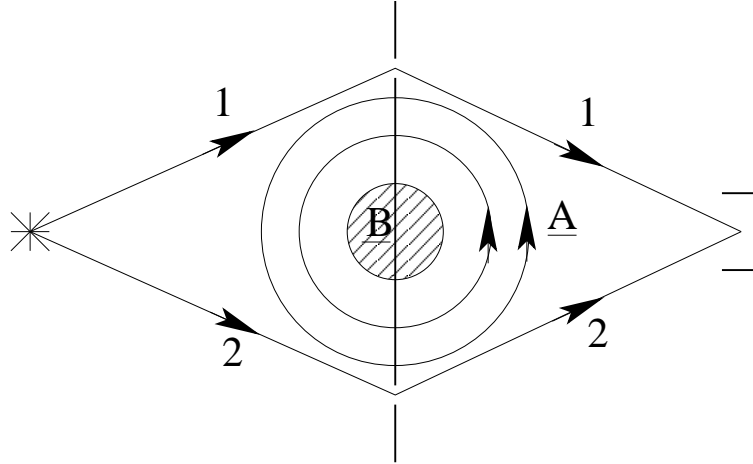
From this we may deduce

$$| \underline{x}, t \rangle \rightarrow \exp \left\{ -\frac{ie}{\hbar c} \chi(\underline{x}, t) \right\} | \underline{x}, t \rangle \quad (2.70)$$

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

2.11. The Aharonov-Bohm effect

Consider a double slit experiment involving charged particles and a magnetic field.



The magnetic field \underline{B} points out of the page and is non-zero in the shaded area only – think of a long thin solenoid – and we assume the particles are shielded from the region of non-zero magnetic field perfectly. The \underline{B} field corresponds to a magnetic vector potential \underline{A} whose field lines form circles around the solenoid as shown.

Classically, we expect the field to have no effect because the particles don't travel through the region of non-zero magnetic field. The \underline{A} field is non-zero along the paths but the vector potential has no direct significance in classical physics.

Quantum mechanically, the dominant contributions to the transition amplitude $\langle f|i\rangle$ will come from paths close to the classical paths $\underline{x}_1(t)$ and $\underline{x}_2(t)$ shown in the figure. In the absence of the field, we add the amplitudes as usual, so the contribution of these paths is

$$e^{iS[x_1]/\hbar} + e^{iS[x_2]/\hbar} = e^{iS[x_1]/\hbar} \left(1 + e^{i(S[x_2]-S[x_1])/ \hbar} \right) \quad (2.71)$$

and we get interference from the relative phase $\phi = (S[x_2] - S[x_1])/ \hbar$.

When we add a magnetic field \underline{B} (assumed time-independent, so that \underline{A} is also time-independent) the Lagrangian changes:

$$L \rightarrow L + \frac{e}{c} \dot{\underline{x}} \cdot \underline{A}$$

so

$$S \rightarrow S + \frac{e}{c} \int_{t_a}^{t_b} dt \frac{d\underline{x}}{dt} \cdot \underline{A} = S + \frac{e}{c} \int_{t_a}^{t_b} d\underline{x}(t) \cdot \underline{A} \quad (2.72)$$

Therefore, when we switch on the magnetic field, there is a change in the relative phase

$$\begin{aligned} \delta\phi &= \frac{e}{\hbar c} \left(\int_{t_a}^{t_b} \underline{A} \cdot d\underline{x}_2(t) - \int_{t_a}^{t_b} \underline{A} \cdot d\underline{x}_1(t) \right) \\ &= \frac{e}{\hbar c} \oint_C \underline{A} \cdot d\underline{x}(t) \equiv \frac{e}{\hbar c} \Phi \end{aligned} \quad (2.73)$$

where the curve C is the closed path x_2-x_1 . This path clearly encircles the region of non-zero magnetic field, but the magnetic field is zero everywhere on the closed path itself. Using Stokes' theorem we may write

$$\Phi = \oint_C \underline{A} \cdot d\underline{x}(t) = \int_S \nabla \times \underline{A} \cdot d\underline{S} = \int_S \underline{B} \cdot d\underline{S} \quad (2.74)$$

where S is any surface bounded by the closed curve x_2-x_1 in the diagram. So Φ is the *total magnetic flux* passing in between the two paths, and the interference pattern shifts upwards (or downwards) due to the relative phase shift $(e/\hbar c) \Phi$ – even though the particle hasn't passed through any region of non-zero magnetic field \underline{B} , and has therefore felt no direct electromagnetic forces!

Notes:

- (1) We get the *same* phase shift $\delta\phi$ for *all* paths $\underline{x}_1(t)$ and $\underline{x}_2(t)$ which don't penetrate the region of non-zero magnetic field \underline{B} , not just for the classical paths. Hence our expression (2.73) for the phase shift holds in the full quantum theory, it's not just a semi-classical approximation.
- (2) Φ is gauge invariant. If $\underline{A} \rightarrow \underline{A} + \nabla\chi$, then

$$\Phi \rightarrow \Phi + \oint_C \nabla\chi \cdot d\underline{x} = \Phi + \oint_C d\chi = \Phi + 0 = \Phi. \quad (2.75)$$

- (3) Only the flux passing *between* the two paths is included.
- (4) The effect is periodic: there is no effect if $\delta\phi = 2n\pi$, i.e. when

$$\Phi = 2\pi n \frac{\hbar c}{e} = n \frac{hc}{e}, \quad n = 0, \pm 1, \pm 2, \dots \quad (2.76)$$

- (5) From the shift in the interference pattern, we deduce that the vector potential $\underline{A}(\underline{x})$ is not just a mathematical artifice, as might be concluded from classical physics.
- (6) The Aharonov-Bohm effect was first observed in 1960.

2.12. Transition Elements

Besides transition amplitudes, we are also interested in *transition elements* where the sum over all paths is weighted by some function(al) of $x(t)$. The simplest example is ($t_a \leq t \leq t_b$):

$$\begin{aligned} \langle x(t) \rangle_S &\equiv \int_{x_a}^{x_b} \mathcal{D}x \, x(t) e^{iS[x]/\hbar} = \int_{-\infty}^{\infty} dx \int_x^{x_b} \mathcal{D}x \int_{x_a}^x \mathcal{D}x \exp \left\{ \frac{i}{\hbar} \int_t^{t_b} L dt \right\} x \exp \left\{ \frac{i}{\hbar} \int_{t_a}^t L dt \right\} \\ &= \int dx \langle x_b, t_b | x, t \rangle x \langle x, t | x_a, t_a \rangle = \int dx \langle x_b, t_b | \hat{x}(t) | x, t \rangle \langle x, t | x_a, t_a \rangle \\ &= \langle x_b, t_b | \hat{x}(t) | x_a, t_a \rangle \end{aligned} \quad (2.77)$$

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, and it's a non-trivial function of t . It is easy to see (exercise) that for any local function $f(x(t))$, we have

$$\langle x_b, t_b | f(\hat{x}(t)) | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \, f(x(t)) e^{iS[x]/\hbar} \quad (2.78)$$

Now consider *correlations* between $x(t)$ and $x(t')$ with $t \neq t'$. For $t > t'$:

$$\begin{aligned} \langle x(t)x(t') \rangle_S &\equiv \int_{x_a}^{x_b} \mathcal{D}x \, x(t)x(t') e^{iS/\hbar} = \int dx \int dx' \langle x_b, t_b | x, t \rangle x \langle x, t | x', t' \rangle x' \langle x', t' | x_a, t_a \rangle \\ &= \int dx \int dx' \langle x_b, t_b | \hat{x}(t) | x, t \rangle \langle x, t | \hat{x}(t') | x', t' \rangle \langle x', t' | x_a, t_a \rangle \\ &= \langle x_b, t_b | \hat{x}(t) \hat{x}(t') | x_a, t_a \rangle \end{aligned}$$

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

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

So, in general we have:

$$\int_{x_a}^{x_b} \mathcal{D}x \, x(t)x(t') e^{iS/\hbar} = \langle x_b, t_b | T(\hat{x}(t) \hat{x}(t')) | x_a, t_a \rangle \quad (2.79)$$

where

$$T(\hat{x}(t) \hat{x}(t')) \equiv \theta(t - t') \hat{x}(t) \hat{x}(t') + \theta(t' - t) \hat{x}(t') \hat{x}(t) \quad (2.80)$$

is called the *time ordered product* - the position operator at the earlier time appears on the right of the one at the later time.

Note that the Heisenberg-picture operators $\hat{x}(t)$ and $\hat{x}(t')$ do not commute (unless $t = t'$).

Clearly, this may be generalised to any number of local insertions:

$$\begin{aligned} \langle f_1(x(t_1)) \dots f_n(x(t_n)) \rangle_S &= \langle x_b, t_b | T(f_1(\hat{x}(t_1)) \dots f_n(\hat{x}(t_n))) | x_a, t_a \rangle \\ &= \int_{x_a}^{x_b} \mathcal{D}x f_1(x(t_1)) \dots f_n(x(t_n)) e^{iS[x(t)]/\hbar} \end{aligned} \quad (2.81)$$

Note that the quantities $f_i(\hat{x}(t_i))$ in the ‘‘operator expression’’ on the RHS of the first line of (2.81) are non-commuting operators, whilst the quantities $f_i(x(t_i))$ in the path integral on the second line are ordinary (commuting) functions.

The time-ordering operator orders *all* of the operators in the product according to time – the operator at the earliest time is on the extreme right, \dots , and the operator at the latest time is on the extreme left.

Between more general states, we simply insert complete sets of position eigenstates: for example

$$\begin{aligned} \langle \psi | T(\hat{x}(t_1) \dots \hat{x}(t_n)) | \phi \rangle &= \int dx_a \int dx_b \langle \psi | x_b, t_b \rangle \langle x_b, t_b | T(\hat{x}(t_1) \dots \hat{x}(t_n)) | x_a, t_a \rangle \langle x_a, t_a | \phi \rangle \\ &= \int dx_a \int dx_b \underbrace{\psi^*(x_b, t_b) \phi(x_a, t_a)}_{\text{wave functions}} \underbrace{\int_{x_a}^{x_b} \mathcal{D}x x(t_1) \dots x(t_n) e^{iS/\hbar}}_{\text{transition elements}} \end{aligned} \quad (2.82)$$

These *transition elements* or *matrix elements* or *Green functions* or *correlation functions* (in statistical mechanics language) will play a central role in what follows.

We can also define transition elements with insertions of time derivatives of $x(t)$. However, these are a little trickier since $\dot{x} = p/m$, and $\hat{p}(t)$ and $\hat{x}(t)$ do not commute. To understand the issues involved, we consider a couple of examples.

We start by going back to the basic definition of the path integral:

$$\langle x_b, t_b | x_a, t_a \rangle = \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \exp \left\{ \frac{i\varepsilon}{\hbar} \sum_{n=1}^{N+1} \left[\frac{m}{2} \left(\frac{x_n - x_{n-1}}{\varepsilon} \right)^2 - V(x_n, t_n) \right] \right\} \quad (2.83)$$

Now, since $\int_{-\infty}^{\infty} dx_p \frac{\partial}{\partial x_p} f(x_p) = 0$ for any function $f(x_p)$ which approaches zero sufficiently quickly as $|x_p| \rightarrow \infty$, and for any $p \in \{1, \dots, N\}$, we must have:

$$\begin{aligned} 0 &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \frac{\partial}{\partial x_p} \left(F(x_p) \exp \left\{ \frac{i\varepsilon}{\hbar} \sum_{n=1}^{N+1} \left[\frac{m}{2} \left(\frac{x_n - x_{n-1}}{\varepsilon} \right)^2 - V(x_n, t_n) \right] \right\} \right) \\ &= \lim_{N \rightarrow \infty} A_N \left(\prod_{n=1}^N \int dx_n \right) \left(\frac{\partial F}{\partial x_p} - \frac{i\varepsilon}{\hbar} F(x_p) \left\{ \frac{m}{\varepsilon^2} (x_{p+1} - 2x_p + x_{p-1}) + \frac{\partial V}{\partial x_p} \right\} \right) \exp \{ \dots \} \end{aligned} \quad (2.84)$$

Technical note: The integral should be considered as the limit of the analytic continuation of an integral with a real part in the exponential argument. So the integral is well-defined although it looks divergent.

As $\varepsilon \rightarrow 0$ we can rewrite terms in (2.84):

$$\lim_{\varepsilon \rightarrow 0} \frac{x_{p+1} - x_p}{\varepsilon} = \dot{x}(t), \quad \text{while} \quad \lim_{\varepsilon \rightarrow 0} \frac{x_{p+1} - 2x_p + x_{p-1}}{\varepsilon^2} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \left(\frac{x_{p+1} - x_p}{\varepsilon} - \frac{x_p - x_{p-1}}{\varepsilon} \right) = \ddot{x}(t) \quad (2.85)$$

If we now set $F = 1$, so $\frac{\partial}{\partial x_p} F = 0$, then as $N \rightarrow \infty$ we get:

$$0 = \int_{x_a}^{x_b} \mathcal{D}x \left(m\ddot{x}(t) + \frac{\partial V}{\partial x} \right) e^{iS/\hbar} \Rightarrow \langle \ddot{x} \rangle_S = -\frac{1}{m} \left\langle \frac{\partial V}{\partial x} \right\rangle_S \quad (2.86)$$

Equation (2.86) is the quantum version of the classical equation of motion and is known as Ehrenfest’s theorem.

If instead we take $F = x_p$, so $\frac{\partial}{\partial x_p} F = 1$, we get:

$$0 = \int_{x_a}^{x_b} \mathcal{D}x e^{iS/\hbar} \lim_{\varepsilon \rightarrow 0} \left(1 - \frac{i}{\hbar} \left\{ mx_p \left[\frac{x_{p+1} - x_p}{\varepsilon} - \frac{x_p - x_{p-1}}{\varepsilon} \right] + \varepsilon x_p \frac{\partial V}{\partial x_p} \right\} \right) \quad (2.87)$$

As $\varepsilon \rightarrow 0$, we write $x_p \rightarrow x(t)$ and hence $x_{p+1} \rightarrow x(t + \varepsilon)$. Remembering the time ordering rule, and writing $m\dot{x}(t) \equiv p(t)$, we get:

$$\begin{aligned} 0 &= \lim_{\varepsilon \rightarrow 0} \langle x_b, t_b | \left\{ 1 - \frac{i}{\hbar} T(\hat{x}(t)\hat{p}(t + \varepsilon/2) - \hat{x}(t)\hat{p}(t - \varepsilon/2)) \right\} | x_a, t_a \rangle \\ &= \langle x_b, t_b | \left\{ 1 - \frac{i}{\hbar} (\hat{p}(t)\hat{x}(t) - \hat{x}(t)\hat{p}(t)) \right\} | x_a, t_a \rangle \quad (t_a < t < t_b) \end{aligned} \quad (2.88)$$

whence the usual equal-time commutation relation

$$[\hat{x}(t), \hat{p}(t)] = i\hbar. \quad (2.89)$$

It follows that we only get the ordering of \hat{x} and \hat{p} correct if we are careful with the time ordering in the path integral. However, since $x_{p+1} = x_p + O(\varepsilon)$ (by continuity),

$$x_p(x_p - x_{p-1}) = x_{p+1}(x_{p+1} - x_p) + O(\varepsilon^2),$$

we may also write (2.87) as

$$0 = \int_{x_a}^{x_b} \mathcal{D}x e^{iS/\hbar} \lim_{\varepsilon \rightarrow 0} \left(1 - \frac{i}{\hbar} m \left\{ x_p \left(\frac{x_{p+1} - x_p}{\varepsilon} \right) - x_{p+1} \left(\frac{x_{p+1} - x_p}{\varepsilon} \right) \right\} \right) + O(\varepsilon),$$

so:

$$\left\langle m \left(\frac{x_{p+1} - x_p}{\varepsilon} \right)^2 \right\rangle_S = -\frac{\hbar}{i\varepsilon} \langle 1 \rangle_S + O(1) \quad (2.90)$$

But if we now take the limit $\varepsilon \rightarrow 0$, we find that $\langle \dot{x}(t)^2 \rangle_S$ and therefore $\langle p(t)^2 \rangle_S$ are infinite! This shows that the paths that we integrate over are not smooth. The action is finite (for paths that count), so from (2.83), $\varepsilon(\delta x/\varepsilon)^2$ is finite, i.e. $\delta x \sim \sqrt{\varepsilon}$, $\delta \dot{x} \sim 1/\sqrt{\varepsilon}$. The paths are continuous but jagged. This phenomenon is called *Zitterbewegung*.

There is a nice illustration on page 177 of the book by Feynman and Hibbs (and Steyer).

How then do we define the kinetic energy? The trick is to use

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{2m} \langle p(t + \varepsilon/2)p(t - \varepsilon/2) \rangle_S \quad (2.91)$$

To see that this is finite, take $F = x_{p+1} - x_p$, so $\frac{\partial}{\partial x_p} F = -1$, and so, from (2.84):

$$\langle -1 \rangle_S = \frac{i\varepsilon m}{\hbar} \left\langle \left(\frac{x_{p+1} - x_p}{\varepsilon} \right) \left(\frac{x_{p+1} - x_p}{\varepsilon} - \frac{x_p - x_{p-1}}{\varepsilon} \right) + \underbrace{(x_{p+1} - x_p)}_{O(\varepsilon)} \frac{\partial V}{\partial x_p} \right\rangle_S \quad (2.92)$$

$$\begin{aligned} \Rightarrow \frac{1}{2m} \langle p(t + \varepsilon/2)p(t - \varepsilon/2) \rangle_S &= \frac{m}{2} \left\langle \left(\frac{x_{p+1} - x_p}{\varepsilon} \right) \left(\frac{x_p - x_{p-1}}{\varepsilon} \right) \right\rangle_S + O(\varepsilon) \\ &= \underbrace{\left\langle \frac{m}{2} \left(\frac{x_{p+1} - x_p}{\varepsilon} \right)^2 \right\rangle_S}_{\simeq -\frac{\hbar}{2i\varepsilon} \langle 1 \rangle_S + O(1) \text{ from (2.90)}} + \frac{\hbar}{2i\varepsilon} \langle 1 \rangle_S + O(\varepsilon) \end{aligned} \quad (2.93)$$

so the limit $\varepsilon \rightarrow 0$ exists. This provides a (trivial) example of *renormalisation* in quantum mechanics - using a 'point-splitting' regularisation.

3. Perturbation Theory

3.1. Perturbation theory from path integrals

Most dynamical systems are not exactly solvable (either classically or quantum mechanically). However, we can often separate the action into a solvable part and a perturbation

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

For example for a particle in a slowly-varying potential:

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

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

where $\tilde{V}(x, t) = V(x, t) - U(x)$, so L_0 is time-independent. Sometimes we take $U = m\omega^2 x^2/2$, so that L_0 is the Lagrangian of a harmonic oscillator. It all depends on the particular problem we wish to solve.

Then the transition amplitude is (using (3.2)):

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} (S_0[x(t)] + S_1[x(t)]) \right\} = \int_{x_a}^{x_b} \mathcal{D}x e^{iS_0[x(t)]/\hbar} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar} S_1[x(t)] \right)^n \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_a}^{t_b} dt_1 \cdots \int_{t_a}^{t_b} dt_n \int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \cdots V(x(t_n), t_n) e^{iS_0[x(t)]/\hbar} \end{aligned} \quad (3.4)$$

assuming that we can exchange the order of the infinite sum and the functional integration. Each term in the series is a transition element.

For $t_a < t_1 < t_2 < \dots < t_n < t_b$, we may write:

$$\begin{aligned} \int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \cdots V(x(t_n), t_n) e^{iS_0/\hbar} &= \\ = \int dx_1 \cdots \int dx_n \langle x_b, t_b | x_n, t_n \rangle_0 V(x_n, t_n) \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle_0 \cdots V(x_1, t_1) \langle x_1, t_1 | x_a, t_a \rangle_0 \end{aligned} \quad (3.5)$$

The subscript zero indicates that these are transition amplitudes evaluated with S_0 . All that remains to be done is to actually evaluate the transition elements.

It is useful to represent the series in (3.4) & (3.5) pictorially. Denoting the transition amplitudes $\langle x, t | x', t' \rangle_0$ by straight lines and insertions of the potential by wiggles, we have:

$$\langle x_b, t_b | x_a, t_a \rangle = \begin{array}{c} t_b \\ \diagup \\ t_a \end{array} + \begin{array}{c} t_b \quad t_a \\ \diagup \quad \diagdown \\ t_1 \\ \text{wiggle} \end{array} + \begin{array}{c} t_b \quad t_a \\ \diagup \quad \diagdown \\ t_1 \quad t_2 \\ \text{wiggle} \quad \text{wiggle} \\ \diagdown \\ t_b \end{array} + \dots \quad (3.6)$$

In words: the full amplitude can be written as a sum of “partial” amplitudes in which the particle is: not scattered + scattered once + scattered twice + \dots .

The integrals over x_i and t_i ensure that we sum over all paths, and the $1/n!$ ensures that paths with different time orderings are not double counted, since:

$$\frac{1}{n!} \int_{t_a}^{t_b} dt_1 \cdots \int_{t_a}^{t_b} dt_n V(t_1) \cdots V(t_n) = \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \cdots \int_{t_a}^{t_3} dt_2 \int_{t_a}^{t_2} dt_1 V(t_1) \cdots V(t_n) \quad (3.7)$$

so $t_a \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq t_b$ is the only one we need to consider.

Proof of (3.7) for $n = 2$. Generalisation to all n can be done by induction (tutorial). Since

$$\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 V(t_1)V(t_2) = \int_{t_a}^{t_b} dt_2 \left(\int_{t_a}^{t_2} dt_1 V(t_1)V(t_2) + \int_{t_2}^{t_b} dt_1 V(t_1)V(t_2) \right),$$

it suffices to show that:

$$\begin{aligned} \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 V(t_1)V(t_2) &= \int_{t_a}^{t_b} dt_1 \int_{t_1}^{t_b} dt_2 V(t_1)V(t_2) \quad (\text{swapped order of integrals}) \\ &= \int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1 V(t_2)V(t_1) \quad (\text{relabelled dummy integrands: } t_1 \leftrightarrow t_2) \end{aligned}$$

This works because the integrand is symmetric under $t_1 \leftrightarrow t_2$, i.e. $V(t_1)V(t_2) = V(t_2)V(t_1)$.

Using the result from (3.5) and (3.7) in (3.4), we obtain the transition amplitude to *all orders* in perturbation theory:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \langle x_b, t_b | x_a, t_a \rangle_0 + \\ &+ \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int dx_1 \cdots \int dx_n \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \cdots \int_{t_a}^{t_2} dt_1 \\ &\quad \langle x_b, t_b | x_n, t_n \rangle_0 V(x_n, t_n) \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle_0 \cdots V(x_1, t_1) \langle x_1, t_1 | x_a, t_a \rangle_0 \end{aligned} \quad (3.8a)$$

We can obtain a formal expression for the sum of this series as follows. First write (3.8a) as

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

where the dots represent all higher-order terms. Now factorise the 2nd, 3rd, \dots , terms:

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

The infinite sum in square brackets is just the perturbation series for $\langle x, t | x_a, t_a \rangle$. Therefore

$$\langle x_b, t_b | x_a, t_a \rangle = \langle x_b, t_b | x_a, t_a \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx \int_{t_a}^{t_b} dt \langle x_b, t_b | x, t \rangle_0 V(x, t) \langle x, t | x_a, t_a \rangle \quad (3.8b)$$

We may interpret equation (3.8b) pictorially:

$$\begin{array}{c} \text{Diagram 1: A double line from } t_a \text{ to } t_b. \\ \text{Diagram 2: A single line from } t_a \text{ to } t_b. \\ \text{Diagram 3: A double line from } t_a \text{ to } t, \text{ a wavy line from } t \text{ to } t, \text{ and a single line from } t \text{ to } t_b. \end{array} = \quad (3.9)$$

Full amplitude = unscattered amplitude + sum of all processes with the last scattering at time t .

We can use (3.8b) to obtain a similar equation for wavefunctions:

$$\begin{aligned}
\langle x, t | \psi \rangle &= \int_{-\infty}^{\infty} dx'' \langle x, t | x'', t_0 \rangle \langle x'', t_0 | \psi \rangle = \int_{-\infty}^{\infty} dx'' \langle x, t | x'', t_0 \rangle_0 \langle x'', t_0 | \psi \rangle \\
&\quad - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' \int_{t_0}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \langle x', t' | x'', t_0 \rangle \langle x'', t_0 | \psi \rangle \\
&= \langle x, t | \psi \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \langle x', t' | \psi \rangle \\
\text{i.e. } \psi(x, t) &= \psi_0(x, t) - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \int_{t_0}^t dt' \langle x, t | x', t' \rangle_0 V(x', t') \psi(x', t')
\end{aligned} \tag{3.10}$$

where $\psi_0(x, t)$ is the *unperturbed* wave function, which satisfies the *unperturbed* Schrödinger equation

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

Relation to Schrödinger's equation: Recall that $G_0(x, x'; t, t') \equiv \theta(t - t') \langle x, t | x', t' \rangle_0$ satisfies

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

(See equations (2.56), etc.) If we rewrite the last line of equation (3.10) as

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

we find

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

The last line of (3.10) is therefore an *integral equation* for ψ , which is equivalent to Schrödinger's equation.

3.2. Fixed target scattering – time-independent transitions

Consider elastic scattering of a particle of mass m in a fixed potential $V(\underline{x}, t)$. We need to find

$$\lim_{\substack{t_b \rightarrow +\infty \\ t_a \rightarrow -\infty}} \langle \underline{x}_b, t_b | \underline{x}_a, t_a \rangle = \lim_{\substack{t_b \rightarrow +\infty \\ t_a \rightarrow -\infty}} \langle \underline{x}_b | \hat{U}(t_b, t_a) | \underline{x}_a \rangle \equiv \langle \underline{x}_b | \hat{S} | \underline{x}_a \rangle$$

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: $\hat{S}^\dagger \hat{S} = \hat{1}$. (What goes in must come out!)

$|\underline{x}_b, \infty\rangle$ is called the *out* state, a free particle state in the far future, and $|\underline{x}_a, -\infty\rangle$ is the *in* state, a free particle state in the far past, where we have assumed that the potential $V(\underline{x}, t)$ is short-ranged: $V(\pm\infty, t) = 0$.

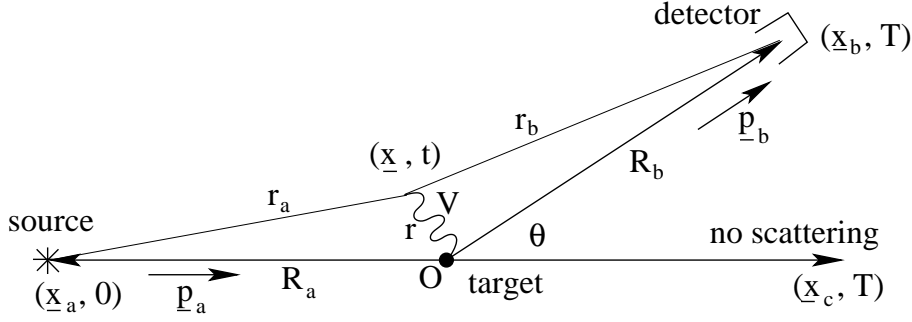
If the interaction is time-independent, (i.e. just $V(\underline{x})$), then

$$\lim_{\substack{t_b \rightarrow +\infty \\ t_a \rightarrow -\infty}} \langle \underline{x}_b, t_b | \underline{x}_a, t_a \rangle = \lim_{T \rightarrow \infty} \langle \underline{x}_b, T/2 | \underline{x}_a, -T/2 \rangle = \lim_{T \rightarrow \infty} \langle \underline{x}_b, T | \underline{x}_a, 0 \rangle$$

by time translation invariance. So, from equation (3.8a) we need to calculate

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

where $\langle \underline{x}_b, T | \underline{x}_a, 0 \rangle_0$ obviously describes the case of no scattering.



We are treating $V(\underline{x})$ as the perturbation, so the unperturbed Lagrangian is simply

$$L_0 = \frac{m}{2} (\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2)$$

In Cartesian coordinates, the path integral for the transition amplitude for a free particle in three dimensions factorises into three one-dimensional path integrals, and hence (exercise)

$$\langle \underline{x}', t' | \underline{x}, t \rangle_0 = \prod_{i=1}^3 \langle x'_i, t' | x_i, t \rangle_0$$

The transition amplitude, A_1 , in first-order perturbation theory is then

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

Performing the integral over t using

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

(see separate handout) gives

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

where we defined $r_a \equiv |\underline{x}_a - \underline{x}|$ and $r_b \equiv |\underline{x}_b - \underline{x}|$.

Since the potential is short-range, if we define $R_a \equiv |\underline{x}_a|$, $R_b \equiv |\underline{x}_b|$, and $r \equiv |\underline{x}|$, then $r \ll R_a, R_b$, and so

$$r_a = (|\underline{x}_a - \underline{x}|^2)^{1/2} = R_a \left(1 - \frac{2\underline{x}_a \cdot \underline{x}}{R_a^2} + \frac{r^2}{R_a^2} \right)^{1/2} = R_a - \underline{n}_a \cdot \underline{x} + O(1/R_a)$$

where $\underline{n}_a = \underline{x}_a/R_a$ is a unit vector in the direction of \underline{x}_a . Similarly

$$r_b = R_b - \underline{n}_b \cdot \underline{x} + O(1/R_b) \quad \text{and} \quad (r_a + r_b)^2 = (R_a + R_b)^2 - 2(R_a + R_b)(\underline{n}_a + \underline{n}_b) \cdot \underline{x} + O(R_{a,b}^0)$$

So

$$\begin{aligned} A_1 &\simeq \frac{-i}{\hbar} \left(\frac{m}{2\pi i \hbar} \right)^{5/2} \frac{1}{T^{3/2}} \left\{ \frac{1}{R_a} + \frac{1}{R_b} + O \left(\frac{1}{R_{a,b}^2} \right) \right\} \exp \left\{ \frac{im}{2\hbar T} (R_a + R_b)^2 \right\} \\ &\quad \times \int_{-\infty}^{\infty} d^3x V(\underline{x}) \exp \left\{ -\frac{im}{\hbar T} (R_a + R_b)(\underline{n}_a + \underline{n}_b) \cdot \underline{x} + O(R_{a,b}^0) \right\} \end{aligned}$$

We can measure R_a , R_b and T , and for a short-range potential (where we can treat it as a free particle most of the time), we deduce from the diagram on the previous page that the particle's total energy, initial momentum and final momentum are

$$E = \frac{1}{2}m \frac{(R_a + R_b)^2}{T^2} = \frac{1}{2}m u^2 \quad \text{and} \quad \underline{p}_a = -p \underline{n}_a, \quad \underline{p}_b = p \underline{n}_b \quad \text{where} \quad p = m \frac{(R_a + R_b)}{T} = mu$$

and u is the particle's speed. Therefore

$$A_1 \simeq \frac{-i}{\hbar} \left(\frac{m}{2\pi i \hbar} \right)^{5/2} \frac{1}{T^{3/2}} \left(\frac{R_a + R_b}{R_a R_b} \right) \exp\{iET/\hbar\} \underbrace{\int_{-\infty}^{\infty} d^3x V(\underline{x}) \exp\left\{i \left((\underline{p}_a - \underline{p}_b) \cdot \underline{x} \right) / \hbar \right\}}_{\equiv \tilde{V}(\underline{q})}$$

where we defined the wave vector transfer $\underline{q} \equiv (\underline{p}_a - \underline{p}_b)/\hbar$, so that the momentum transfer is $\hbar \underline{q}$. The transition probability (per unit volume – see tutorial) is then

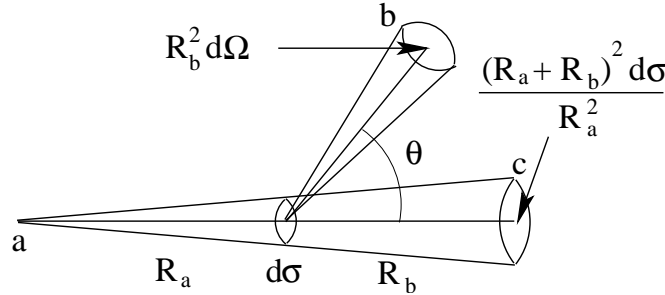
$$P(a \rightarrow b) = |A_1|^2 = \frac{1}{\hbar^2} \left(\frac{m}{2\pi \hbar} \right)^5 \frac{1}{T^3} \left(\frac{R_a + R_b}{R_a R_b} \right)^2 |\tilde{V}(\underline{q})|^2 = \frac{1}{\hbar^2} \left(\frac{m}{2\pi \hbar} \right)^5 \frac{1}{T} \frac{u^2}{R_a^2 R_b^2} |\tilde{V}(\underline{q})|^2$$

$$\text{Similarly } P(a \rightarrow c) = |A_0|^2 = |\langle \underline{x}_c, T | \underline{x}_a, 0 \rangle_0|^2 = \left(\frac{m}{2\pi \hbar} \right)^3 \frac{1}{T^3} = \left(\frac{m}{2\pi \hbar} \right)^3 \frac{1}{T} \frac{u^2}{(R_a + R_b)^2}$$

where $\underline{x}_c \equiv -R_b \underline{n}_a$, is the probability (per unit volume) for *no scattering* (i.e. for $V(\underline{x}) = 0$). The ratio of the scattering and no-scattering probabilities is then:

$$\frac{P(a \rightarrow b)}{P(a \rightarrow c)} = \left(\frac{m}{2\pi \hbar} \right)^2 \left(\frac{R_a + R_b}{R_a R_b} \right)^2 |\tilde{V}(\underline{q})|^2$$

Following classical ideas, we describe the scattering process in terms of an effective target area known as the *scattering cross section*.



If particles starting from \underline{x}_a were to hit a small target of area $d\sigma$, at distance R_a , these particles would be removed from the region around \underline{x}_c , where they would be spread out over area $[(R_a + R_b)/R_a]^2 d\sigma$. Instead, they are scattered into solid angle $d\Omega$ and are spread out over area $R_b^2 d\Omega$ there. Hence

$$P(a \rightarrow b) R_b^2 d\Omega = P(a \rightarrow c) \frac{(R_a + R_b)^2}{R_a^2} d\sigma$$

Rearranging gives

$$\frac{P(a \rightarrow b)}{P(a \rightarrow c)} = \left(\frac{R_a + R_b}{R_a R_b} \right)^2 \frac{d\sigma}{d\Omega}$$

Comparing our two expressions for this ratio gives

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi \hbar} \right)^2 |\tilde{V}(\underline{q})|^2$$

which is called the *differential cross section* in the *Born approximation*.

A more conventional wording of the definition of the differential cross section is (see, for example, *Quantum Physics*):

$$\begin{aligned} & \text{(Number of particles scattered into } d\Omega \text{ / unit time)} \\ & = \\ & d\sigma \times \text{(Number of incident particles crossing scattering region / unit area / unit time)} \end{aligned}$$

Again, this gives

$$P(a \rightarrow b) R_b^2 d\Omega = d\sigma \left(P(a \rightarrow c) \left(\frac{R_a + R_b}{R_a} \right)^2 \right)$$

which reproduces our previous result for $d\sigma/d\Omega$.

Notes:

- (1) All factors of T , R_a , R_b cancel when we construct $d\sigma/d\Omega$, so we can send them to infinity with impunity.
- (2) We assumed initial and final states with definite *position*. However, we get the same result for *any* initial and final states, provided sufficiently localised wave functions cancel when we take the ratio $P(a \rightarrow b)/P(a \rightarrow c)$.
- (3) For a *central* potential $V(r)$, $r = |\underline{x}|$, we choose spherical polars with \underline{q} parallel to the z -axis, and the expression for $\tilde{V}(\underline{q})$ simplifies to

$$\int_{-\infty}^{\infty} d^3x V(r) \exp(i\underline{q} \cdot \underline{x}) = 2\pi \int_0^{\infty} r^2 dr \int_{-1}^{+1} d(\cos\theta) \exp(iqr \cos\theta) V(r) = \frac{4\pi}{q} \int_0^{\infty} rV(r) \sin(qr) dr$$

Hence

$$\frac{d\sigma}{d\Omega} = \frac{4m^2}{\hbar^4 q^2} \left| \int_0^{\infty} rV(r) \sin(qr) dr \right|^2$$

with $q = |\underline{p}_a - \underline{p}_b|/\hbar = (2p/\hbar) \sin\theta/2$ where θ is the *scattering angle* as shown in the figure.

- (4) For the Coulomb potential $V(r) = -e^2/(4\pi\epsilon_0 r)$

$$\int_0^{\infty} rV(r) \sin(qr) dr = \frac{-e^2}{4\pi\epsilon_0 q}$$

so

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

which is not only independent of \hbar , but is the *same* as the classical Rutherford cross section. This “quantum cross section = classical cross section” result is unique to the $1/r$ potential – Rutherford got lucky!

Technical note (1): For the integral over the Coulomb potential to converge, we need to define $V(r) = -e^2 \exp(-\mu r)/(4\pi\epsilon_0 r)$, and take the limit $\mu \rightarrow 0$ at the end. (See tutorial.)

Technical note (2): For compatibility with most standard texts, we have used *SI units* in the expression for the Coulomb potential. In *Heaviside-Lorentz units* $V(r) = -e^2/(4\pi r)$, i.e. just remove the ϵ_0 .

- (5) The *total cross-section*, σ , is

$$\sigma \equiv \int_{4\pi} \frac{d\sigma}{d\Omega} d\Omega = \iint \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi$$

in spherical polar coordinates, where θ is the *scattering angle* shown in the figure, and ϕ is the angle measured about the the ‘beam axis’ which runs through the origin and \underline{x}_c

- (6) These results may be obtained using time-dependent perturbation theory for plane wave states – see *Quantum Physics*.
- (7) We may use (3.8a) to generate the $O(V^n)$ (with $n > 1$) contributions to the scattering amplitude. The resulting perturbation expansion is known as the *Born Series*.

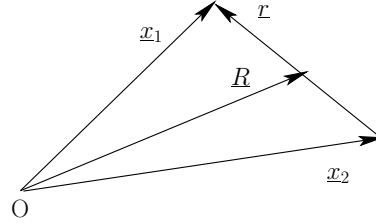
3.3. Colliding Beams

Consider two particles of masses m_1 and m_2 interacting through a mutual potential. The Lagrangian is

$$\begin{aligned} L &= \frac{1}{2}m_1|\dot{\underline{x}}_1|^2 + \frac{1}{2}m_2|\dot{\underline{x}}_2|^2 - V(\underline{x}_1 - \underline{x}_2) \\ &= \frac{1}{2}M|\dot{\underline{R}}|^2 + \frac{1}{2}\mu|\dot{\underline{r}}|^2 - V(\underline{r}) \end{aligned}$$

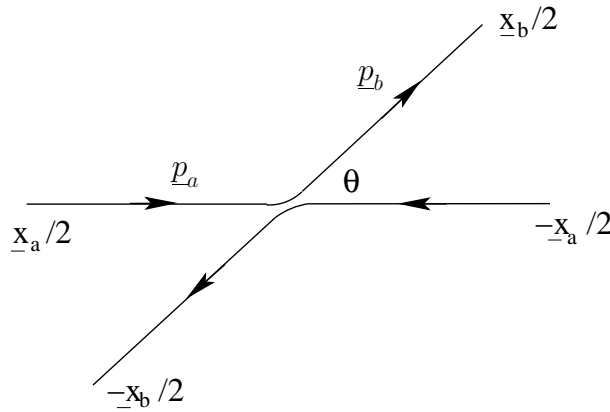
where

$$\underbrace{\underline{R} = \frac{m_1\underline{x}_1 + m_2\underline{x}_2}{m_1 + m_2}, \quad M = m_1 + m_2,}_{\text{centre-of-mass motion}} \quad \underbrace{\underline{r} = \underline{x}_1 - \underline{x}_2, \quad \mu = \frac{m_1m_2}{m_1 + m_2}}_{\text{relative motion}}$$



In the centre-of-mass frame, $\underline{R} \equiv 0$, so the first term drops out, and we have simply $L = \frac{1}{2}\mu|\dot{\underline{r}}|^2 - V(\underline{r})$, i.e. it's the same as in fixed-particle scattering but with $\underline{x} \rightarrow \underline{r}$ and $m \rightarrow \mu$.

So if we consider a colliding beam scattering experiment,



the differential cross section is simply

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

where $\underline{q} = (\underline{p}_a - \underline{p}_b)/\hbar$ as before, and we have defined the *scattering amplitude* $f(\theta, \phi)$, via

$$\frac{d\sigma}{d\Omega} \equiv |f(\theta, \phi)|^2$$

If $m_2 \rightarrow \infty$, then $\mu \rightarrow m_1 = m$, say, and we recover the fixed target result (Born-Oppenheimer approximation.)

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

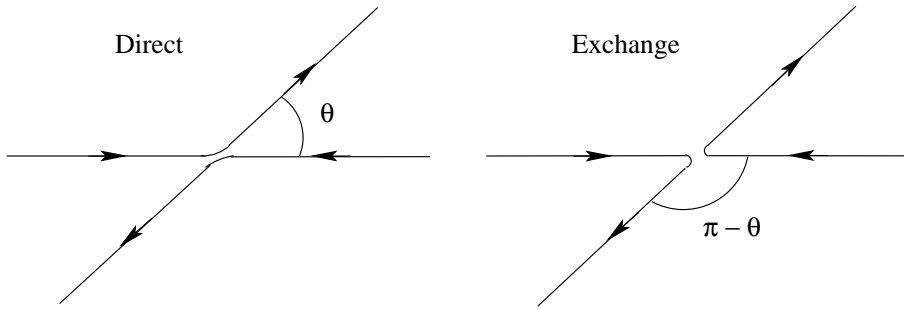
$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{4\pi\hbar^2} \right)^2 |\tilde{V}(\underline{q})|^2$$

For central potentials, we have already shown that the scattering amplitude depends only on θ (see Note (3) above), hence

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

Scattering of identical particles

If the particles are identical, we have two indistinguishable possibilities:



Classically, we add *probabilities*, so in a mythical world of classical “identical” particles we would have

$$\frac{d\sigma_{cl}}{d\Omega} = |f(\theta)|^2 + |f(\pi - \theta)|^2$$

But in quantum mechanics, we must add *amplitudes*, therefore for identical bosons

$$\frac{d\sigma_b}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2$$

so, for example, for the Coulomb potential,

$$\frac{d\sigma_b}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{16E^2} \left(\frac{1}{\sin^2(\theta/2)} + \frac{1}{\cos^2(\theta/2)}\right)^2 = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{E^2} \frac{1}{\sin^4\theta}$$

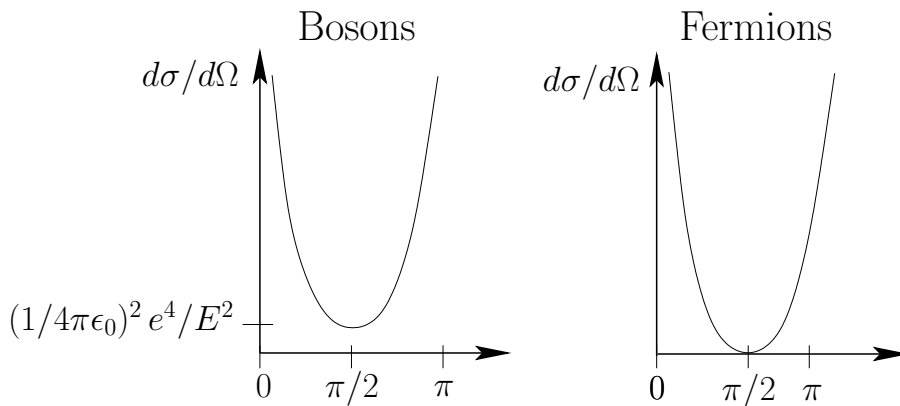
For identical spinless ‘fermions’ (*i.e.* ignoring spin – see tutorial for spin dependence)

$$\frac{d\sigma_f}{d\Omega} = |f(\theta) - f(\pi - \theta)|^2 = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{16E^2} \left(\frac{1}{\sin^2(\theta/2)} - \frac{1}{\cos^2(\theta/2)}\right)^2$$

This gives

$$\frac{d\sigma_f}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{E^2} \frac{\cos^2\theta}{\sin^4\theta}$$

which vanishes when $\theta = \pi/2$, as it must.



So we can tell whether particles are bosons or fermions by studying the *shape* of the differential cross section.

3.4. Perturbation theory in the operator formalism

Consider the transition amplitude $\langle x_b, t_b | x_a, t_a \rangle$, where the position eigenstates are in the Heisenberg picture. From (2.52) and the unitarity of \hat{U} , we have

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \left(\hat{U}^\dagger(t_b, t_0) |x_b\rangle \right)^\dagger \hat{U}^\dagger(t_a, t_0) |x_a\rangle = \langle x_b | \hat{U}(t_b, t_0) \hat{U}(t_0, t_a) |x_a\rangle \\ &= \langle x_b | \hat{U}(t_b, t_a) |x_a\rangle \end{aligned} \quad (3.11)$$

where $|x_a\rangle$ and $|x_b\rangle$ are position eigenstates in the Schrödinger picture. We shall develop perturbation theory for $\hat{U}(t_b, t_a)$

Firstly, we use (2.81) to write (3.5) as

$$\int_{x_a}^{x_b} \mathcal{D}x V(x(t_1), t_1) \cdots V(x(t_n), t_n) e^{iS_0/\hbar} = {}_0\langle x_b, t_b | T(V(\hat{x}_0(t_1), t_1) \cdots V(\hat{x}_0(t_n), t_n)) |x_a, t_a\rangle_0 \quad (3.12)$$

where the states $|x, t\rangle_0$ and the operators $\hat{x}_0(t)$ are in the Heisenberg picture with respect to S_0 rather than S ,

$$\hat{x}_0(t) = \hat{U}_0^\dagger(t, t_0) \hat{x} \hat{U}_0(t, t_0).$$

In this expression, \hat{x} is the position operator in the Schrödinger picture, and the unperturbed time-evolution operator $\hat{U}_0(t, t_0)$ therefore satisfies

$$i\hbar \frac{\partial}{\partial t} \hat{U}_0 = \hat{H}_0 \hat{U}_0,$$

where \hat{H}_0 is the unperturbed Hamiltonian. This is known as the *Dirac* or *interaction picture* for time dependence in quantum mechanics.

Using (3.8a) the perturbative expansion (3.4) may then be written as:

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_a}^{t_b} dt_1 \cdots \int_{t_a}^{t_b} dt_n {}_0\langle x_b, t_b | T(V(\hat{x}_0(t_1), t_1) \cdots V(\hat{x}_0(t_n), t_n)) |x_a, t_a\rangle_0 \\ &= \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int_{t_a}^{t_b} dt_n \int_{t_a}^{t_n} dt_{n-1} \cdots \int_{t_a}^{t_2} dt_1 {}_0\langle x_b, t_b | V(\hat{x}_0(t_n), t_n) \cdots V(\hat{x}_0(t_1), t_1) |x_a, t_a\rangle_0 \end{aligned} \quad (3.13)$$

Note that

$$V(\hat{x}_0(t), t) = \hat{U}_0^\dagger(t, t_0) V(\hat{x}, t) \hat{U}_0(t, t_0) \quad (3.14a)$$

is the potential energy operator in the interaction picture, and $V(\hat{x}, t)$ is its Schrödinger-picture equivalent.

Since the time dependence in (3.12) and (3.13) is governed by S_0 , the interaction-picture states $|x_b, t_b\rangle_0$ and $|x_a, t_a\rangle_0$ on the RHS of (3.13) are related to the Schrödinger-picture states by

$$|x_a, t_a\rangle_0 = \hat{U}_0^\dagger(t_a, t_0) |x_a\rangle \quad \text{and hence} \quad {}_0\langle x_b, t_b | = \langle x_b | \hat{U}_0(t_b, t_0) \quad (3.14b)$$

Furthermore we shall need

$$\hat{U}_0(t_n, t_0) \hat{U}_0^\dagger(t_{n-1}, t_0) = \hat{U}_0(t_n, t_0) \hat{U}_0(t_0, t_{n-1}) = \hat{U}_0(t_n, t_{n-1}) \quad (3.14c)$$

Starting from (3.13), and using (3.11) and (3.14a/b/c), we obtain another representation for equation (3.8a) in terms of the unperturbed time-evolution operators $\hat{U}_0(t_n, t_{n-1})$ and the Schrödinger-picture operators $V(\hat{x}, t_n)$

$$\begin{aligned} \langle x_b | \hat{U}(t_b, t_a) |x_a\rangle &= \langle x_b | \hat{U}_0(t_b, t_a) |x_a\rangle \\ &+ \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int_{t_a}^{t_b} dt_n \cdots \int_{t_a}^{t_2} dt_1 \langle x_b | \hat{U}_0(t_b, t_n) V(\hat{x}, t_n) \hat{U}_0(t_n, t_{n-1}) V(\hat{x}, t_{n-1}) \cdots \\ &\cdots V(\hat{x}, t_2) \hat{U}_0(t_2, t_1) V(\hat{x}, t_1) \hat{U}_0(t_1, t_a) |x_a\rangle \end{aligned}$$

The equation above holds for all states $|x_a\rangle$ and $|x_b\rangle$, so we can write it in purely operator form

$$\hat{U}(t_b, t_a) = \hat{U}_0(t_b, t_a) + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_a}^{t_b} dt_n \cdots \int_{t_a}^{t_2} dt_1 \hat{U}_0(t_b, t_n) V(\hat{x}, t_n) U_0(t_n, t_{n-1}) V(\hat{x}, t_{n-1}) \cdots \\ \cdots V(\hat{x}, t_2) \hat{U}_0(t_2, t_1) V(\hat{x}, t_1) \hat{U}_0(t_1, t_a) \quad (3.15a)$$

This is usually referred to as the *Dyson series*. We can sum this series formally (exercise) to obtain the operator equivalent of (3.8b)

$$\hat{U}(t_b, t_a) = \hat{U}_0(t_b, t_a) - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{U}_0(t_b, t) V(\hat{x}, t) \hat{U}(t, t_a) \quad (3.15b)$$

Equivalently, we can obtain (3.15b) by expressing (3.8b) in terms of time evolution operators and Schrödinger-picture position eigenstates (exercise). We leave it as an exercise to show that (3.15b) is the “solution” of the Schrödinger equation. Indeed, (3.15b) can be derived directly from the Schrödinger equation (tutorial).

Note that all of the potential-energy operators $V(\hat{x}, t)$, etc, in (3.15a) and (3.15b) are in the Schrödinger picture.

3.4. Time dependent transitions

A common situation is where the Lagrangian L_0 (corresponding to the action S_0) is time independent, whilst the Lagrangian L_1 of the perturbation (corresponding to S_1) is time dependent. Let us further assume that the Hamiltonian \hat{H}_0 of the unperturbed system has a discrete spectrum of bound-state energies E_n and (Schrödinger-picture) eigenstates $|n\rangle$

$$\hat{H}_0 |n\rangle = E_n |n\rangle$$

(For the Heisenberg-picture, we simply replace $|n\rangle \rightarrow |n, t\rangle$.) Rather than working in the position basis, it is easier to use the energy eigenbasis, because then the unperturbed transition amplitude is diagonal:

$$\langle m, t | n, t' \rangle_0 = \langle m | \hat{U}_0(t, t') | n \rangle = \langle m | e^{-i(t-t')\hat{H}_0/\hbar} | n \rangle = \exp\left\{-i(t-t')\frac{E_n}{\hbar}\right\} \delta_{mn} \quad (3.16)$$

It follows from (3.15a) that the perturbed amplitude in the energy eigenbasis is:

$$\langle b, t_b | a, t_a \rangle = \langle b | \hat{U}(t_b, t_a) | a \rangle = \langle b | \hat{U}_0(t_b, t_a) | a \rangle - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \langle b | \hat{U}_0(t_b, t) V(\hat{x}, t) \hat{U}_0(t, t_a) | a \rangle + \cdots \\ = \langle b | \hat{U}_0(t_b, t_a) | a \rangle - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \sum_{m,n} \langle b | \hat{U}_0(t_b, t) | m \rangle \langle m | V(\hat{x}, t) | n \rangle \langle n | \hat{U}_0(t, t_a) | a \rangle + \cdots \\ = e^{-i(t_b-t_a)E_a/\hbar} \delta_{ab} - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \sum_{m,n} e^{-i(t_b-t)E_b/\hbar} \delta_{mb} V_{mn}(t) e^{-i(t-t_a)E_a/\hbar} \delta_{na} + \cdots \\ = e^{-i(t_b-t_a)E_a/\hbar} \delta_{ab} - \frac{i}{\hbar} e^{-i(E_b t_b - E_a t_a)/\hbar} \int_{t_a}^{t_b} dt e^{it(E_b - E_a)/\hbar} V_{ba}(t) + \cdots \quad (3.17)$$

where $V_{mn}(t)$ is the matrix element of the potential

$$V_{mn}(t) \equiv \langle m | V(\hat{x}, t) | n \rangle = \int_{-\infty}^{\infty} dx \langle m | V(\hat{x}, t) | x \rangle \langle x | n \rangle = \int_{-\infty}^{\infty} dx u_m^*(x) V(x, t) u_n(x)$$

The second order term in the expansion is (check this for yourself)

$$\left(-\frac{i}{\hbar}\right)^2 \sum_n \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 e^{-i(t_b-t_2)E_b/\hbar} V_{bn}(t_2) e^{-i(t_2-t_1)E_n/\hbar} V_{na}(t_1) e^{-i(t_1-t_a)E_a/\hbar}$$

It is easy to see how this will generalise to higher orders. Diagrammatically, we have (for $a \neq b$):

$$\langle b, t_b | a, t_a \rangle = \begin{array}{c} V_{ba}(t) \\ \text{---} \\ \text{---} \\ a \quad b \\ t_a \quad t_b \end{array} + \sum_n \begin{array}{c} V_{na}(t_1) \\ \text{---} \\ \text{---} \\ a \quad n \quad b \\ t_a \quad t_2 \quad t_b \\ V_{bn}(t_2) \end{array} + \sum_{n,m} \begin{array}{c} V_{na}(t_1) \quad V_{bm}(t_3) \\ \text{---} \quad \text{---} \\ \text{---} \\ a \quad n \quad m \quad b \\ t_a \quad t_2 \quad t_b \\ V_{mn}(t_2) \end{array} + \dots$$

All intermediate ‘virtual’ states n, m, \dots are summed over, and the ‘interaction times’ $t_1 < t_2 < \dots < t_n$ are integrated over. For example, at third order: $a \rightarrow n \rightarrow m \rightarrow b$ for all possible intermediate values of n and m .

If $a \neq b$, the first (trivial) term vanishes, and the transition probability becomes:

$$p(a \rightarrow b) = |\langle b, t_b | a, t_a \rangle|^2 = \frac{1}{\hbar^2} \left| \int_{t_a}^{t_b} dt e^{i\omega_{ba}t} V_{ba}(t) + \mathcal{O}(V^2) \right|^2 \quad (3.18)$$

where $\omega_{ba} \equiv (E_b - E_a)/\hbar$ is the *transition frequency*. This should be familiar from *Quantum Physics*. Note that higher order terms interfere: from (3.18), the next correction to $p(a \rightarrow b)$ is $\mathcal{O}(V^3)$, not $\mathcal{O}(V^4)$. Writing

$$\tilde{V}_{ba} = \int_{t_a}^{t_b} dt e^{i\omega_{ba}t} V_{ba}(t),$$

we obtain

$$p(a \rightarrow b) = \frac{1}{\hbar^2} |\tilde{V}_{ba}|^2 - \frac{2}{\hbar^3} \text{Re} \left(\tilde{V}_{ba}^* \sum_n \tilde{V}_{bn} \tilde{V}_{na} \right). \quad (3.19)$$

When the perturbation is time *independent*, we can do the t integrals, and the transition amplitude through second order becomes

$$e^{-iT E_a/\hbar} \delta_{ab} + \frac{(e^{-i T E_b/\hbar} - e^{-i T E_a/\hbar})}{E_b - E_a} V_{ba} + \sum_n \frac{(e^{-i T E_b/\hbar} - e^{-i T E_n/\hbar})(e^{-i T E_n/\hbar} - e^{-i T E_a/\hbar})}{(E_b - E_n)(E_n - E_a)} V_{bn} V_{na}$$

where $T = t_b - t_a$, as usual.

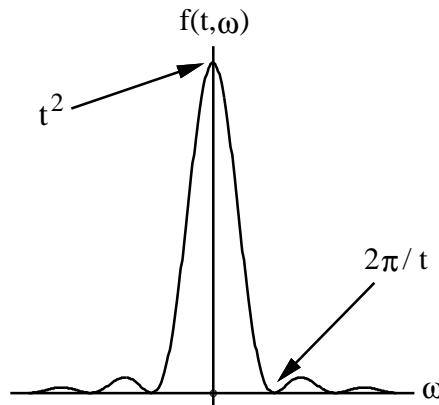
To first order, the transition probability (for the time-independent case with $a \neq b$) is simply

$$p(a \rightarrow b) = \frac{|e^{-i T E_a/\hbar} (e^{-i T \omega_{ba}} - 1)|^2}{\hbar^2 \omega_{ba}^2} |V_{ba}|^2 = \frac{\sin^2(\omega_{ba} T/2)}{\hbar^2 (\omega_{ba}/2)^2} |V_{ba}|^2 \equiv \frac{f(T, \omega_{ba})}{\hbar^2} |V_{ba}|^2 \quad (3.20)$$

The function

$$f(t, \omega) = \frac{\sin^2(\omega t/2)}{(\omega/2)^2} = \frac{\sin^2(\omega t/2)}{(\omega t/2)^2} t^2$$

consists essentially of a large peak, centred on $\omega = 0$, with height t^2 and width $\simeq 2\pi/t$, as indicated in the figure. Thus there is only a significant transition probability to those states whose energy lies in a band of width $\delta E \simeq 2\pi\hbar/t$ about the initial energy, E_a .



Using the standard integral $\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi$ we have

$$\int_{-\infty}^{\infty} f(t, \omega) d\omega = 2\pi t.$$

Therefore $f(t, \omega)$ reduces to an infinite “spike” of area $2\pi t$ as $t \rightarrow \infty$, and we have

$$\lim_{t \rightarrow \infty} f(t, \omega) \sim 2\pi t \delta(\omega).$$

Now consider the case of a transition not to a single final state but to a range \mathcal{R} of final states around E_b . Then we have

$$p(a \rightarrow \mathcal{R}) = \int_{\mathcal{R}} p(a \rightarrow E) \varrho(E) dE, \quad (3.21)$$

where $\varrho(E) dE$ is the number of states in the interval $E \rightarrow E + dE$. The function $\varrho(E)$ is called the *density of final states*.

Let us assume that the range \mathcal{R} is small enough so that we can consider $\varrho(E)$ and V_{ba} to be constant in \mathcal{R} . Since

$$\lim_{t \rightarrow \infty} \sin^2(\omega_{ba}T/2)/(\omega_{ba}/2)^2 = 2\pi T \delta(\omega_b - \omega_a) \quad (3.22)$$

then, for sufficiently large T , the only significant contributions to the integral come from the energy range corresponding to the narrow central peak of the function $f(T, \omega_{ba})$, so we can safely extend the limits on the integral to infinity without affecting the result. This gives

$$\begin{aligned} p(a \rightarrow \mathcal{R}) &= \frac{1}{\hbar^2} \int_{-\infty}^{\infty} \varrho(E) \frac{\sin^2(\omega_{ba}T/2)}{(\omega_{ba}/2)^2} |V_{ba}|^2 dE = \frac{|V_{ba}|^2 \varrho(E_b)}{\hbar^2} \int_{-\infty}^{\infty} \frac{\sin^2(\omega_{ba}T/2)}{(\omega_{ba}/2)^2} \hbar d\omega_{ba} \\ &= \frac{2\pi}{\hbar} |V_{ba}|^2 \varrho(E_b) T \end{aligned} \quad (3.23)$$

The transition *rate* is then

$$R = \frac{2\pi}{\hbar} |V_{ba}|^2 \varrho(E_b) \quad (3.24)$$

This result is known as *Fermi's Golden Rule*.

3.4. Feynman Perturbation Theory

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

$$L = L_0 + L_1 = \underbrace{\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2 + Jx}_{\text{forced SHO}} - \underbrace{\frac{\lambda}{4}x^4}_{\text{anharmonic}} \quad (3.41)$$

where $J = J(t)$ is an arbitrary function of t . The classical equation of motion is:

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) x = \frac{J}{m} - \frac{\lambda}{m} x^3 \quad (3.42)$$

The homogeneous equation

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) x = 0$$

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

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) \Delta(t, t') = -\delta(t - t')$$

which satisfies the boundary conditions $\Delta(t_b, t') = \Delta(t_a, t') = 0$. It is straightforward (tutorial) to show that

$$\Delta(t, t') = \frac{1}{\omega \sin \omega T} \left[\begin{aligned} &\theta(t - t') \sin \omega(t_b - t) \sin \omega(t' - t_a) \\ &+ \theta(t' - t) \sin \omega(t - t_a) \sin \omega(t_b - t') \end{aligned} \right] \quad (3.44)$$

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 $\Delta(t, t') = \Delta(t', t)$.

The full solution of (3.42) with the correct boundary conditions is then

$$\bar{x}(t) = \bar{x}_0(t) + \frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') (-J(t') + \lambda \bar{x}(t')^3) \quad (3.51)$$

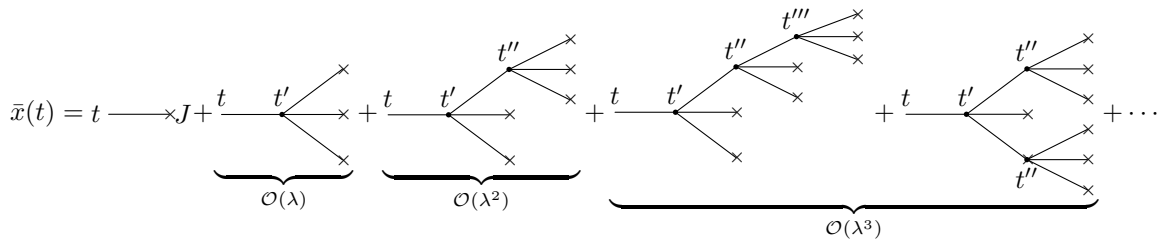
The second term on the RHS is the solution of the full inhomogeneous equation with trivial (zero) boundary conditions (check this explicitly), whilst the first term “fixes up” the boundary conditions.

More precisely, equation (3.51) is an integral equation for $\bar{x}(t)$ which we can solve iterately:

$$\bar{x}(t) = \bar{x}_0(t) - \frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') J(t') + \frac{\lambda}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') \left(\bar{x}_0(t') - \frac{1}{m} \int_{t_a}^{t_b} dt'' \Delta(t', t'') J(t'') \right)^3 + \dots \quad (3.52)$$

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 (3.52) 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 (3.51) that must be evaluated explicitly.

Notes:

- (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. . .

Quantum mechanics: An interesting question is whether we can find a similar expansion for the corresponding quantum problem, e.g. in the evaluation of transition elements.

For the forced anharmonic oscillator, we again define $S[x, J] = S_0[x, J] + S_1[x]$, where

$$S_0[x, J] = \int_{t_a}^{t_b} dt \left(\frac{m}{2} (\dot{x}^2 - \omega^2 x^2) + Jx \right) \quad \text{and} \quad S_1[x] = -\frac{\lambda}{4} \int_{t_a}^{t_b} d\tau x^4, \quad (3.53)$$

Consider the transition element

$$\langle x_b, t_b | T(\hat{x}(t_1) \cdots \hat{x}(t_m)) | x_a, t_a \rangle_J = \int_{x_a}^{x_b} \mathcal{D}x x(t_1) \cdots x(t_m) \exp \left\{ \frac{i}{\hbar} S[x, J] \right\} \quad (3.54)$$

where the subscript J on the LHS indicates that the transition element is evaluated in the presence of the force or “source” $J(t)$.

Functional differentiation: For a set of independent real variables $\{J_i, x_j \in \mathbb{R} \mid i, j = 0 \dots N\}$, we have the usual results for partial derivatives

$$\frac{\partial}{\partial J_i} J_j = \delta_{ij} \quad \text{and} \quad \frac{\partial}{\partial J_i} \sum_{j=0}^N J_j x_j = x_i \quad (3.55)$$

We may generalise the second result to define differentiation with respect to a *function* $J(t)$ of a continuous variable t . Define the *functional derivative* of the functional $X[J] = \int_{t_a}^{t_b} J(t) x(t) dt$ with respect to the value of the function $J(t)$ at the point t' to be

$$\frac{\delta X[J]}{\delta J(t')} \equiv \frac{\delta}{\delta J(t')} \int_{t_a}^{t_b} J(t) x(t) dt = x(t') \quad \text{when } t_a < t' < t_b, \quad \text{and zero otherwise.} \quad (3.56)$$

For this to hold for arbitrary functions $x(t)$, we must have $\frac{\delta}{\delta J(t')} J(t) = \delta(t - t')$.

The usual rules of differentiation apply, for example

$$\frac{\hbar}{i} \frac{\delta}{\delta J(t')} \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} J(t) x(t) dt \right\} = x(t') \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} J(t) x(t) dt \right\} \quad (3.57)$$

when $t_a < t' < t_b$ (which will always be the case in what follows), and zero otherwise.

Now use (3.53) and (3.57) to rewrite the transition element (3.54) in terms of functional derivatives

$$\begin{aligned} \langle x_b, t_b | T(\hat{x}(t_1) \cdots \hat{x}(t_m)) | x_a, t_a \rangle_J &= \int_{x_a}^{x_b} \mathcal{D}x x(t_1) \cdots x(t_m) \exp \frac{i}{\hbar} \left\{ S[x, 0] + \int_{t_a}^{t_b} J(t) x(t) dt \right\} \\ &= \int_{x_a}^{x_b} \mathcal{D}x \frac{\hbar}{i} \frac{\delta}{\delta J(t_1)} \cdots \frac{\hbar}{i} \frac{\delta}{\delta J(t_m)} \exp \frac{i}{\hbar} \left\{ S[x, 0] + \int_{t_a}^{t_b} J(t) x(t) dt \right\} \\ &= \hbar^m \frac{\delta^m}{i \delta J(t_1) \cdots i \delta J(t_m)} \langle x_b, t_b | x_a, t_a \rangle_J \end{aligned} \quad (3.58)$$

In the last line, we took the functional derivatives outside the path integral to obtain an expression for the m -point transition element (with $J \neq 0$) in terms of functional derivatives of the exact transition amplitude, also with $J \neq 0$.

If we set $J = 0$ at the *end* of the calculation, i.e. after performing *all* the functional derivatives, we get the transition element in the *absence* of the source $J(t)$

$$\langle x_b, t_b | T(\hat{x}(t_1) \cdots \hat{x}(t_m)) | x_a, t_a \rangle_{J=0} = \hbar^m \left[\frac{\delta^m}{i \delta J(t_1) \cdots i \delta J(t_m)} \langle x_b, t_b | x_a, t_a \rangle_J \right]_{J=0} \quad (3.59)$$

Perturbation theory: To obtain a perturbation expansion, we expand $\exp\{iS_1/\hbar\}$ as a power series in λ , just as we did for ordinary time-dependent perturbation theory in (3.4):

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle_J &= \int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} (S_0[x, J] + S_1[x]) \right\} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\lambda}{4\hbar} \right)^n \int_{t_a}^{t_b} d\tau_1 \cdots \int_{t_a}^{t_b} d\tau_n \int_{x_a}^{x_b} \mathcal{D}x x(\tau_1)^4 \cdots x(\tau_n)^4 \exp \frac{i}{\hbar} \left\{ S_0[x, 0] + \int_{t_a}^{t_b} J(t) x(t) dt \right\} \end{aligned} \quad (3.60)$$

We can replace all the factors of $x(\tau_i)^4$ by functional derivatives with respect to $J(\tau_i)$ using

$$x(\tau_i)^4 \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} J(t) x(t) dt \right\} = \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau_i)} \right)^4 \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} J(t) x(t) dt \right\} \quad (3.61)$$

Taking the functional derivatives outside the path integral and resumming the series gives

$$\langle x_b, t_b | x_a, t_a \rangle_J = \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} S_0[x, J] \right\} \quad (3.62)$$

The remaining path integral in (3.62) is just the forced harmonic oscillator. From (2.40) we have

$$\int_{x_a}^{x_b} \mathcal{D}x \exp \left\{ \frac{i}{\hbar} S_0[x, J] \right\} = F_\omega(T) \exp \left\{ \frac{i}{\hbar} S_0[\bar{x}, J] \right\} \quad (2.40a)$$

where $S_0[\bar{x}, J]$ is the *classical* action for the forced harmonic oscillator, which satisfies boundary conditions $x(t_a) = x_a$ and $x(t_b) = x_b$, with $T = t_b - t_a$.

Substituting (2.40a) and (3.62) into (3.58) gives us an expression for *all* transition elements to *all* orders in perturbation theory in terms of functional derivatives of the transition amplitude for the forced harmonic oscillator!

$$\begin{aligned} \langle x_b, t_b | T(\hat{x}(t_1) \cdots \hat{x}(t_m)) | x_a, t_a \rangle_J \\ = \hbar^m \frac{\delta^m}{i\delta J(t_1) \cdots i\delta J(t_m)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} F_\omega(T) \exp \left\{ \frac{i}{\hbar} S_0[\bar{x}, J] \right\} \end{aligned} \quad (3.63)$$

We evaluated $S_0[\bar{x}, J]$ for arbitrary x_a and x_b explicitly in tutorial-problem (2.3) (or Feynman and Hibbs Problem 3-11), but things are much simpler if we choose $x_a = x_b = 0$, as we did for classical mechanics. Let $\bar{x}(t)$ satisfy

$$\ddot{\bar{x}} + \omega^2 \bar{x} = \frac{J}{m} \quad \text{with} \quad \bar{x}(t_a) = \bar{x}(t_b) = 0. \quad (3.64)$$

From our discussion of classical mechanics (3.51), this has solution

$$\bar{x}(t) = -\frac{1}{m} \int_{t_a}^{t_b} dt' \Delta(t, t') J(t') \quad (3.65)$$

Integrating the classical action $S_0[\bar{x}, J]$ by parts, and using (3.64) and (3.65), we obtain (exercise)

$$S_0[\bar{x}, J] = \int_{t_a}^{t_b} dt \left(\frac{m}{2} (\dot{\bar{x}}^2 - \omega^2 \bar{x}^2) + J\bar{x} \right) = \frac{1}{2} \int_{t_a}^{t_b} dt J(t) \bar{x}(t) = -\frac{1}{2m} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \quad (3.66)$$

Substituting (3.66) into (3.63) gives an explicit expression for the (quantum) transition elements (with $x_a = x_b = 0$) to *all* orders in perturbation theory in terms of the *classical* Green function $\Delta(t, t')$

$$\begin{aligned} \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \cdots \hat{x}(t_m)) | 0, t_a \rangle_J \\ = \frac{\hbar^m \delta^m}{i\delta J(t_1) \cdots i\delta J(t_m)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar}{i} \frac{\delta}{\delta J(\tau)} \right)^4 \right\} \exp \left\{ \frac{-i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \end{aligned} \quad (3.67)$$

Harmonic oscillator: As a first example, let us evaluate the *two-point correlation function* for $\lambda = 0$ and set the source to zero at the end.

$$\begin{aligned}
 \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2)) | 0, t_a \rangle_{J=0} &= \left[\frac{\hbar^2 \delta^2}{i\delta J(t_1) i\delta J(t_2)} \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \\
 &= \left[\frac{\hbar^2 \delta^2}{i\delta J(t_1) i\delta J(t_2)} \left\{ 1 - \frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') + O(J^4) \right\} \right]_{J=0} \\
 &= \frac{i\hbar}{2m} \frac{\delta}{\delta J(t_1)} 2 \int_{t_a}^{t_b} dt J(t) \Delta(t, t_2) = \frac{i\hbar}{m} \Delta(t_1, t_2) \\
 &= \frac{\quad}{t_1 \quad \quad \quad t_2}
 \end{aligned} \tag{3.68}$$

where we have again introduced an obvious diagrammatic notation. Note that we don't need to evaluate the $O(J^4)$ term in the expansion of the exponential because its contribution vanishes when we set $J = 0$ at the end. And since $\Delta(t, t') = \Delta(t', t)$, we also have

$$\int_{t_a}^{t_b} dt' \Delta(t_2, t') J(t') = \int_{t_a}^{t_b} dt J(t) \Delta(t, t_2) \tag{3.68}$$

Similarly, for the *four-point function* (exercise)

$$\begin{aligned}
 \frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2) \hat{x}(t_3) \hat{x}(t_4)) | 0, t_a \rangle_{J=0} &= \left[\frac{\hbar^4 \delta^4}{i\delta J(t_1) \cdots i\delta J(t_4)} \exp \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \\
 &= \frac{\hbar^4 \delta^4}{i\delta J(t_1) \cdots i\delta J(t_4)} \frac{1}{2!} \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}^2 \\
 &= \left(\frac{i\hbar}{m} \right)^2 \left[\Delta(t_1, t_2) \Delta(t_3, t_4) + \Delta(t_1, t_3) \Delta(t_2, t_4) + \Delta(t_1, t_4) \Delta(t_2, t_3) \right] \\
 &= \frac{\quad}{t_1 \quad \quad \quad t_2} + \frac{\quad}{t_1 \quad \quad \quad t_2} + \frac{\quad}{t_1 \quad \quad \quad t_2}
 \end{aligned} \tag{3.70}$$

Note that we only need the contributions from the $O(J^4)$ term in the third line: the $O(J^2)$ term gives zero when we perform the four derivatives, and all terms $O(J^n)$ with $n > 4$ vanish when we set $J = 0$ at the end.

Note that the final result is symmetric with respect to interchange of any pair of $\{t_1, \dots, t_4\}$. In general, for $\lambda = 0$

$$\frac{1}{F_\omega(T)} \langle 0, t_b | \hat{x}(t_1) \cdots \hat{x}(t_m) | 0, t_a \rangle_{J=0} = \left(\frac{i\hbar}{m} \right)^{m/2} \sum_{\text{all pairings}} \Delta(t_{i_1}, t_{i_2}) \Delta(t_{i_3}, t_{i_4}) \cdots \Delta(t_{i_{m-1}}, t_{i_m}) \tag{3.71}$$

when m is even, and zero when m is odd. The sum is over all possible pairings of times t_1 to t_m . This result is known as *Wick's Theorem*.

Anharmonic oscillator: Now let's evaluate the four-point function in perturbation theory to first-order in λ for $J = 0$

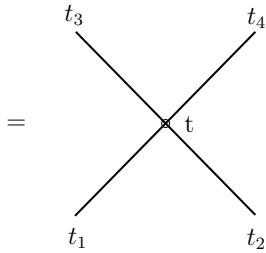
$$\frac{1}{F_\omega(T)} \langle 0, t_b | T(\hat{x}(t_1) \hat{x}(t_2) \hat{x}(t_3) \hat{x}(t_4)) | 0, t_a \rangle_{J=0} = \left[\frac{\hbar^4 \delta^4}{i\delta J(t_1) \cdots i\delta J(t_4)} \exp \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar \delta}{i\delta J(\tau)} \right)^4 \right\} \exp \left\{ \frac{-i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\} \right]_{J=0} \quad (3.72)$$

The $O(\lambda)$ contribution may be obtained by expanding the first exponential to first order, giving a total of eight functional derivatives. So we need only the $O(J^8)$ term from the second exponential

$$\frac{\hbar^4 \delta^4}{i\delta J(t_1) \cdots i\delta J(t_4)} \left\{ -\frac{i\lambda}{4\hbar} \int_{t_a}^{t_b} d\tau \left(\frac{\hbar \delta}{i\delta J(\tau)} \right)^4 \right\} \frac{1}{4!} \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' J(t) \Delta(t, t') J(t') \right\}^4 \quad (3.73)$$

Clearly, this will result in many different terms. Let us first perform the derivatives with respect to $J(\tau)$, keeping only those terms in which each derivative acts on a *different* $\int J \Delta J$ term in $\{\int J \Delta J\}^4$, which gives

$$\begin{aligned} & \frac{\hbar^4 \delta^4}{i\delta J(t_1) \cdots i\delta J(t_4)} \left(-\frac{i\lambda}{4\hbar} \right) \left(\frac{\hbar}{i} \right)^4 \frac{8 \cdot 6 \cdot 4 \cdot 2}{4!} \int_{t_a}^{t_b} d\tau \left\{ -\frac{i}{2m\hbar} \int_{t_a}^{t_b} dt' \Delta(\tau, t') J(t') \right\}^4 \\ &= -i \frac{3! \lambda}{\hbar} \int_{t_a}^{t_b} dt \prod_{i=1}^4 \left(\frac{i\hbar}{m} \Delta(t, t_i) \right) \end{aligned} \quad (3.74)$$



where we changed the dummy integration variable from τ to t in the last expression. All the other terms give rise to disconnected diagrams, which we ignore - see below.

To keep track of the form of each term, diagrams are *very* useful. The *Feynman Rules* for drawing Feynman diagrams (or graphs) are collected in table 3.1. Note that in the diagrams the binomial coefficients are omitted.

vertices	$\times t$	$-i \frac{3! \lambda}{\hbar} \int_{t_a}^{t_b} dt$
propagator	$t \text{ --- } t'$	$\frac{i\hbar}{m} \Delta(t, t')$
external field	$t \times \text{---}$	$\frac{i}{\hbar} \int_{t_a}^{t_b} dt J(t)$

Table 3.1: Feynman rules

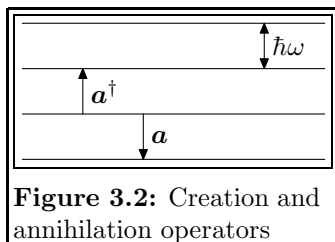


Figure 3.2: Creation and annihilation operators

Interpretation: Remember, that for a harmonic oscillator we may write (in the Heisenberg picture)

$$\begin{aligned} \hat{x}(t) &= \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger(t) + \hat{a}(t)) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger(0) e^{-i\omega t} + \hat{a}(0) e^{i\omega t}) \end{aligned} \quad (3.83)$$

Think of the insertions $\hat{x}(t)$ as creating or destroying a quantum at time t . $a^\dagger(t)$ creates a mode with energy $E > 0$ at time t , $\hat{a}(t)$ destroys it. The transition element in (3.74) describes how two quanta interact and scatter off each other due to the anharmonic perturbation, which gives us the basis of a *multi-particle* quantum theory.

For coupled oscillators, the anharmonic term describes phonon-phonon scattering in simple models of crystals.

This brings us to the end of the examinable material for the non-relativistic part of the course. What follows should be useful for Modern Quantum Field Theory.

End of examinable material on non-relativistic quantum theory

Loops and legs: We can represent the perturbation expansion of equation (3.67) for $\langle 0, t_b | 0, t_a \rangle_J$ by setting the index $m = 0$ and using Feynman diagrams. For $J = 0$, we find, through $\mathcal{O}(\lambda^2)$ (not proven here)

$$\langle 0, t_b | 0, t_a \rangle_0 = F_\omega(T) \left(1 + \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots \right) \quad (3.75)$$

Curved lines in the diagrams above represent propagators $i\hbar/m \Delta(t, t')$ as before. Curved lines which begin and end at the *same* point represent propagators $i\hbar/m \Delta(t, t)$, i.e with $t = t'$.

If $J(t) \neq 0$, we must perform the derivatives without expanding the exponential of the $\iint J \Delta J$ term. We find, for example,

$$\langle 0, t_b | 0, t_a \rangle_J = F_\omega(T) e^{iS_0[\bar{x}, J]/\hbar} \left(1 + \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots \right) \quad (3.76)$$

If instead we consider a ratio, the factors $F_\omega(T) e^{iS_0[\bar{x}, J]/\hbar}$ cancel not proven here – see MQFT). For example, expanding up to order $\mathcal{O}(\lambda^2)$, we get

$$\frac{\langle 0, t_b | \hat{x}(t) | 0, t_a \rangle_J}{\langle 0, t_b | 0, t_a \rangle_J} =$$

classical $\text{---} \times + \text{---} \times + \text{---} \times + \dots$

$\mathcal{O}(\hbar)$ $+ \text{---} \text{[loop]} + \text{---} \text{[loop]} + \text{---} \text{[loop]} + \text{---} \text{[loop]} + \dots$

$\mathcal{O}(\hbar^2)$ $+ \text{---} \text{[loop]} + \text{---} \text{[loop]} + \text{---} \text{[loop]} + \dots$

Notes:

- (1) We have only drawn the “connected” diagrams because all the “disconnected” ones cancel between numerator and denominator. The proof, however, needs more machinery.
- (2) The new graphs which we didn’t encounter in the diagrammatic version of (3.52) for the classical solution $\bar{x}(t)$ contain propagator “loops”, and these give the quantum corrections to the classical result. To show this, we need to count the powers of \hbar . Each propagator brings an \hbar , each source

brings a \hbar^{-1} , while each vertex gives us a factor of \hbar^{-1} . Hence, for a graph of order \hbar^n , the number P of propagators, the number V of vertices, and the number S of sources are related by

$$n = P - V - S. \quad (3.77)$$

But, from the diagrams above, this is also equal to the number of loops (the proof is by induction). Thus in the classical limit all loop graphs are suppressed as $\hbar \rightarrow 0$ and the tree graphs sum to the classical solution as in (3.52).

- (3) To calculate scattering amplitudes, we need to take $t_a \rightarrow -\infty$ and $t_b \rightarrow \infty$. We also require to pick out definite “in” and “out” states in this limit, but $\Delta(t, t')$ oscillates wildly for large times. The trick is to take $\omega'^2 \equiv \omega^2 - i\varepsilon$, with infinitesimal (but non-zero) $\varepsilon > 0$, in the action, so

$$S' = S + i\varepsilon \int_{-\infty}^{\infty} x^2 dt \quad \Rightarrow \quad e^{iS'/\hbar} = e^{iS/\hbar - \varepsilon/\hbar \int x^2 dt}. \quad (3.78)$$

So states with $x \neq 0$ as $t_{b,a} \rightarrow \pm\infty$ are exponentially suppressed. We have

$$\begin{aligned} \omega' &= \sqrt{\omega^2 - i\varepsilon} = \omega \left(1 - \frac{i\varepsilon}{\omega^2}\right)^{\frac{1}{2}} \simeq \omega \left(1 - \frac{i\varepsilon}{2\omega^2}\right) = \left(\omega - \frac{i\varepsilon}{2\omega}\right) \\ &= (\omega - i\varepsilon'). \end{aligned} \quad (3.79)$$

where $\varepsilon' = \varepsilon/(2\omega) > 0$.

In the limit $t_{b,a} \rightarrow \pm\infty$ the first term in $\Delta(t, t')$ in (3.44) becomes

$$\begin{aligned} \lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \frac{\sin \omega'(t_b - t) \sin \omega'(t' - t_a)}{\sin \omega' T} &= \lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \frac{\frac{1}{2i} e^{i\omega'(t_b - t)} \frac{1}{2i} e^{i\omega'(t' - t_a)}}{\frac{1}{2i} e^{i\omega' T}} \\ &= \frac{1}{2i} e^{-i\omega'(t - t')} \end{aligned} \quad (3.80)$$

This, together with a similar analysis for the second term in (3.44), gives

$$\lim_{t_b \rightarrow \infty} \lim_{t_a \rightarrow -\infty} \Delta(t, t') = \frac{1}{2i\omega'} (e^{-i\omega'(t - t')} \theta(t - t') + e^{i\omega'(t - t')} \theta(t' - t)) \equiv \Delta_F(t - t') \quad (3.81)$$

which is the “standard” Feynman propagator. We can now drop the prime on ω' (until we need it again.) Adding a small imaginary term to the action is called the *i-epsilon prescription*.

Since “in” and “out” states with $x(t) \neq 0$ are suppressed, the in and out states are just ground or “vacuum” states of the SHO. (This argument can be refined.) To calculate the “scattering amplitude”, we have to find the vacuum expectation value with $J = 0$. For $m = 4$, we find

$$\frac{\langle 0 | T(\hat{x}(t_1) \cdots \hat{x}(t_4)) | 0 \rangle}{\langle 0 | 0 \rangle} = \text{tree} + \text{loop} + \text{self-energy} + \cdots \quad (3.82)$$

The first “tree level” diagram is $O(\lambda)$ whilst the next two (and all permutations thereof) are $O(\lambda^2)$ and carry one more power of \hbar associated with the loop.

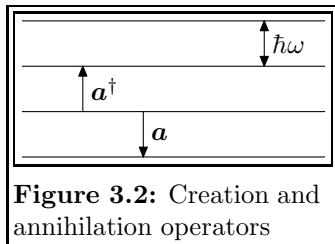


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Think of the insertions $\hat{x}(t)$ as creating or destroying a quantum out of the vacuum at time t . $\hat{a}^\dagger(t)$ creates a mode with energy $E > 0$ at time t , $\hat{a}(t)$ destroys it. The scattering amplitude in (3.82)

describes how two quanta interact and scatter off each other due to the anharmonic perturbation, which gives us the basis of a multi-particle quantum theory.

For coupled oscillators, the anharmonic term describes phonon-phonon scattering in simple models of crystals.

Note that the Feynman propagator $\Delta_F(t - t')$ takes modes with $E > 0$ forwards in time, $t > t'$: “retarded”; whilst it takes modes with $E < 0$ backwards in time, $t < t'$: “advanced”. The $E < 0$ modes are like $E > 0$ modes moving backwards in time - but everything adds up to give a causal answer!

Quantum field theory is constructed by replacing the position operators $\hat{x}(t)$ by scalar field operators $\hat{\phi}(\underline{x}, t)$. These create and destroy field quanta, which we now interpret as particles, and the Feynman propagator $\Delta_F(t - t')$ gets replaced by its four-dimensional equivalent. Then (3.82) gives us the amplitude for scattering of pairs of Higgs bosons! (See MQFT or Standard Model courses.)
