The University of Edinburgh
School of Physics and Astronomy

Lecture Notes

Quantum Theory

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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 and particle physics are better suited to a more intuitive formulation of quantum mechanics based on the ideas of Dirac and Feynman, namely the the path integral or "sum over histories" approach. In this course we begin with a review of the fundamental ideas of quantum mechanics, the path integral for a non-relativistic point particle is introduced and used to derive time-dependent perturbation theory and the Born series for nonrelativistic scattering. The course concludes with an introduction to relativistic quantum mechanics and the 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 Schrödinger in 1926, and thereafter unified into a more general formulation 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.)

Structure of the course:

(1) Elements of Quantum Mechanics;

(2) Path integrals for single particles;

(3) Perturbation Theory and Scattering;

(4) Relativistic Quantum Theory – wave mechanics, field theory.

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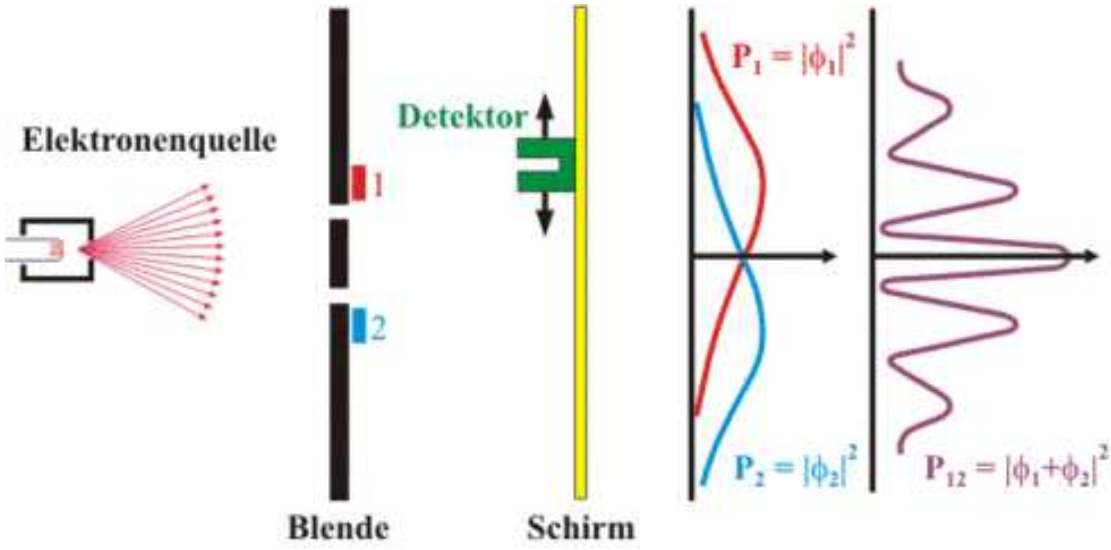
Brian Pendleton Edinburgh, January 2010.

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* (which are 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

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 - this is called 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

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

This is called *linear superposition* of states.

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

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

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

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

(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:*

$$\|\,|\psi\rangle\,\|^2 = \langle\psi|\psi\rangle = 1. \tag{1.3}$$

This fixes $|c|^2 = 1$, so $c = \mathrm{e}^{\mathrm{i}\alpha}$. 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:

$$|1\rangle \quad \text{(the particle goes through slit 1)}$$
$$|2\rangle \quad \text{(the particle goes through slit 2)}$$

The state observed in the detector will in general be some linear combination of these:

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

There are *many* 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

$$P(\psi \to \phi) = |\langle\phi|\psi\rangle|^2 \tag{1.4}$$

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

- The amplitude for $\psi \to \phi$ and *then* $\phi \to \chi$ is $\langle\chi|\phi\rangle\,\langle\phi|\psi\rangle$.
- The amplitude for $\psi \to \phi$ *or* $\psi \to \chi$ is $\langle\phi|\psi\rangle + \langle\chi|\psi\rangle$;

This means that:

$$P(\psi \to \phi \to \chi) = P(\psi \to \phi)\, P(\phi \to \chi)$$

but

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

because

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

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

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 be detected in the final state $|f\rangle$ (on the second screen) is:

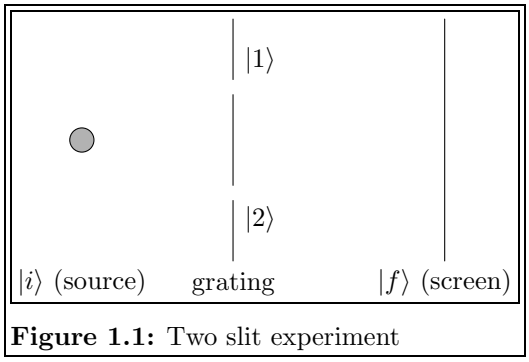


Figure 1.1: Two slit experiment

$$\langle f|i\rangle = \langle f|1\rangle\,\langle 1|i\rangle + \langle f|2\rangle\,\langle 2|i\rangle$$

The first (second) term is the amplitude for the path through slit 1 (2). For the probability, we have:

$$\begin{aligned} P(i \to f) &= |\langle f|i\rangle|^2 \\ &= |\langle f|1\rangle\,\langle 1|i\rangle + \langle f|2\rangle\,\langle 2|i\rangle|^2 \\ &\neq |\langle f|1\rangle\,\langle 1|i\rangle|^2 + |\langle f|2\rangle\,\langle 2|i\rangle|^2 \end{aligned}$$

Question: Why?

Answer: The probability $P(i \to f) \neq P(i \to f \text{ via } 1) + P(i \to f \text{ via } 2)$ because $P(i \to f)$ can vanish if amplitudes for the different paths cancel.

Question: For a given $i \to f$, 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

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

and there is no interference.

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

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 $|\psi\rangle \in \mathcal{H}$:

$$|\psi\rangle = \sum_n \psi_n |n\rangle \tag{1.5}$$

for some complex numbers ψ_n (the *components* of $|\psi\rangle$). The basis vectors may be chosen to be *orthonormal:*

$$\langle m|n\rangle = \delta_{mn}. \tag{1.6}$$

Then the following equation holds:

$$\langle m|\psi\rangle = \sum_n \psi_n \langle m|n\rangle = \psi_m. \tag{1.7}$$

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

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle \tag{1.8}$$

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

$$\sum_n |n\rangle \langle n| = \hat{1} \tag{1.9}$$

where $\hat{1}$ is the unit or identity operator. 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:

$$1 = \langle\psi|\psi\rangle = \sum_n \langle\psi|n\rangle \langle n|\psi\rangle = \sum_n |\langle n|\psi\rangle|^2 = \sum_n P(\psi \to n) \tag{1.10}$$

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

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

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. However, 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:*

$$\hat{\xi} \equiv \sum_n \xi_n |n\rangle \langle n| \tag{1.11}$$

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:

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

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

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

$$\hat{\xi}\,|n\rangle = \sum_m \xi_m\,|m\rangle\,\langle m|n\rangle = \xi_n\,|n\rangle \tag{1.12}$$

(d) if we have a second observable which takes values ζ_n on $|n\rangle$, then $\hat{\xi}$ and $\hat{\zeta}$ commute:

$$\hat{\xi}\hat{\zeta}\,|n\rangle = \xi_n\zeta_n\,|n\rangle = \zeta_n\xi_n\,|n\rangle = \hat{\zeta}\hat{\xi}\,|n\rangle \;\;\forall n,\;\; \text{so } [\hat{\xi},\,\hat{\zeta}] = 0.$$

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:

$$\begin{aligned}\overline{\xi} &= \sum_n \xi_n |\,\langle n|\psi\rangle\,|^2 = \sum_n \xi_n\,\langle\psi|n\rangle\,\langle n|\psi\rangle \\ &= \langle\psi|\,\hat{\xi}\,|\psi\rangle\end{aligned} \tag{1.13}$$

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*. (The basis states may often 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 $\{|n\rangle\} \mapsto \{|\bar{n}\rangle\}$. Expressing the new basis states in terms of the old ones gives:

$$|\bar{n}\rangle = \sum_m |m\rangle\,\langle m|\bar{n}\rangle \equiv \sum_m |m\rangle\,U_{mn} \tag{1.14}$$

Orthonormality then implies that

$$\begin{aligned}\delta_{nn'} = \langle\bar{n}|\bar{n}'\rangle &= \sum_{m,m'} \langle\bar{n}|m\rangle\,\langle m|m'\rangle\,\langle m'|\bar{n}'\rangle = \sum_{m,m'} \langle\bar{n}|m\rangle\,\delta_{mm'}\,\langle m'|\bar{n}'\rangle \\ &= \sum_m U^\dagger_{nm}U_{mn'} \qquad (\text{where } U^\dagger_{nm} \equiv U^*_{mn})\end{aligned}$$

So U_{mn} is the mn element of a *unitary* matrix. In operator notation we define

$$|\bar{n}\rangle \equiv \hat{U}\,|n\rangle \quad \text{which gives} \quad U_{mn} = \langle m|\,\hat{U}\,|n\rangle$$

(brief exercise for the student). Clearly, $\hat{U}$ is a *unitary operator:* $\hat{U}^\dagger\hat{U} = \hat{1}$. Note that 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. if we let $n \to \infty$, we will need a *continuous* label x. We get the usual transition from discrete to continuous variables

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

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

$$|\psi\rangle = \int_a^b \psi(x)\,|x\rangle\ \mathrm{d}x$$

If we normalise our states so that

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

then

$$\langle x' | \psi\rangle = \int_a^b \psi(x)\,\langle x' | x\rangle\ \mathrm{d}x = \psi(x')$$

so

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

We may write

$$|\psi\rangle = \int_a^b \mathrm{d}x\,|x\rangle\,\langle x | \psi\rangle \qquad \text{and thus} \qquad \hat{1} = \int_a^b \mathrm{d}x\,|x\rangle\,\langle x| \tag{1.15}$$

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

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

$$1 = \langle \psi | \psi\rangle = \int_a^b \mathrm{d}x\,\langle \psi | x\rangle\,\langle x | \psi\rangle = \int_a^b \mathrm{d}x\,\psi^*(x)\,\psi(x),$$

so $|\psi|^2\,\mathrm{d}x$ is the probability that the particle is between x and $x+\mathrm{d}x$. Therefore $\psi(x)$ is the usual (time-independent) wavefunction of wave mechanics.

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

$$\hat{x} = \int_a^b \mathrm{d}x\,x\,|x\rangle\,\langle x| \tag{1.16}$$

and verify that

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

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

$$\langle \psi|\,\hat{x}\,|\psi\rangle = \int_a^b \mathrm{d}x\,\langle \psi | x\rangle\,x\,\langle x | \psi\rangle = \int_a^b \mathrm{d}x\,\psi^*(x)\,x\,\psi(x) \tag{1.17}$$

There is of course no need to restrict ourselves to a finite interval (a, b). We can let $a \to -\infty$ and $b \to \infty$ and take $x \in (-\infty, \infty)$. Furthermore we do not have to stay in the position basis. For example consider the Fourier transform basis:

$$|k\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}}\,\mathrm{e}^{+\mathbb{i}kx}\,|x\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\,|x\rangle\,\langle x | k\rangle\,, \tag{1.18}$$

from which we may read off:

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathbb{i}kx} \quad ; \quad \langle k|x\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\mathbb{i}kx}. \tag{1.19}$$

Then we obtain the following relation:

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

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

$$\hat{k} = \int \mathrm{d}k\, k\, |k\rangle\, \langle k| \quad \Rightarrow \quad \hat{k}\,|k\rangle = k\,|k\rangle\,.$$

It follows that

$$\begin{aligned} \hat{k}\,|x\rangle &= \int \mathrm{d}k\, k\, |k\rangle\, \langle k|x\rangle = \mathbb{i}\frac{\partial}{\partial x}\int \mathrm{d}k\, |k\rangle\, \langle k|x\rangle \\ &= \mathbb{i}\frac{\partial}{\partial x}\,|x\rangle\,. \end{aligned} \tag{1.21}$$

where we used (1.19) which implies

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

to obtain the last expression on the first line of (1.21).

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

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

Finally

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

which should look familiar from wave mechanics.

Similarly, if we define

$$\tilde{\psi}(k) = \langle k|\psi\rangle = \int \mathrm{d}x\,\langle k|x\rangle\,\langle x|\psi\rangle = \int \frac{\mathrm{d}x}{\sqrt{2\pi}}\mathrm{e}^{-\mathbb{i}kx}\psi(x) \tag{1.23}$$

we easily find

$$\langle k|\,\hat{k}\,|\psi\rangle = k\tilde{\psi}(k), \tag{1.24}$$

while (exercise)

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

and hence

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

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

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

Table 1.1: Operators in different bases

$$\left[\hat{x},\hat{k}\right] = \mathbb{i} \tag{1.26}$$

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

$$\Delta x \Delta k \geq \frac{1}{2}. \tag{1.27}$$

Later we will show that momentum $p = \hbar k$. All of the above can easily generalised to 3 space dimensions:

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

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

$$\begin{aligned}\langle f|i\rangle &= \int \mathrm{d}x_1 \, \langle f|x_1,t_1\rangle \, \langle x_1,t_1|i\rangle \\ &= \int \mathrm{d}x_1 \int \mathrm{d}x_2 \\ &\qquad \langle f|x_2,t_2\rangle \, \langle x_2,t_2|x_1,t_1\rangle \, \langle x_1,t_1|i\rangle \\ &= \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_N \, \langle f|x_N,t_N\rangle \cdots \langle x_1,t_1|i\rangle \end{aligned} \tag{1.28}$$

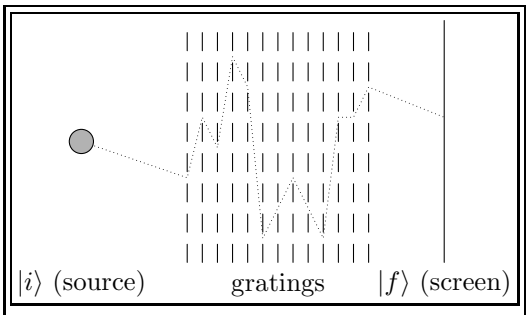


Figure 1.2: Sketch of the slit experiment with more gratings

By adding more and more gratings the time intervals get smaller and smaller and we fix the 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

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

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

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

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 $N \to \infty$ (*i.e.* $\varepsilon \to 0$) this becomes:

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

where the 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 integrate ('sum') 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 ($t_n = t_{n-1} + \varepsilon$):

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

where ϕ is real. This is because:

(a) in the limit $\varepsilon \to 0$, the amplitude should be constant (continuity);

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

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

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

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

where L is the Lagrangian. For a non-relativistic point particle in a potential V in one dimension this is:

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

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

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

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

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

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

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

Consider now the *value* of the action S on the classical path: $S_{\mathrm{cl}} = S[\bar{x}(t)]$. 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 (for $\delta t_b = 0$)

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

Hence

$$\frac{\partial S_{\mathrm{cl}}}{\partial x_b} = p_b \tag{2.6}$$

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

Now consider $\frac{\mathrm{d}S_{\mathrm{cl}}}{\mathrm{d}t_b}$. From (2.1) we get:

$$\frac{\mathrm{d}S_{\mathrm{cl}}}{\mathrm{d}t_b} = L(x_b, \dot{x}_b, t_b) = \frac{\partial S_{\mathrm{cl}}}{\partial t_b} + \frac{\partial S_{\mathrm{cl}}}{\partial x_b}\dot{x}_b$$

This gives

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

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 and Lagrange's equation of motion (EoM) are

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

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

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

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

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

and, using the Hamilton-Jacobi equations, we get

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

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

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

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,

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

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

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

2.2. The Amplitude for a Path

We saw already in (1.33) that we expect the amplitude to be:

$$\langle x_b, t_b | x_a, t_a\rangle\,\big|_{x(t)} \sim \exp\left\{\,\mathbb{i}\int_{t_a}^{t_b} {\rm d}t\;\phi(x, \dot{x}, t)\right\}. \tag{2.8}$$

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:

$$S[x(t)] = \int_{t_a}^{t_b} {\rm d}t\; L(x, \dot{x}, t) \tag{2.9}$$

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 $\int \phi\,{\rm d}t = S/\hbar$, *i.e.* we assume:

$$\langle x_b, t_b | x_a, t_a\rangle\,\big|_{x(t)} = {\rm e}^{\mathbb{i}S[x(t)]/\hbar}. \qquad \text{(Dirac)} \tag{2.10}$$

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:

(1) If $S \to S + c$ (where c is a constant), all amplitudes change by ${\rm e}^{\mathbb{i}c/\hbar}$, 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:

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

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

$$\int_{x_a}^{x_b} \mathcal{D}x = \lim_{N\to\infty} A_N \prod_{n=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}x_n$$

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

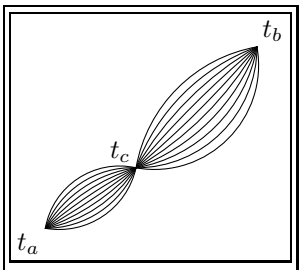


Figure 2.1: Split one path in two

Note also the fundamental property: if we split the path in two, as shown pictorially in figure 2.1, we get

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

as required. This may be used to fix the normalisation $\nu(t)$ (see below.)

2.4. The classical limit (heuristic)

For quantum situations, t_b & t_a, and x_b & x_a are "close", $S[x(t)] = \mathcal{O}(\hbar)$, and the phases are of order $\mathcal{O}(1)$.

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 $\hbar \to 0$.) Now consider paths "very close" to a given path $x(t)$. Even though δx is small, δS will in general be large compared with $\hbar$, because S is so large. So $\mathrm{e}^{\mathbb{i}\delta S/\hbar} = \cos(\delta S/\hbar) + i\sin(\delta S/\hbar)$ 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 $\hbar \to 0$ the classical path gives the dominant contribution (*i.e.* we derive the principle of least action and hence classical mechanics) and therefore

$$\langle x_b, t_b | x_a, t_a \rangle \sim \mathrm{e}^{\mathbb{i}S_{\mathrm{cl}}/\hbar} \qquad (\text{'semiclassical approximation'})$$

2.5. Momentum and Energy

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

$$S_{\mathrm{cl}} \to S_{\mathrm{cl}} + \frac{\partial S_{\mathrm{cl}}}{\partial x_b} \delta x_b.$$

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

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

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):

$$[\hat{x}, \hat{p}] = \mathbb{i}\hbar. \tag{2.13}$$

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

$$S_{\mathrm{cl}} \to S_{\mathrm{cl}} + \frac{\partial S_{\mathrm{cl}}}{\partial t_b} \delta t_b.$$

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

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

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 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

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

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

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

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

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

and note that

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

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

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

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

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

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

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

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

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

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

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

since, as we showed above for the free particle,

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

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

Notes:

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

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

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

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

$$G_0(x_b - x_a, t_b - t_a) \equiv \langle x_b, t_b | x_a, t_a \rangle \tag{2.21}$$

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)

$$\begin{aligned}\tilde{G}_0(p,t) &\equiv \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{\mathbb{i}xp/\hbar} G_0(x,t) = \sqrt{\frac{m}{2\pi\mathbb{i}\hbar t}} \int_{-\infty}^{\infty} \mathrm{d}x\, \exp\left\{\frac{\mathbb{i}xp}{\hbar} + \frac{\mathbb{i}mx^2}{2\hbar t}\right\} \\ &= \exp\left(-\mathbb{i}\frac{p^2 t}{2m\hbar}\right) = \exp\left(-\mathbb{i}\frac{Et}{\hbar}\right)\end{aligned} \tag{2.22}$$

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

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

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

must be finite, and we *must* choose $\nu(\varepsilon) = \sqrt{\frac{m}{2\pi\mathbb{i}\hbar\varepsilon}}(1 + O(\varepsilon))$, (so that the $O(\varepsilon)$ term goes to zero as $\varepsilon \to 0$). 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 $t_b \to t_a$

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

as required.

Finally, it is easy to check that with this normalisation

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, \langle x_b, t_b | x, t \rangle\, \langle x, t | x_a, t_a \rangle \tag{2.23}$$

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

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

To see this, consider an alternative method of calculation: write $x(t) = \bar{x}(t) + \eta(t)$, 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 $\frac{\delta S}{\delta x}\big|_{x=\bar{x}} = 0$ 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

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

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

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

$$\langle x_b, t_b | x_a, t_a\rangle = \mathrm{e}^{\mathrm{i}S_{\rm cl}/\hbar}\int_0^0 \mathcal{D}\eta\,\mathrm{e}^{\mathrm{i}S[\eta]/\hbar} \equiv F_0(T)\,\mathrm{e}^{\mathrm{i}S_{\rm cl}/\hbar}, \tag{2.25}$$

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 is

$$F_0(T) = \langle 0, t_b | 0, t_a\rangle = \langle 0, T | 0, 0\rangle \tag{2.26}$$

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)

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

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

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

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

2.7. The Harmonic Oscillator

The Lagrangian is:

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

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

$$S[\bar{x}+\eta] = S[\bar{x}] + S[\eta] \tag{2.30}$$

because the cross-term

$$\int_{t_a}^{t_b} \mathrm{d}t\,\left(\dot{\bar{x}}\dot{\eta} - \omega^2\bar{x}\eta\right) = -\int_{t_a}^{t_b} \mathrm{d}t\,\eta\left(\ddot{\bar{x}} + \omega^2\bar{x}\right) + \big[\eta\dot{\bar{x}}\big]_{t_a}^{t_b} = 0 \tag{2.31}$$

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

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

$$\langle x_b, t_b | x_a, t_a \rangle = F_\omega(t_b - t_a) \mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar}, \tag{2.32}$$

where S_{cl} is the classical action

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

and the normalisation factor is

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

which is again independent of the boundary conditions. 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:

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

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

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

Note that as $\omega \to 0$, $F_\omega(t) \to F_0(t)$, as it must.

2.8. The Forced Harmonic Oscillator

Consider the forced harmonic oscillator with Lagrangian

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

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

$$\ddot{\bar{x}} + \omega^2 \bar{x} = \frac{J}{m}. \tag{2.38}$$

The action depends on both $x(t)$ and $J(t)$, but since it is still quadratic we get

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

The *fluctuation term* $S[\eta, 0]$ is independent of J because the coupling of J to x (and hence to η) is linear. Thus

$$\langle x_b, t_b | x_a, t_a \rangle = F_\omega(T) \, \mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar} \tag{2.40}$$

where now $S_{\mathrm{cl}} = S[\bar{x}, J]$, 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:

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

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

$$|p\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi\hbar}} \mathrm{e}^{+\mathrm{i}px/\hbar}\,|x\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\,|x\rangle\,\langle x|p\rangle\,, \tag{2.42}$$

from which we may read off

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar} \quad ; \qquad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}px/\hbar}\,. \tag{2.43}$$

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

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

Now consider the infinitesimal amplitude

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

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 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 rewrite (2.45) as

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

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

Finally, we use the Baker-Campbell-Hausdorff formula

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

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

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

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 $\varepsilon = t_{n+1} - t_n$, then for infinitesimal $t - t_0$, this result may be written in the form

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

If we differentiate (2.49) with respect to time t, we get the following differential equation:

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

where we used $\hat{H}(t_0) \approx \hat{H}(t)$ for infinitesimal $t - t_0$. Now define $\psi(x,t) = \langle x,t|\psi\rangle$, so $\langle\psi|x,t\rangle = \psi^*(x,t)$, then (exercise)

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

Equation (2.50) is of course known as the *Schrödinger 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:

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

   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 is particularly useful in statistical mechanics.
3. We can use (2.51) to give yet another derivation of the free particle amplitude:

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

   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. The equation (2.49) may be regarded as a solution of the Schrödinger equation for infinitesimal $t - t_0$. If the Hamiltonian were time-independent, (2.49) would hold for all t,

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

whereas, for a general time-dependent Hamiltonian, we must write:

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

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

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

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

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

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

5. **The Schrödinger and Heisenberg pictures**

We may now 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 satisfies the Schrödinger equation

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

We say that $|\psi,t\rangle$ and $|x\rangle$ are the state vector and position eigenstate in the *Schrödinger picture* for time dependence in quantum mechanics, whereas $|\psi\rangle$ 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 $\hat{x} = \int \mathrm{d}x\; x\,|x\rangle\,\langle x|$ are time-independent while in the Heisenberg picture $\hat{x}(t) = \int \mathrm{d}x\; x\,|x,t\rangle\,\langle x,t|$ 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

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

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

However, since

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

we must have $\hat{U}\hat{H} = \hat{H}\hat{U} \;\Rightarrow\; \hat{H} = \hat{U}^\dagger\hat{H}\hat{U}$, *i.e.* the Hamiltonian is the *same* in both pictures.

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

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

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

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

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

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

$$\psi(x,t) = \langle x, t | \psi \rangle = \int \mathrm{d}x' \, \langle x, t | x', t' \rangle \, \langle x', t' | \psi \rangle$$

So if we define

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

$$\text{then} \qquad \theta(t-t')\,\psi(x,t) = \int \mathrm{d}x' \, G(x, x'; t, t')\, \psi(x', t')$$

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

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) - \mathrm{i}\hbar\frac{\partial}{\partial t}\right)\theta(t-t')\,\psi(x,t) = -\mathrm{i}\hbar\delta(t-t')\,\psi(x,t)$$

$$\text{so} \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) - \mathrm{i}\hbar\frac{\partial}{\partial t}\right) G(x, x'; t, t') = -\mathrm{i}\hbar\delta(t-t')\,\delta(x-x') \qquad \forall\, t, t'$$

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

Note that 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 usual to expand in a basis of energy eigenstates $|n\rangle$ with $n = 0, 1, 2, 3, \ldots$

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

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

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

Let us take the Fourier transform of $G(x, y; t)$ with respect to t:

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

The $\mathrm{i}\epsilon$ ($\epsilon > 0$, infinitesimal) is introduced to ensure that for positive real energies the integral converges at the upper limit. 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 $E_n - \mathrm{i}\epsilon$, 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 $\mathrm{i}\epsilon$ is also necessary for the convergence of the path integral, *e.g.* for the harmonic oscillator, $E_n \to E_n - \mathrm{i}\epsilon$ if $\omega \to \omega - \mathrm{i}\epsilon, \omega > 0$, *i.e.* $\omega^2 \to \omega^2 - \mathrm{i}\epsilon$, so

$$S[x] \to S[x] + \mathrm{i}\epsilon m \int \mathrm{d}t\, x^2, \quad \text{and} \quad \exp\{\mathrm{i}S/\hbar\} \to \exp\{\mathrm{i}S/\hbar\} \exp\left\{-\epsilon(m/\hbar)\int \mathrm{d}t x^2\right\}$$

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 $t > 0$):

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \langle x, t | x, 0 \rangle = \int \mathrm{d}x \, G(x, x; t) = \sum_n \mathrm{e}^{-\mathrm{i}tE_n/\hbar} \int \mathrm{d}x \, |u_n(x)|^2 = \sum_n \mathrm{e}^{-\mathrm{i}tE_n/\hbar} \tag{2.60}$$

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:

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}x\, \langle x,t|x,0\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, \sqrt{\frac{m\omega}{2\pi \mathbb{i}\hbar \sin\omega t}}\, \exp\left\{ \underbrace{\frac{\mathbb{i}m\omega}{2\hbar\sin\omega t} 2x^2(\cos\omega t - 1)}_{\mathbb{i}S_{\mathrm{cl}}/\hbar,} \right\} \\ &= \frac{1}{2\mathbb{i}} \frac{1}{\sin\frac{\omega t}{2}} \qquad \text{(gaussian integral)} \\ &= \frac{\mathrm{e}^{-\mathbb{i}\omega t/2}}{1-\mathrm{e}^{-\mathbb{i}\omega t}} = \mathrm{e}^{-\mathbb{i}\omega t/2} \sum_{n=0}^{\infty} \mathrm{e}^{-\mathbb{i}n\omega t} = \sum_n \mathrm{e}^{-\mathbb{i}tE_n/\hbar} \qquad \text{(using (2.60))}\end{aligned} \tag{2.61}$$

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)

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

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

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

The classical Hamiltonian is

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

Exercise: verify explicitly that the Lagrangian (2.62) gives the Lorentz force and the classical Hamiltonian above. (See Junior Honours *Lagrangian Dynamics* notes & tutorials if necessary.)

One can then derive the quantum Hamiltonian $H(\hat{\underline{x}}, \hat{\underline{p}}, t)$ and the corresponding Schrödinger equation. However, this is tricky because $\left[\hat{\underline{p}},\, \underline{A}(\hat{\underline{x}},t)\right] \neq 0$ (tutorial).

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

$$\underline{A} \to \underline{A} + \underline{\nabla}\chi \qquad \text{and} \qquad \phi \to \phi - \frac{1}{c}\frac{\partial\chi}{\partial t} \tag{2.66}$$

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

$$L \to L + \frac{e}{c}\,\dot{\underline{x}}\cdot\underline{\nabla}\chi + \frac{e}{c}\frac{\partial\chi}{\partial t} = L + \frac{e}{c}\frac{d\chi}{dt} \tag{2.67}$$

where we noted that $\dot{\underline{x}}\cdot\underline{\nabla}\chi + \frac{\partial\chi}{\partial t} = \frac{d\chi}{dt}$, 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.

However, the action does change:

$$S = \int_{t_a}^{t_b} \mathrm{d}t\, L \to S + \frac{e}{c}\int_{t_a}^{t_b} \mathrm{d}t\, \frac{d\chi}{dt} = S + \frac{e}{c}\,\left(\chi(\underline{x}_b,t_b) - \chi(\underline{x}_a,t_a)\right) \tag{2.68}$$

so the transition *amplitude* also changes:

$$\langle \underline{x}_b, t_b|\underline{x}_a, t_a\rangle = \int_{\underline{x}_a}^{\underline{x}_b} \mathcal{D}\underline{x}\, e^{\mathbb{i}S/\hbar} \to \left(\int_{\underline{x}_a}^{\underline{x}_b} \mathcal{D}\underline{x}\, e^{\mathbb{i}S/\hbar}\right) \exp\left\{\frac{\mathbb{i}e}{\hbar c}\left(\chi(\underline{x}_b,t_b) - \chi(\underline{x}_a,t_a)\right)\right\} \tag{2.69}$$

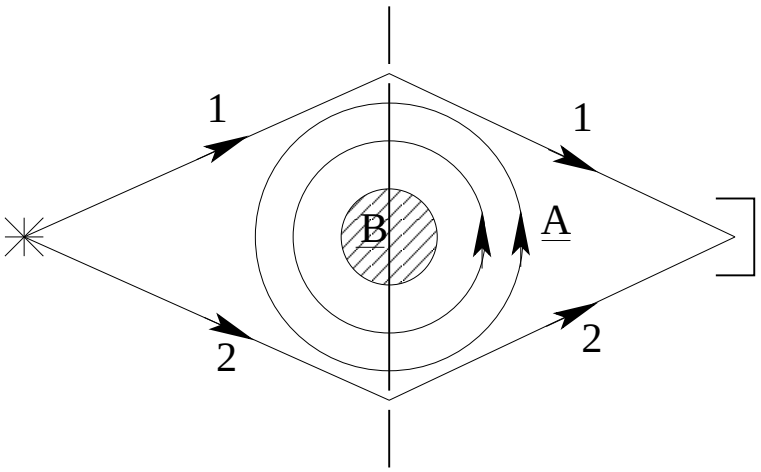
From this we may deduce

$$|\underline{x},t\rangle \to \exp\left\{-\frac{\mathbb{i}e}{\hbar c}\chi(\underline{x},t)\right\}|\underline{x},t\rangle \tag{2.70}$$

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 slits are shielded from the 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

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

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

When we add a magnetic field (assumed time-independent) the Lagrangian changes:

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

so

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

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

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

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

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

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 by $(e/\hbar c)\,\Phi$ 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! 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.

Notes:

(1) Φ is gauge invariant. If $\underline{A} \to \underline{A} + \underline{\nabla}\chi$, then

$$\Phi \to \Phi + \oint_C \underline{\nabla}\chi \cdot \mathrm{d}\underline{x} = \Phi + \oint_C \mathrm{d}\chi = \Phi + 0 = \Phi \,. \tag{2.75}$$

(2) Only the flux passing *between* the two paths is included.

(3) The effect is periodic: there is no effect if $\delta\phi = 2n\pi$, *i.e.* when

$$\Phi = 2\pi n \,\frac{\hbar c}{e} = n\,\frac{hc}{e}\,, \qquad n = 0,\, \pm 1,\, \pm 2,\, \ldots \tag{2.76}$$

(4) 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.

(5) 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 ($t_a \le t \le t_b$):

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

which is the matrix element of the operator $\hat{x}(t)$ in the Heisenberg picture. It is easy to see that for any local function $f(x(t))$:

$$\langle x_b, t_b |\, f(\hat{x}(t))\, | x_a, t_a\rangle = \int_{x_a}^{x_b} \mathcal{D}x\; f(x(t))\; \mathrm{e}^{\mathrm{i}S[x(t)]/\hbar}\,. \tag{2.78}$$

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

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

For $t < t'$, we get the same thing with $t \leftrightarrow t'$, *i.e.*

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

So, in general we have:

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

where

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

is called the *time ordered product*. Note, that $\hat{x}(t)$ and $\hat{x}(t')$ do not commute (unless $t = t'$) because they are Heisenberg-picture operators.

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

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

Note that the quantities $f_i(\hat{x}(t_i))$ in the "quantum" 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 numbers.

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

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

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 more tricky 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:

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

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

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

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

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

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

$$0 = \int \mathcal{D}x\;\left(m\ddot{x}(t) + \frac{\partial V}{\partial x}\right)\mathrm{e}^{\mathbb{i}S/\hbar} \quad\Rightarrow\quad \langle\ddot{x}\rangle_S = -\frac{1}{m}\left\langle\frac{\partial V}{\partial x}\right\rangle_S \tag{2.86}$$

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:

$$0 = \int \mathcal{D}x\;\mathrm{e}^{\mathbb{i}S/\hbar}\lim_{\varepsilon\to 0}\left(1 - \frac{\mathbb{i}}{\hbar}\left\{mx_p\left[\frac{x_{p+1}-x_p}{\varepsilon} - \frac{x_p-x_{p-1}}{\varepsilon}\right] + \varepsilon x_p\frac{\partial V}{\partial x_p}\right\}\right) \tag{2.87}$$

So, remembering the time ordering rule, and writing $m\dot{x}(t) \equiv p(t)$, we get:

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

whence the usual commutation relation

$$[\hat{x}, \hat{p}] = \mathbb{i}\hbar\,. \tag{2.89}$$

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),

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

we may also write (2.87) as

$$0 = \int \mathcal{D}x \; \mathrm{e}^{\mathbb{i}S/\hbar} \lim_{\varepsilon\to 0} \left(1 - \frac{\mathbb{i}}{\hbar} m \left\{ x_p \frac{x_{p+1} - x_p}{\varepsilon} - x_{p+1} \frac{x_{p+1} - x_p}{\varepsilon}(1 - \mathcal{O}(\varepsilon)) \right\}\right),$$

so:

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

But if we now want to take the limit $\varepsilon \to 0$, we get that $\langle \dot{x}(t)^2 \rangle_S$ or $\langle p(t)^2 \rangle_S$ are infinite! This shows that the paths that we integrate over are not smooth. The action is finite (for paths that count), so from (2.84), $\varepsilon(\delta x/\varepsilon)^2$ 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*.

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

$$\lim_{\varepsilon\to 0} \frac{1}{2m} \langle \hat{p}(t+\varepsilon/2)\hat{p}(t-\varepsilon/2) \rangle \tag{2.91}$$

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):

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

$$\begin{aligned} \text{so} \qquad \frac{1}{2m} \langle \hat{p}(t+\varepsilon/2)\hat{p}(t-\varepsilon/2) \rangle &\simeq \frac{m}{2} \left\langle \left(\frac{x_{p+1} - x_p}{\varepsilon} \right) \left(\frac{x_p - x_{p-1}}{\varepsilon} \right) \right\rangle + O(\varepsilon) \\ &= \Bigg\langle \underbrace{\frac{m}{2} \left(\frac{x_{p+1} - x_p}{\varepsilon} \right)^2}_{\simeq -\frac{\hbar}{2\mathbb{i}\varepsilon} + O(1) \text{ using } (2.90)} + \frac{\hbar}{2\mathbb{i}\varepsilon} \Bigg\rangle + O(\varepsilon) \end{aligned} \tag{2.93}$$

so the limit $\varepsilon \to 0$ exists. This is getting rather technical but it gives a (trivial) example of *renormalisation* in quantum mechanics - using a "point-splitting" *regularisation*.

3. Perturbation Theory

3.1. Time independent transitions

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

$$S[x(t)] = S_0[x(t)] + S_1[x(t)]. \tag{3.1}$$

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

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

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

where $\tilde{V}(x,t) = V(x,t) - U(x)$, so L_0 is time-independent. Sometimes we take $U = (m/2)\omega^2 x^2$, so that L_0 is the Lagrangian of a harmonic oscillator. It all depends on the problem we want to solve. Then the transition amplitude is (using (3.2)):

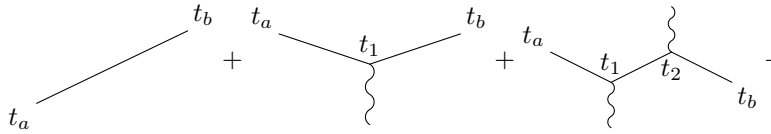
$$\begin{aligned}\langle x_b, t_b | x_a, t_a\rangle &= \int \mathcal{D}x\ \exp\left\{\frac{\mathrm{i}}{\hbar}\left(S_0[x(t)] + S_1[x(t)]\right)\right\} = \int \mathcal{D}x\ \mathrm{e}^{\mathrm{i}S_0[x(t)]/\hbar} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\mathrm{i}}{\hbar}S_1[x(t)]\right)^n \\ &= \sum_{n=0}^{\infty}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

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 $t_a < t_1 < t_2 < \ldots < t_n < t_b$, we have

$$\begin{aligned}&\int_{x_a}^{x_b} \mathcal{D}x\ V(x(t_1),t_1)\cdots V(x(t_n),t_n)\ \mathrm{e}^{\mathrm{i}S_0/\hbar} = \\ &= \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_n\ \ \langle x_b, t_b | x_n, t_n\rangle_0\, V(x_n,t_n)\, \langle x_n, t_n | x_{n-1}, t_{n-1}\rangle_0 \cdots V(x_1,t_1)\, \langle x_1, t_1 | x_a, t_a\rangle_0\end{aligned} \tag{3.5}$$

where the subscript zero indicates that these are transition amplitudes evaluated with S_0. All that remains to be done is to 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:

$\langle x_b, t_b | x_a, t_a\rangle =$ 

(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 + $\cdots$.

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:

$$\frac{1}{n!}\int_{t_a}^{t_b}\mathrm{d}t_1\cdots\int_{t_a}^{t_b}\mathrm{d}t_n\;V(t_1)\cdots V(t_n)=\int_{t_a}^{t_b}\mathrm{d}t_n\int_{t_a}^{t_n}\mathrm{d}t_{n-1}\cdots\int_{t_a}^{t_3}\mathrm{d}t_2\int_{t_a}^{t_2}\mathrm{d}t_1\;V(t_1)\cdots V(t_n) \tag{3.7}$$

so $t_a\le t_1\le t_2\le\cdots\le t_n\le t_b$ 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

$$\int_{t_a}^{t_b}\mathrm{d}t_2\int_{t_a}^{t_b}\mathrm{d}t_1\;V(t_1)V(t_2)=\int_{t_a}^{t_b}\mathrm{d}t_2\left(\int_{t_a}^{t_2}\mathrm{d}t_1\;V(t_1)V(t_2)+\int_{t_2}^{t_b}\mathrm{d}t_1\;V(t_1)V(t_2)\right),$$

it suffices to show that:

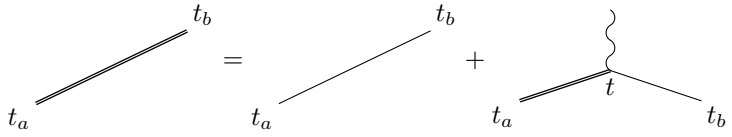
$$\begin{aligned}\int_{t_a}^{t_b}\mathrm{d}t_2\int_{t_a}^{t_2}\mathrm{d}t_1\;V(t_1)V(t_2)&=\int_{t_a}^{t_b}\mathrm{d}t_1\int_{t_1}^{t_b}\mathrm{d}t_2\;V(t_1)V(t_2)\quad\text{(swapped order of integrals)}\\&=\int_{t_a}^{t_b}\mathrm{d}t_2\int_{t_2}^{t_b}\mathrm{d}t_1\;V(t_2)V(t_1)\quad\text{(relabelled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

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

Using the result from (3.5) and (3.7) in (3.4), we have:

$$\begin{aligned}\langle x_b,t_b|x_a,t_a\rangle&=\langle x_b,t_b|x_a,t_a\rangle_0+\sum_{n=1}^{\infty}\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int\mathrm{d}x_1\cdots\int\mathrm{d}x_n\int_{t_a}^{t_b}\mathrm{d}t_n\int_{t_a}^{t_n}\mathrm{d}t_{n-1}\cdots\int_{t_a}^{t_2}\mathrm{d}t_1\\&\qquad\langle x_b,t_b|x_n,t_n\rangle_0\,V(x_n,t_n)\,\langle x_n,t_n|x_{n-1},t_{n-1}\rangle_0\cdots V(x_1,t_1)\,\langle x_1,t_1|x_a,t_a\rangle_0\\\Rightarrow\quad\langle x_b,t_b|x_a,t_a\rangle&=\langle x_b,t_b|x_a,t_a\rangle_0-\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}x\int_{t_a}^{t_b}\mathrm{d}t\,\langle x_b,t_b|x,t\rangle_0\,V(x,t)\,\langle x,t|x_a,t_a\rangle\end{aligned} \tag{3.8}$$

To see this last result, expand the second line iteratively by repeatedly substituting the left-hand side into the right-hand side. It is easy to understand equation (3.8) pictorially:



(3.9)

The full amplitude = unscattered amplitude + sum of processes with the last scattering at time t.

In terms of wavefunctions we can express (3.8) as follows:

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

where $\psi_0(x,t)=\langle x,t|\psi\rangle_0$ satisfies the unperturbed Schrödinger equation.

Using

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

and

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \hat{H}_0(x,t)\right)\langle x,t|x',t'\rangle_0 = \mathrm{i}\hbar\delta(t-t')\,\delta(x-x') \quad (t \geq t')$$

(see the equation above (2.57)), equation (3.10) becomes

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \hat{H}_0(x,t)\right)\psi(x,t) = 0 - \frac{\mathrm{i}}{\hbar}\,\mathrm{i}\hbar\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}t'\,\delta(t-t')\delta(x-x')V(x',t')\psi(x',t') = V(x,t)\psi(x,t)$$

$$\Rightarrow \qquad \mathrm{i}\hbar\frac{\partial}{\partial t}\psi = (\hat{H}_0 + V)\psi = \hat{H}\psi$$

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

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

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

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!)

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

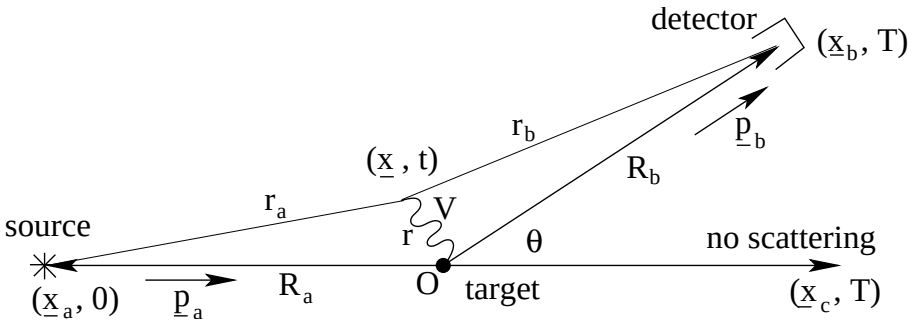
If the interaction is time-independent, (*i.e.* just $V(\underline{x})$), then

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

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

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

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



The unperturbed Lagrangian is just

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

so the path integral for the transition amplitude for a free particle in three dimensions in Cartesian coordinates factorises into 3 one-dimensional path integrals, and hence (exercise)

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

So the *scattering amplitude* A in first-order perturbation theory is

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

Performing the integral over t using

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

(see separate handout) gives

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

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

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

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

$$r_b=R_b-\underline{n}_b\cdot\underline{x}+\ldots\qquad\text{and}\qquad(r_a+r_b)^2=(R_a+R_b)^2-2(R_a+R_b)\,(\underline{n}_a+\underline{n}_b)\cdot\underline{x}+\ldots$$

So

$$\begin{aligned}A &\simeq \frac{-\mathbb{i}}{\hbar}\left(\frac{m}{2\pi\mathbb{i}\hbar}\right)^{5/2}\frac{1}{T^{3/2}}\left(\frac{1}{R_a}+\frac{1}{R_b}\right)\exp\left\{\frac{im}{2\hbar T}\left(R_a+R_b\right)^2\right\}\\ &\qquad\times\int_{-\infty}^{\infty}\mathrm{d}^3x\,V(\underline{x})\,\exp\left\{-\frac{im}{\hbar T}(R_a+R_b)\,(\underline{n}_a+\underline{n}_b)\cdot\underline{x}\right\}\end{aligned}$$

We can measure R_a, R_b and T, and for a short-range potential, we deduce from the diagram on the previous page, that

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

so

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

where we defined the *momentum transfer* $\hbar\underline{q}\equiv(\underline{p}_a-\underline{p}_b)$. The transition probability per unit volume is then

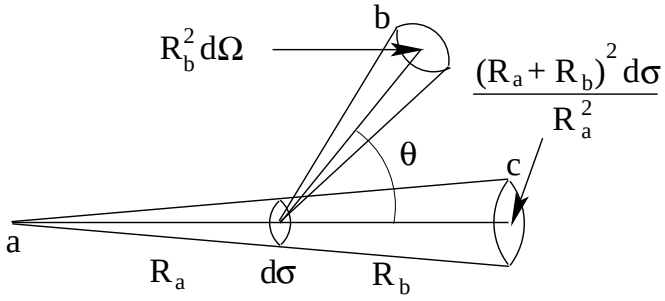
$$P(a\to b)=|A|^2=\frac{1}{\hbar^2}\left(\frac{m}{2\pi\hbar}\right)^5\frac{1}{T^3}\left(\frac{R_a+R_b}{R_aR_b}\right)^2|\tilde{V}(\underline{q})|^2$$

$$\text{Now note}\quad P(a\to c)=|A_0|^2=|\,\langle\underline{x}_c,T|\underline{x}_a,0\rangle_0\,|^2=\left(\frac{m}{2\pi\hbar}\right)^3\frac{1}{T^3}\,,$$

where $\underline{x}_c = -R_b \underline{n}_a$, is the probability (per unit volume) for no scattering (*i.e.* for $V(\underline{x}) = 0$). So

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

Now if we scatter into solid angle $\mathrm{d}\Omega$



Define the differential cross section as

$$\mathrm{d}\sigma = \frac{\#\text{ of particles scattered into } \mathrm{d}\Omega \text{ from unit area of scattering region / unit time}}{\#\text{ of incident particles crossing scattering region / unit area / unit time}}$$

$$= \frac{P(a \to b)\, R_b^2\, \mathrm{d}\Omega}{P(a \to c)\, (R_a + R_b)^2 / R_a^2}$$

whence

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

Notes:

(1) All factors of T, R_a, R_b cancel when we construct $\mathrm{d}\sigma/\mathrm{d}\Omega$, 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 $P(a \to b)/P(a \to c)$.

(3) For a *central* potential $V(r)$, $r = |\underline{x}|$, the expression for $\tilde{V}(\underline{q})$ simplifies to

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

Hence

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

with $q = |\underline{p}_a - \underline{p}_b|/\hbar = (2p/\hbar)\,\sin\theta/2$ where θ is the *scattering angle*. This is of course the same as the Born approximation result obtained in Section 11 of *Quantum Physics*.

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

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

so

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

which is the same as the classical Rutherford cross section. (This "quantum = classical" cross section doesn't happen for any potential other than the $1/r$ potential!)

Technical note: 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 $\mu \to 0$ at the end.

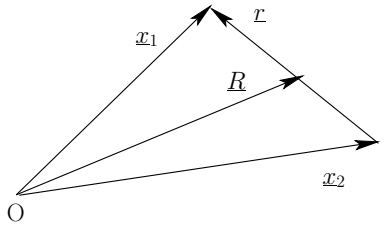
3.3. Colliding Beams

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

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

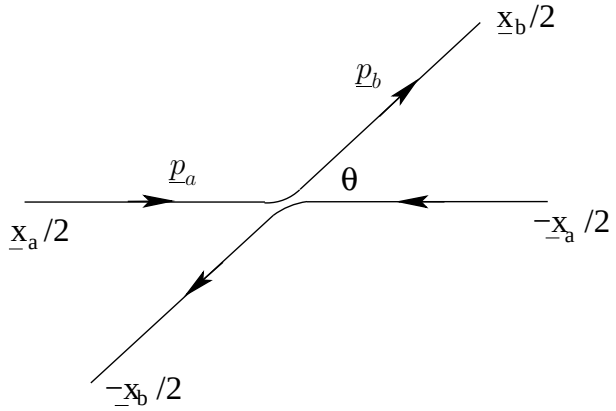
where

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



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

So if we consider a colliding beam scattering experiment,



the differential cross section is simply

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

with $\underline{q} = (\underline{p}_a - \underline{p}_b)/\hbar$ as before.

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

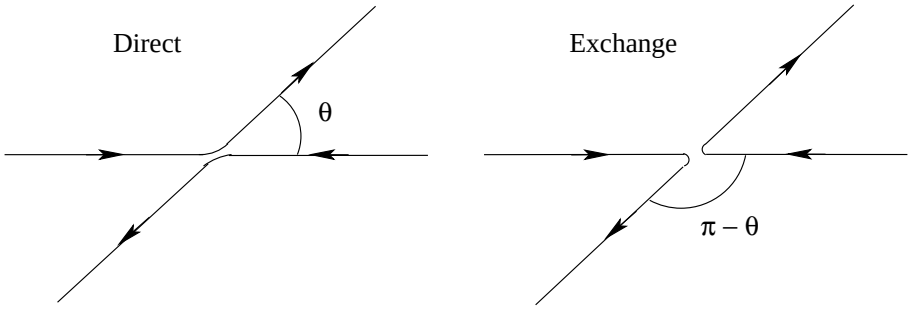
However, for particles of the same mass $m_1 = m_2 = m$, then $\mu = m/2$ and

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

where $f(\theta)$ is called the scattering amplitude.

Scattering of identical particles

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



Classically:

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

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

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

so, for example, for the Coulomb potential,

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

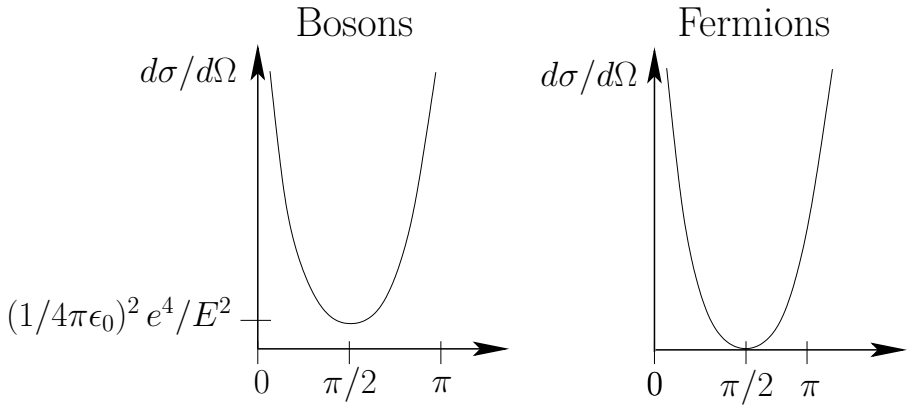
For identical fermions (ignoring spin – see tutorial for spin dependence)

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

For the Coulomb potential

$$\frac{\mathrm{d}\sigma_{\mathrm{tot}}}{\mathrm{d}\Omega} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{e^4}{E^2}\,\cos^2\theta\,\mathrm{cosec}^4\theta$$

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 states are in the Heisenberg picture. From (2.52) and the unitarity of $\hat{U}$, we have

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

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 (3.5) to write

$$\int_{x_a}^{x_b} \mathcal{D}x\; V(x(t_1), t_1)\cdots V(x(t_n), t_n)\mathrm{e}^{\mathbb{i}S_0/\hbar} = {}_0\langle x_b, t_b|\,T(V(\hat{x}_0(t_1), t_1)\cdots V(\hat{x}_0(t_n), t_n)\,|x_n, t_n\rangle_0 \tag{3.12}$$

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,

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

and the unperturbed evolution operator therefore satisfies

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

where $\hat{H}_0$ is the unperturbed Hamiltonian. This is known as the *Dirac* or *interaction picture*.

The perturbative expansion (3.4) may then be written as:

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

which is usually referred to as the *Dyson series*.

Note that

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

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 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 states by

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

Furthermore we shall need

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

Starting from (3.13), and using (3.11) and (3.14a/b/c) we get another representation for the first of equations (3.8)

$$\begin{aligned}\langle x_b|\,\hat{U}(t_b, t_a)\,|x_a\rangle &= \langle x_b|\,\hat{U}_0(t_b, t_a))\,|x_a\rangle \\ &\quad + \sum_{n=1}^{\infty}\left(-\frac{\mathbb{i}}{\hbar}\right)^n\int_{t_a}^{t_b}\mathrm{d}t_n\cdots\int_{t_a}^{t_2}\mathrm{d}t_1\ \langle x_b|\,\hat{U}_0(t_b, t_n)V(\hat{x}, t_n)U_0(t_n, t_{n-1})V(\hat{x}, t_{n-1})\cdots \\ &\qquad \cdots\ V(\hat{x}, t_2)\hat{U}_0(t_2, t_1)V(\hat{x}, t_1)\hat{U}_0(t_1, t_a)\,|x_a\rangle\end{aligned}$$

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

$$\hat{U}(t_b,t_a) = \hat{U}_0(t_b,t_a) + \sum_{n=1}^{\infty}\left(-\frac{\mathbb{i}}{\hbar}\right)^n \int_{t_a}^{t_b} \mathrm{d}t_n \cdots \int_{t_a}^{t_2} \mathrm{d}t_1\; \hat{U}_0(t_b,t_n)V(\hat{x},t_n)U_0(t_n,t_{n-1})V(\hat{x},t_{n-1})$$
$$\cdots\; V(\hat{x},t_2)\hat{U}_0(t_2,t_1)V(\hat{x},t_1)\hat{U}_0(t_1,t_a)$$

$$\Rightarrow \quad \hat{U}(t_b,t_a) = \hat{U}_0(t_b,t_a) - \frac{\mathbb{i}}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\; \hat{U}_0(t_b,t)V(\hat{x},t)\hat{U}(t,t_a) \tag{3.15}$$

To see this, expand the second line iteratively by substituting the left-hand side into the right-hand side – exactly as we did in (3.8). We leave it as an exercise to show that this last expression is the "solution" of the Schrödinger equation.

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 $|n\rangle$

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

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

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

It follows that the perturbed amplitude in the energy eigenbasis is:

$$\begin{aligned}
\langle b,t_b\big|a,t_a\rangle &= \langle b|\,\hat{U}(t_b,t_a)\,|a\rangle = \langle b|\,\hat{U}_0(t_b,t_a)\,|a\rangle - \frac{\mathbb{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\langle b|\,\hat{U}_0(t_b,t)V(\hat{x},t)\hat{U}_0(t,t_a)\,|a\rangle + \cdots \\
&= \langle b|\,\hat{U}_0(t_b,t_a)\,|a\rangle - \frac{\mathbb{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\sum_{m,n}\langle b|\,\hat{U}_0(t_b,t)\,|m\rangle\,\langle m|\,V(\hat{x},t)\,|n\rangle\,\langle n|\,\hat{U}_0(t,t_a)\,|a\rangle + \cdots \\
&= \mathrm{e}^{-\mathbb{i}(t_b-t_a)E_a/\hbar}\delta_{ab} - \frac{\mathbb{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\sum_{m,n}\mathrm{e}^{-\mathbb{i}(t_b-t)E_b/\hbar}\delta_{mb}V_{mn}(t)\mathrm{e}^{-\mathbb{i}(t-t_a)E_a/\hbar}\delta_{na} \\
&= \mathrm{e}^{-\mathbb{i}(t_b-t_a)E_a/\hbar}\delta_{ab} - \frac{\mathbb{i}}{\hbar}\mathrm{e}^{-\mathbb{i}(E_bt_b-E_at_a)/\hbar}\int_{t_a}^{t_b}\mathrm{d}t\;\mathrm{e}^{\mathbb{i}t(E_b-E_a)/\hbar}V_{ba}(t) + \cdots
\end{aligned} \tag{3.17}$$

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

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

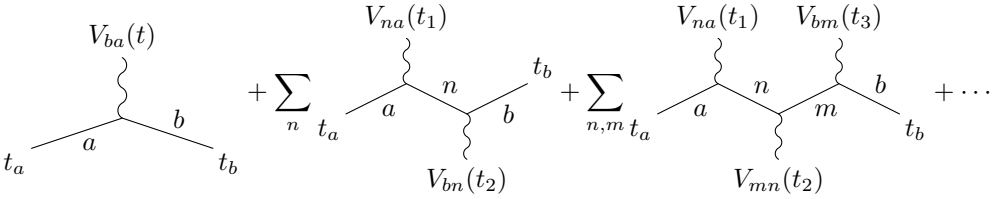
The second order term in the expansion is (check this):

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

The intermediate 'virtual' states $n,m,\cdots$ are summed over: $a \to n \to b$ for all possible intermediate values of n.

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

$\langle b,t_b\big|a,t_a\rangle =$



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

$$p(a \to b) = |\langle b, t_b | a, t_a \rangle|^2 = \frac{1}{\hbar^2} \left| \int_{t_a}^{t_b} \mathrm{d}t \; \mathrm{e}^{\mathbb{i} t \omega_{ba}} V_{ba}(t) + \mathcal{O}(V^2) \right|^2 \tag{3.18}$$

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 is $\mathcal{O}(V^3)$, not $\mathcal{O}(V^4)$. Writing

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

we have

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

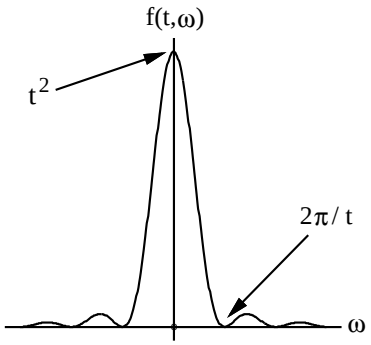
When the perturbation is time independent, we can do the t integrals, and the transition amplitude becomes

$$e^{-\mathbb{i}TE_a/\hbar}\delta_{ab} + \frac{\left(e^{-\mathbb{i}TE_b/\hbar} - e^{-\mathbb{i}TE_a/\hbar}\right)}{E_b - E_a} V_{ba} + \sum_n \frac{\left(e^{-\mathbb{i}TE_b/\hbar} - e^{-\mathbb{i}TE_n/\hbar}\right)\left(e^{-\mathbb{i}TE_n/\hbar} - e^{-\mathbb{i}TE_a/\hbar}\right)}{(E_b - E_n)(E_n - E_a)} V_{bn} V_{nb}$$

The transition probability is simply (to first order)

$$p(a \to b) = \frac{\left|\mathrm{e}^{-\mathbb{i}T\omega_{ba}} - 1\right|^2}{\hbar^2 \omega_{ba}^2} |V_{ba}|^2 = \frac{\sin^2(\omega_{ba} T/2)}{\hbar^2 (\omega_{ba}/2)^2} |V_{ba}|^2 \equiv \frac{f(T, \omega_{ba})}{\hbar^2} |V_{ba}|^2 \tag{3.20}$$

where $T = t_b - t_a$, as usual, and the function $f(t, \omega)$ looks like:



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

$$p(a \to \mathcal{R}) = \int_{\mathcal{R}} p(a \to E) \varrho(E) \, \mathrm{d}E, \tag{3.21}$$

where $\varrho(E)$ is 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. Since

$$\lim_{t \to \infty} 4 \sin^2(\omega_{ba} t/2)/(\omega_{ba})^2 = 2\pi t \delta(\omega_b - \omega_a) \tag{3.22}$$

We can extend the limits on the integral to infinity for T large enough, and this gives

$$\begin{aligned} p(a \to \mathcal{R}) &= \int_{-\infty}^{\infty} \varrho(E) \frac{4}{\hbar^2 \omega_{ba}^2} \sin^2(\omega_{ba} T/2) |V_{ba}|^2 \, \mathrm{d}E = \frac{\varrho(E_b)}{\hbar^2} |V_{ba}|^2 \int_{-\infty}^{\infty} 4 \frac{\sin^2(\omega_{ba} t/2)}{\omega_{ba}^2} \hbar \, \mathrm{d}\omega_{ba} \\ &= \frac{2\pi}{\hbar} \varrho(E_b) |V_{ba}|^2 T \end{aligned} \tag{3.23}$$

Equation (3.23) is known as *Fermi's Golden Rule*.