Chapter 1

Quantum Dynamics

1.1 Time Evolution

Physical system given by $|\alpha\rangle$ at time $t_0$. At some later time $t > t_0$ state is given by $|\alpha, t_0; t\rangle$. Since time is a continuous parameter

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle \equiv |\alpha\rangle . \quad (1.1)$$

Two Kets at different times can be related by an operator, called the time-evolution operator $u(t, t_0)$.

$$|\alpha, t_0; t\rangle = u(t, t_0) |\alpha, t_0\rangle . \quad (1.2)$$

Properties of the time-evolution operator? First important property is the unitarily requirement, follows from probability conservation. Suppose at $t_0$ the state Ket is expanded in terms of eigenkets of same observable $A$:

$$|\alpha, t_0\rangle = \sum_{a'} c_{a'} (t_0) |a'\rangle \quad (1.3)$$

then at a later time $t$
\[ |\alpha, t_0; t \rangle = \sum_{\alpha'} c_{\alpha'} (t) |\alpha' \rangle . \] (1.4)

In general

\[ |c_{\alpha'} (t)| \neq |c_{\alpha'} (t_0)| \] (1.5)

(Unless \(A\) commutes with \(H\)). Probability conservation requires

\[ \sum_{\alpha'} |c_{\alpha'} (t_0)|^2 = \sum_{\alpha'} |c_{\alpha'} (t)|^2 . \] (1.6)

Stated in a different way, this means if the state \(Ket\) is normalized to unity at a time \(t_0\), it must remain normalized to unity at all later times. This property is guaranteed if the time-evolution operator is taken to be unitary

\[ u \implies U^+ (t, t_0) U(t, t_0) = 1 . \] (1.7)

Unitarily is often synonymous with probability conservation. A further requirement is the composition property

\[ U(t_2, t_0) = U(t_2, t_1) U(t_1, t_0) ; \ t_2 \ ) t_2 \ ) t_0 . \] (1.8)

Consider an infinitesimal time-evolution at

\[ |\alpha, t_0; t_0 + dt \rangle = U(t_0 + dt, t_0) |\alpha, t_0 \rangle . \] (1.9)

Because of continuity, the infinitesimal time-evolution operator must reduce to the identity operator if \(dt \to 0\)

\[ \lim_{dt \to 0} U(t_0 + dt, t_0) = 1 . \] (1.10)

We expect the difference between \(U(t_0 + dt, t_0)\) and \(1\) to be of first order in \(dt\).
\[ U (t_0 + dt, t_0) = 1 - i\Omega \, dt \]  

(1.11)

where \( \Omega \) is a Hermitian operator, \( \Omega^+ \Omega = 1 \). Unitarily property can be checked as follows:

\[
U^+ (t_0 + dt, t_0) U(t_0 + dt, t_0) = (1 + i\Omega \, dt) \, (1 - i\Omega \, dt) = 1
\]

(1.12)

to the extent that terms \( (dt)^2 \) can be neglected.

The operator \( \Omega \) has the dimension of frequency or inverse time. From Planck-Einstein relation \( E = \hbar \omega \), it is natural to relate \( \Omega \) to the Hamiltonian \( H \)

\[ \Omega = \frac{H}{\hbar} . \]  

(1.13)

So, the infinitesimal time-evolution operator can be written as

\[ U(t + dt, t_0) = 1 - \frac{i}{\hbar} H \, dt . \]  

(1.14)

Exploit the composition property to derive an equation of \( U \) and consider

\[ U(t + dt, t_0) = U(t + dt, t) \, U(t, t_0) = (1 - \frac{i}{\hbar} H \, dt) \, U(t, t_0) \]  

(1.15)

where the time difference \( t - t_0 \) does not need to be infinitesimal. From (1.15) follows

\[ U(t + dt, t_0) - U(t, t_0) = -\frac{i}{\hbar} H \, dt \, U(t, t_0) \]  

(1.16)

or equivalently

\[ i \, \hbar \, \frac{\partial}{\partial t} \, U(t, t_0) = H \, U(t, t_0) . \]  

(1.17)

This is the Schrödinger equation for the time-evolution operator.
Applying (1.17) to a state $\text{Ket}$ leads immediately to the Schrödinger equation for the state $\text{Ket}$

$$i \, \hbar \, \frac{\partial}{\partial t} \, U \left( t, t_0 \right) \, | \alpha, t_0 \rangle = H \, U \left( t, t_0 \right) \, | \alpha, t_0 \rangle . \quad (1.18)$$

Since per definition $| \alpha, t_0 \rangle$ does not depend on $t$, this gives with (1.2)

$$i \, \hbar \, \frac{\partial}{\partial t} \, | \alpha, t_0 ; t \rangle = H \, | \alpha, t_0 ; t \rangle . \quad (1.19)$$

If we are given $U(t, t_0)$ and in addition know how $U \left( t, t_0 \right)$ acts on the initial state $| \alpha, t_0 \rangle$ it is not necessary to bother with the Schrödinger equation for the state $\text{Ket}$ (1.19). All one has to do is apply $U(t, t_0)$ to $| \alpha, t_0 \rangle$ and obtain the state $\text{Ket}$ or any time $t$. The first task is to derive formal solutions for the time-evolution operator (1.17). There are three cases to be considered.

**Case 1:** The Hamiltonian operator $H$ is independent of time. This means even when the parameter $t$ changes, the $H$ operator remains unchanged.

**Example:** Hamiltonian for a spin-magnetic moment interaction with time-independent magnetic field.

In this case, the solution of (1.17) is given by

$$U(t, t_0) = \exp \left[ - \frac{i}{\hbar} H(t - t_0) \right] . \quad (1.20)$$

To proceed this expand the potential

$$\exp \left[ - \frac{i}{\hbar} H \left( t - t_0 \right) \right] = 1 - \frac{i}{\hbar} H \left( t - t_0 \right) + \frac{1}{2} \left( - \frac{i}{\hbar} \right)^2 [H \left( t - t_0 \right)]^2 + \cdots \quad (1.21)$$

The derivation is given by

$$\frac{\partial}{\partial t} \exp \left[ - \frac{i}{\hbar} H(t - t_0) \right] = - \frac{i}{\hbar} H + \frac{1}{2} \cdot 2 \left( - \frac{i}{\hbar} \right)^2 H^2 \left( t - t_0 \right) + \cdots \quad (1.22)$$
Comparison with (1.17) shows that (1.20) fulfills the differential equation. For \( t \to t_0 \) (1.20) reduces to the identity thus the boundary conditions we fulfilled.

**Case 2:** The Hamiltonian is time-dependent, but the \( H' \)'s at different times commute.

**Example:** Spin magnetic moment with magnetic field, whose strength varies with time, but the direction is unchanged.

The formal solution of (1.17) is given by

\[
U(t, t_0) = \exp \left[ -\frac{i}{\hbar} \int_{t_0}^{t} dt' \ H(t') \right].
\]  

(1.23)

For a proof replace in (1.20) \( H(t - t_0) \) with \( \int_{t_0}^{t} dt' \ H(t') \).

**Case 3:** The \( H' \)'s at different times do **not** commute. In the example above that would involve a magnetic field whose direction changes with time. Since, e.g., \( S_x \) and \( S_y \) do not commute, a Hamiltonian with a term \( \vec{S} \cdot \vec{B} \) would fall in this category.

The formal solution in this case is given by

\[
U(t, t_0) = 1 + \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \ H(t_1) \ H(t_2) \cdots \ H(t_n)
\]

(1.24)

which is sometimes known as **Dyson Series**. Dyson developed a perturbative expansion of this form in quantum field theory.

In usual applications, one considers Case 1. Then the effect of the time-evolution operator is particularly straightforward to obtain, if the basis states are eigenstates to an operator \( A \) with

\[
[A, H] = 0
\]

(1.25)

such that the eigenstates of \( A \) are also eigenstates of \( H \) with

\[
H \ |a'\rangle = E_{a'} \ |a'\rangle.
\]

(1.26)
Expanding (1.20) in terms of $|a'\rangle \langle a'|$ (at $t_0 = 0$ for simplicity) gives

$$
\exp \left( -\frac{i}{\hbar} H t \right) = \sum_{a'} \sum_{a''} |a'\rangle \langle a'| \exp \left( -\frac{i}{\hbar} \frac{E_{a''}}{E_{a'} t} \right) \langle a'| a'' \rangle \quad \text{(1.27)}
$$

The time-evolution operator written in this form allows to solve any initial value problem once the expansion of the initial \textit{Ket} in terms of \{\{a'\} is known. Suppose

$$
|\alpha, t_0 = 0 \rangle = \sum_{a'} |a'\rangle \langle a'| \alpha \rangle = \sum_{a'} c_{a'} |a'\rangle .
$$

(1.28)

We then have

$$
|\alpha, t_0 = 0 ; t \rangle = \exp \left( -\frac{i}{\hbar} H t \right) |\alpha, t_0 = 0 \rangle = \sum_{a'} |a'\rangle \langle a'| \alpha \rangle \exp \left( -\frac{i}{\hbar} \frac{E_{a''}}{E_{a'} t} \right) .
$$

(1.29)

In other words, the expansion coefficient changes with time as

$$
c_{a'} (t = 0) \longrightarrow c_{a'} (t) = c_{a'} (t = 0) \exp \left( -\frac{i}{\hbar} \frac{E_{a'}}{E_{a'} t} \right) .
$$

(1.30)

It is modulus unchanged. The relative phases among the various components vary with time since the oscillation frequencies are different. If the initial state \{\{|a'\}\}, i.e., $|\alpha, t_0 = 0 \rangle = |a'\rangle$ then

$$
|\alpha, t_0 = 0 ; t \rangle = |a'\rangle \exp \left( -\frac{i}{\hbar} \frac{E_{a'}}{E_{a'} t} \right) ,
$$

(1.31)

thus, if the system is initially a simultaneous eigenstate of $A$ and $H$, it remains so at all times, within a phase modulation. In this sense the observable $A$ is compatible with $H$ and is a constant of motion.
It is instructive to study how the expectation value of an observable changes as function of time. Suppose at $t = 0$ the initial state is eigenstate of an observable $A$ with $[A, H] = 0$, and we look at the expectation value of an observable $B$, which does not commute with $A$ or $H$. Because of $|\alpha', t_0 = 0 ; t \rangle = U(t, 0) |\alpha' \rangle$ we have

\[
\langle B \rangle \equiv \langle \alpha' | U^\dagger (t, 0) B U(t, 0) | \alpha' \rangle \\
= \langle \alpha' | \exp \left( \frac{i}{\hbar} E' t \right) B \exp \left( -\frac{i}{\hbar} E_{\alpha'} t \right) | \alpha' \rangle \\
= \langle \alpha' | B | \alpha' \rangle
\]  

which is independent of $t$. For this reason energy eigenstates are called stationary states.

The situation is more interesting when the expectation value is taken with respect to a superposition of energy eigenstates or a non-stationary state. Suppose the initial state is given by

\[
|\alpha, t = 0 \rangle = \sum_{\alpha'} c_{\alpha'} |\alpha' \rangle .  
\]  

Then

\[
\langle B \rangle = \left[ \sum_{\alpha'} c_{\alpha'}^* \langle \alpha' | \exp \left( \frac{i}{\hbar} E_{\alpha'} t \right) \right] B \left[ \sum_{\alpha''} c_{\alpha''} \exp \left( -\frac{i}{\hbar} E_{\alpha''} t \right) | \alpha'' \rangle \right] \\
= \sum_{\alpha'} \sum_{\alpha''} c_{\alpha'}^* c_{\alpha''} \langle \alpha' | B | \alpha'' \rangle \exp \left( -\frac{i}{\hbar} (E_{\alpha''} - E_{\alpha}) t \right) .
\]  

Thus the expectation value consists of oscillating terms whose frequencies are determined by

\[
\omega_{\alpha'\alpha''} = \frac{(E_{\alpha''} - E_{\alpha})}{\hbar}.
\]  

8
1.2 Time-Dependent Wave Equation

Consider the Schrödinger picture and study the time-evolution of \(|\alpha, t_0; t\rangle\) in the coordinate representation, i.e., examine the behavior of the wave function

\[
\psi (\vec{x}, t) = \langle \vec{x} | \alpha, t_0; t \rangle
\]

as function of time. The Hamiltonian is given by

\[
H = \frac{\hat{p}^2}{2m} + V(\vec{x})
\]

(1.37)

where \(V(\vec{x})\) is a local operator, i.e., \(\langle \vec{x}' | V(\vec{x}) | \vec{x} \rangle = V(\vec{x}) \delta^3 (\vec{x}' - \vec{x})\), and \(V(\vec{x})\) be a real function. The Schrödinger equation for the state (1.19) written in coordinate representation is

\[
i \hbar \frac{\partial}{\partial t} \langle \vec{x}' | \alpha, t_0; t \rangle = \langle \vec{x}' | H | \alpha, t_0; t \rangle.
\]

(1.38)

Inserting the Hamiltonian (1.37) leads to

\[
i \hbar \frac{\partial}{\partial t} \langle \vec{x}' | \alpha, t_0; t \rangle = -\frac{\hbar^2}{2m} \nabla^2 \langle \vec{x}' | \alpha, t_0; t \rangle + V(\vec{x}') \langle \vec{x}' | \alpha, t_0; t \rangle.
\]

(1.39)

This represents the time-dependent Schrödinger equation and is the starting point for the so-called wave mechanics.

Eigenfunctions of the Hamiltonian have the simple time dependence of (1.31),

\[
\langle \vec{x}' | \alpha', t_0; t \rangle = \langle \vec{x}' | \alpha' \rangle \exp \left( -\frac{i}{\hbar} E_{\alpha'} t \right),
\]

(1.40)

where it is understood that initially the system is prepared in a simultaneous eigenstate of \(A\) and \(H\) with eigenvalues \(a'\) and \(E_{a'}\). Substituting (1.40) into (1.39) leads to the time-independent Schrödinger equation

\[
-\frac{\hbar^2}{2m} \nabla^2 \langle \vec{x}' | \alpha' \rangle + V(\vec{x}') \langle \vec{x}' | \alpha' \rangle = E_{\alpha'} \langle \vec{x}' | \alpha' \rangle.
\]

(1.41)
This partial differential equation is satisfied by the energy eigenfunctions \( \langle \vec{x}' | \alpha' \rangle \) with energy eigenvalues \( E_{\alpha'} \).

Let us turn to the interpretation of the wave function. The expression \( \langle \vec{x}' | \alpha, t_0; t \rangle \) is to be considered as the expansion coefficient of \( |\alpha, t_0; t \rangle \) in terms of the position eigenstates \( \{ |\vec{x}' \rangle \} \). The quantity \( \rho (\vec{x}', t) \) defined by

\[
\rho (\vec{x}', t) = |\psi (\vec{x}', t)|^2 = |\langle \vec{x}' | \alpha, t_0; t \rangle|^2
\]

(1.42)

is, therefore, regarded as the probability density in quantum mechanics, e.g., when using a detector to ascertain the presence of the particle within a volume element \( d^3 x' \) around \( \vec{x}' \), the probability of recording a positive result at time \( t \) is given by \( \rho (\vec{x}', t) \, d^3 x' \).

Defining a probability flux \( j(\vec{x}, t) \) by

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

(1.43)

\[
= \frac{\hbar}{m} \Im (\psi^* \nabla \psi)
\]

we can derive the continuity equation

\[
\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0.
\]

(1.44)

In obtaining this result, the Hermiticity of \( V \) (a reality of \( V \)) plays a crucial role. A complex potential can phenomenologically account for the disappearance of particles.

Rewrite the wave function as

\[
\psi(\vec{x}, t) = \sqrt{\rho(\vec{x}, t)} \exp \left( \frac{i}{\hbar} S(\vec{x}, t) \right)
\]

(1.45)

with \( S \) real and \( \rho > 0 \). Any complex function of \( \vec{x} \) and \( t \) can be represented this way. Consider
\[
\psi^* \nabla \psi = \sqrt{\rho} \exp\left(-\frac{i}{\hbar} S\right) \left[ \nabla \sqrt{\rho} \exp\left(\frac{i}{\hbar} S\right) + \sqrt{\rho} \frac{i}{\hbar} \nabla S \exp\left(\frac{i}{\hbar} S\right)\right] (1.46)
= \sqrt{\rho} \nabla \sqrt{\rho} + \frac{i}{\hbar} \rho \nabla S
\]

and

\[
\psi \nabla \psi^* = \sqrt{\rho} \nabla \sqrt{\rho} - \frac{i}{\hbar} \rho \nabla \rho
\]

(1.47)

follows from (1.44)

\[
\vec{j}(\vec{x}, t) = \frac{\rho(\vec{x}, t)}{m} \vec{\nabla} S(\vec{x}, t) .
\]

(1.48)

Thus, the gradient of the phase \( S \), i.e., the \textit{spatial variation of the phase} of the wave function characterizes the probability flux. The stronger the phase variations, the more intense the flux. The direction of \( \vec{j} \) at some point \( \vec{x} \) is seen to be normal to the surface of a constant phase that goes through that point.

Consider simple case of plane wave

\[
\psi(\vec{x}, t) \approx \exp\left(\frac{i}{\hbar} \vec{p} \cdot \vec{x} - \frac{i}{\hbar} E t\right).
\]

(1.49)

Then \( \vec{\nabla} S = \vec{\rho} \). It is tempting to regard \( \vec{\nabla} S/m \) as some kind of velocity, so that the continuity equation reads

\[
\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0
\]

(1.50)

as in fluid dynamics. But caution!
\section*{1.3 Propagators}

In Section 1.1 we showed that the most general time-evolution with a time-independent Hamiltonian can be solved once the initial state is expanded in terms of eigenstates of an observable that commutes with $H$.

\begin{equation}
|\alpha, t_0; t\rangle = \exp \left[-\frac{i}{\hbar} H (t - t_0) \right] |\alpha, t_0\rangle \\
= \sum_{a'} |a'\rangle \langle a' | \alpha, t_0 \rangle \exp \left[-\frac{i}{\hbar} E_{a'} (t - t_0) \right]
\end{equation}

Multiplying with $\langle \bar{x}' |$ gives

\begin{equation}
\langle \bar{x}' | \alpha, t_0; t \rangle = \sum_{a'} \langle \bar{x}' | a' \rangle \langle a' | \alpha, t_0 \rangle \exp \left[-\frac{i}{\hbar} E_{a'} (t - t_0) \right]
\end{equation}

which is of the form

\begin{equation}
\psi (\bar{x}, t) = \sum_{a'} c_{a'} (t_0) u_{a'} (\bar{x}) \exp \left[-\frac{i}{\hbar} E_{a'} (t - t_0) \right],
\end{equation}

where $u_{a'} (\bar{x}) = \langle \bar{x}' | a' \rangle$ stands for the eigenfunctions of an operator $A$ with eigenvalue $a'$. Note also that

\begin{equation}
\langle a' | \alpha, t_0 \rangle = \int d^3 x' \langle a' | \bar{x}' \rangle \langle \bar{x}' | \alpha, t_0 \rangle
\end{equation}

which corresponds to the usual rule for obtaining the expansion coefficients of an initial state:

\begin{equation}
c_{a'} (t_0) = \int d^3 \bar{x}' u^*_{a} (\bar{x}') \psi (\bar{x}', t_0).
\end{equation}

Combining (1.52) and (1.54) can be written as some kind of integral operator, which acts on the initial wave function to yield a final wave function:
\[
\psi (\vec{x}'', t) = \int d^3 \vec{x}' \ K (\vec{x}'', t ; \vec{x}', t_0) \psi (\vec{x}', t_0)
\]  
(1.56)

where the kernel of the integral operator is given by

\[
K (\vec{x}'', t ; \vec{x}', t_0) = \sum_{a'} \langle \vec{x}'' | a' \rangle \langle a' | \vec{x}' \rangle \exp \left[ - \frac{i}{\hbar} E_{a'} (t - t_0) \right]
\]  
(1.57)

and is known as \textbf{propagator}.

In any given problem the propagator depends only on the potential (via \( H \)) and is independent of the initial wave function. The time-evolution of the wave function is completely determined once \( K (\vec{x}'', t ; \vec{x}', t) \) is known and \( \psi (\vec{x}', t_0) \) is given. In this sense, the Schrödinger theory is a \textit{perfectly causal theory}. The time development of a wave function subject to some potential is as deterministic as classical mechanics \textit{provided the system is left undisturbed}. If a measurement is intervenes, the wave function changes abruptly.

\textbf{Properties of the propagator:}

1. For \( t > t_0, K (\vec{x}'', \vec{x}', t_0) \) satisfies Schrödinger’s time-dependent wave equation in variables \( \vec{x}' \) and \( t \) with \( \vec{x}'' \) and \( t_0 \) fixed (via construction).

2. For \( t \to t_0 \)

\[
\lim_{t \to t_0} K (\vec{x}'', t ; \vec{x}', t_0) = \delta^3 (\vec{x}' - \vec{x}')
\]  
(1.58)

because of the completeness of \( \{|a'\} \} \)

In fact, (1.57) can be written as

\[
K (\vec{x}'', t ; \vec{x}', t_0) = \langle \vec{x}'' | \exp \left[ - \frac{i}{\hbar} H (t - t_0) \right] | \vec{x}' \rangle .
\]  
(1.59)

This means the propagator acts on a state \( |\vec{x}' \rangle \) at a given \( t_0 \) and propagates it to state \( |\vec{x}'' \rangle \) at time \( t \).

To obtain information over the wave function \( \psi (\vec{x}', t_0) \) distributed over a finite space, one multiples \( \psi (\vec{x}', t_0) \) with \( K \) and integrates over the entire space.
The propagator is the Green’s function for the time-dependent Schrödinger equation satisfying

\[
\left[ -\left( \frac{\hbar^2}{2m} \right) \nabla^2 + V(x'^t) - i\hbar \frac{\partial}{\partial t} \right] \mathbf{K} \left( x'^t, t; x'^t, t_0 \right) = -i\hbar \, d^3(x'^t - x'^t) \, \delta \left( t - t_0 \right) \quad (1.60)
\]

with the boundary condition

\[
\mathbf{K} \left( x'^t, t; x'^t, t_0 \right) = 0 \quad \text{for} \quad t < t_0 . \quad (1.61)
\]

The \( \delta \)-function \( \delta \left( t - t_0 \right) \) is needed in (1.60), since \( \mathbf{K} \) varies discontinuous at \( t = t_0 \).

The particular form of \( \mathbf{K} \) depends on the potential in the Hamiltonian. Consider the simplest case of free propagation, i.e.,

\[
H_0 = \frac{p^2}{2m} . \quad (1.62)
\]

The obvious observable to commute with \( H \) are the momentum eigenstates with \( p | p' \rangle = p' | p \rangle \) Starting from (1.59) and setting \( t_0 = 0 \) for convenience, one obtains

\[
\mathbf{K} \left( x'^t, t; x'^t, 0 \right) = \langle x'^t \rangle e^{\left[ -\frac{i}{\hbar} H_0 t \right]} \langle | x'^t \rangle \\
= \int d^3 p' \langle x'^t | \exp \left[ -\frac{i}{\hbar} \frac{p^2}{2m} t \right] | p' \rangle \langle p' \rangle \exp \left[ -\frac{i}{\hbar} \frac{p^2}{2m} t \right] \\
= \int d^3 p' \frac{1}{(2\pi \hbar)^3} e^{\frac{i}{\hbar} \cdot \left( x'^t - x'^t \right)} e^{-\frac{p^2}{2m} t} \\
= \frac{1}{(2\pi \hbar)^3} \int d^3 p' e^{\frac{i}{\hbar} \cdot \left( x'^t - x'^t \right) - \frac{p^2}{2m} t} .
\]

Splitting up the integral into \( \int d p_1' \cdots \int d p_2' \cdots \int d p_3' \cdots \), one has to solve

\[
\int d p \, e^{\frac{i}{\hbar} \cdot \left( p \cdot x - \frac{p^2}{2m} t \right)} . \quad (1.64)
\]
Consider exponent
\[
\left(-\frac{p^2}{2m} t + px\right) = -\frac{t}{2m} \left(+p^2 - \frac{2m}{t} px + \frac{x^2 m^2}{t^2}\right) + \frac{x^2 m}{2t} \tag{1.65}
\]
\[
= -\frac{t}{2m} \left(+p - \frac{m x}{t}\right)^2 + \frac{x^2 m}{2t}
\]
\[
= -\left(x^2 \frac{2m}{t} - \sqrt{\frac{t}{2m} p}\right)^2 + \frac{x^2 m}{2t}.
\]

Thus
\[
\int \, dp \, e^{i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}} \left(\frac{px - \frac{p^2}{2m} t}{\hbar}\right) = \int \, dp \cdot \sqrt{\frac{t}{2m \hbar}} e^{i \frac{m x}{\hbar} \frac{\sqrt{t}}{\sqrt{2m \hbar}}} e^{-i \left(\frac{e}{\sqrt{2m \hbar}} - p \sqrt{\frac{m}{\hbar}}\right)^2} \tag{1.66}
\]
\[
= e^{i \frac{m x}{\hbar} \frac{2m \hbar}{t}} \int \, dp \cdot \sqrt{\frac{t}{2m \hbar}} \sqrt{\frac{x^2 m}{2t}} e^{-i \left(\frac{e}{\sqrt{2m \hbar}} - p \sqrt{\frac{m}{\hbar}}\right)^2}
\]
\[
= e^{i \frac{m x}{\hbar} \frac{2m \hbar}{t}} \int \, dp \cdot \sqrt{\frac{t}{2m \hbar}} \sqrt{\frac{2m \hbar}{i \pi}}
\]
\[
= e^{i \frac{m x}{\hbar} \frac{2m \hbar}{it}} \sqrt{\frac{2m \hbar}{it}}
\]

Thus
\[
\frac{1}{2\pi \hbar} \int \, dp e^{i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}} = \left(\frac{m}{2\pi i \hbar}\right)^{1/2} e^{i \frac{m x}{\hbar} \frac{2m \hbar}{it}}. \tag{1.67}
\]

Thus for (1.64) one obtains
\[
\mathbf{K} \left(\mathbf{x}'', t, \mathbf{x}', 0\right) = \frac{1}{(2\pi \hbar)^3} \int d^3 p' \, e^{i \frac{m \mathbf{p}' \cdot (\mathbf{x}' - \mathbf{x}'')}{2\hbar}} e^{-i \frac{p'^2}{2m \hbar} \frac{t}{i \hbar}} \tag{1.68}
\]
\[
= \left(\frac{m}{2\pi i \hbar}\right)^{3/2} e^{i \frac{m x}{\hbar} \frac{2m \hbar}{it}} (x'' - x')^2
\]

This expression can be used to study the spreading of a Gaussian wave packet over time.
Certain space and time integrals derivable from $\mathbf{K}(\bar{x}''; \bar{x}', t_0)$ are of special interest. Set again $t_0 = 0$ and consider $\bar{x}'' = \bar{x}'$ and integrate over space, i.e.,

$$
G(t) = \int d^3 x' \mathbf{K}(\bar{x}', t, \bar{x}', 0)
= \int d^3 x' \sum_{a'} |\langle \bar{x}'|a' \rangle|^2 \exp \left[ - \frac{i}{\hbar} E_{a'} t \right]
= \sum_{a'} \exp \left[ - \frac{i}{\hbar} E_{a'} t \right].
$$

(1.69)

Notice that setting $\bar{x}'' = \bar{x}'$ is equivalent to taking the trace of the time-evolution operator in the $\bar{x}$ representation. The trace is independent of the representation, thus one can use a basis in which $H$ is diagonal. In a sense (1.70) is just a sum over states, reminiscent of a partition function in statistical mechanics. Continue the variable $t$ analytically into the complex plane and define

$$
\beta = \frac{it}{\hbar}
$$

(1.70)

to be real and positive. Then (1.70) can be identified with the partition function

$$
Z = \sum_{a'} \exp(-\beta E_{a'}).
$$

(1.71)

For this reason, some of the techniques used in statistical mechanics can provide useful in dealing with propagators in quantum mechanics.

Consider the Laplace-Fourier transform of $G(t)$

$$
\tilde{G}(E) = - \frac{i}{\hbar} \int_0^\infty dt \, G(t) \exp \left( \frac{i}{\hbar} Et \right)
= - \frac{i}{\hbar} \int_0^\infty dt \sum_{a'} \exp \left( - \frac{i}{\hbar} E_{a'} t \right) \exp \left( \frac{i}{\hbar} Et \right).
$$

(1.72)

The integrand is indefinitely oscillatory. Thus let $E$ acquire a small imaginary part $E \rightarrow e + i\epsilon$. Then one obtains in the limit $\epsilon \rightarrow 0$

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\[ \hat{G} (E) = \sum_{\alpha'} \frac{1}{E - E_{\alpha'}} . \]  

(1.73)

Here the entire energy spectrum is exhibited as simple poles of \( \hat{G}(E) \) in the complex \( E \)-plane. Thus, to find the energy spectrum of a physical system, it is sufficient to study the analytic properties of \( \hat{G} (E) \).

To gain further insight into the physical meaning of the propagator, we wish to relate it to the concept of a transition amplitude. According to (1.59) \( \mathbf{K} (\vec{x}''', t; \vec{x}', t_0) \) can be written as

\[
\mathbf{K} (\vec{x}''', t; \vec{x}', t_0) = \langle \vec{x}' | \exp \left[ - \frac{i}{\hbar} H (t - t_0) \right] \vec{x}'') \langle \vec{x}'' | \exp \left[ \frac{i}{\hbar} H t_0 \right] | \vec{x}'') \rangle \\
= \langle \vec{x}'' | t \vec{x}', t_0 \rangle .
\]

(1.74)

where the states \( | \vec{x}', t_0 \rangle \) and \( \langle \vec{x}''', t \rangle \) are to be understood as eigenket (bra) in the Heisenberg picture.

In this notation \( \langle \vec{x}''', t \mid \vec{x}, t \rangle \) can be identified as the probability amplitude for the particle prepared at time \( t_0 \) with position eigenvalue \( \vec{x}'' \) to be found at a later time \( t \) with position eigenvalue \( \vec{x}'''. \)

Roughly speaking, \( \langle \vec{x}''', t \mid \vec{x}', t_0 \rangle \) is the \textbf{transition amplitude} for the particle to go from space time point \( (\vec{x}', t_0) \) to another space time point \( (\vec{x}''', t) \).

Yet another way to interpret \( \langle \vec{x}''', t \mid \vec{x}', t_0 \rangle \) is to view \( | \vec{x}', t_0 \rangle \) as position \textit{Ket} at \( t_0 \) with eigenvalue \( \vec{x}' \). Thus \( \langle \vec{x}''', t \mid \vec{x}', t_0 \rangle \) is a transformation function that connects two sets of base \textit{Kets} at different times, i.e., the time-evolution can be viewed as unitary transformation that connects one set of basis \textit{Kets} \( \{ | \vec{x}', t_0 \rangle \} \) to one formed by \( \{ | \vec{x}''', t \rangle \} \).

To use a more systematic notation, we write \( \langle \vec{x}''', t'; \vec{x}', t \rangle \). Since at any given time those sets form a complete basis, the identity can be represented as

\[
\int d^3 x'' | x''', t' \rangle \langle x'', t' | = 1 .
\]

(1.75)
Thus the time-evolution from $t'$ to $t'''$ can be divided into two intervals:

$$(t', t'') \cup (t'', t''')$$

with $t''' > t'' > t'$ as

$$
\langle \bar{x}^{\prime\prime\prime}, t''' | \bar{x}', t' \rangle = \int d^3 x'' \langle \bar{x}^{\prime\prime\prime}, t''' | \bar{x}'', t' \rangle \langle \bar{x}'', t'' | \bar{x}', t' \rangle \tag{1.76}
$$

We call this the composition property of the transition amplitude. Clearly, the considered time interval can be divided into as many smaller subintervals as desired

$$
\langle \bar{x}^{\prime\prime\prime}, t''' | \bar{x}', t' \rangle = \int d^3 x'' \int d^3 x'' \langle \bar{x}^{\prime\prime\prime}, t''' | \bar{x}^{\prime\prime}, t'' \rangle \langle \bar{x}^{\prime\prime}, t'' | \bar{x}', t' \rangle \tag{1.77}
$$
1.4 Feynman Path Integral Formulation

Without loss of generality, consider here only one-dimensional problems. Consider the transition amplitude for a particle going from an initial space time point \((x_1, t_1)\) to a final space time point \((x_n, t_n)\). The entire time interval between \(t_1\) and \(t_N\) is divided into \(N - 1\) equal parts

\[
t_j - t_{j-1} \equiv \Delta t = \frac{(t_N - t_n)}{N - 1}
\]  

(1.78)

Exploiting the composition property gives

\[
\langle x_n, t_N | x_1, t_1 \rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \langle x_n, t_N | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_2, t_2 | x_1, t_1 \rangle .
\]  

(1.79)

To visualize, consider the \(x - t\) plane in Fig. 1.1.

The initial and final space-time points \((x_1, t_1)\) and \((x_N, t_N)\) are fixed. For each time segment, i.e., between \(t_{n-1}\) and \(t_n\), we are instructed to consider the transition amplitude
to go from \((x_{n-1}, t_{n-1})\) to \((x_n, t_n)\) and then integrate over \(x_2, x_3, \cdots x_{N-1}\). This means that we must sum over all possible paths in the space time plane with the end points fixed.

Short review of path integrals in classical mechanics:

The classical Lagrangian is written as

\[
L_{\text{classical}}(x, \dot{x}) = \frac{m\dot{x}^2}{2} - V(x). \tag{1.80}
\]

Given this Lagrangian with fixed end points \((x_1, t_1)\) and \((x_N, t_N)\), we do not consider just any path joining the end points. There exists a unique path that corresponds to the actual path of a classical particle. E.g., for

\[
V(x) = mgx, \quad (x_1, t_1) = (h, 0), \quad (x_N, t_N) = \left(0, \sqrt{\frac{2h}{g}}\right)
\]

the classical path in the \(x - t\)-plane can only be

\[
x = h - \frac{g\tau^2}{2}. \tag{1.82}
\]

According to Hamilton’s principle, the unique path that minimizes the action is defined as

\[
\delta \int_{t_1}^{t_2} dt \, L_{\text{classical}}(x, \dot{x}) = 0 \tag{1.83}
\]

from which the equations of motion are obtained.

The basic difference between classical mechanics and quantum mechanics is that in classical mechanics a definite path is associated with the particle’s motion. In contrast, in quantum mechanics all possible paths are included. Yet, classical mechanics must be reproduced in a smooth manner in the limit \(\hbar \to 0\).
Introduce the notation

\[ S(n, n - 1) \equiv \int_{t_{n-1}}^{t_n} dt \ L_{\text{classical}}(x, \dot{x}) . \]  \hspace{1cm} (1.84)

Because \( L_{\text{classical}} \) is a function of \( x \) and \( \dot{x} \), \( S(n, n - 1) \) is defined only after a definite path is specified along which the integration is to be carried out.

Consider a small segment between \( (n_{n-1}, t_{n-1}) \). According to a suggestion by Dirac an "evolution operator" \( \exp \left( \frac{i}{\hbar} S(n, n - 1) \right) \) should be associated with that segment. Going along a definite path, successively expressions of this type need to be multiplied:

\[ \prod_{n=2}^{N} \exp \left[ \frac{i}{\hbar} S(n, n - 1) \right] = \exp \left[ \frac{i}{\hbar} \sum_{n=2}^{N} S(n, n - 1) \right] = \exp \left[ \frac{i}{\hbar} S(N, 1) \right] . \]  \hspace{1cm} (1.85)

This does not yet give \( \langle x_n, t_n | x_1, t_1 \rangle \) rather describes the contribution along a particular path. One still needs to integrate over \( x_2, x_3, \cdots x_{N-1} \). At the same time, let time interval \( \Delta t \) be infinitesimally small. Thus, in a loose sense we may write

\[ \langle x_N, t_N | x_1, t_1 \rangle \approx \sum_{\text{all paths}} \exp \left[ \frac{1}{\hbar} S(N, 1) \right] , \]  \hspace{1cm} (1.86)

where the sum is to be taken over an infinite set of paths.

Qualitative remarks:

As \( \hbar \to 0 \) exponent in (1.82) oscillates strongly, thus destructive interference for most paths.

Consider a path that satisfies \( \delta S(N, 1) = 0 \), where the change in \( S \) is due to a slight deformation of the path with the end point fixed (i.e., the classical path of Hamilton’s principle). As long as a deformation of the classical path is small, there will be constructive interference, even if \( \hbar \) is small. For larger deformations, destructive interference. As a result, as long as we stay near the classical path constructive interference between neighboring paths is possible. In the limit \( \hbar \to 0 \) the major contributions must arise from a very narrow stripe containing the classical paths.

To formulate Feynman’s conjecture more precisely, write
\[ \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \frac{1}{\omega(\Delta t)} \exp \left[ \frac{i}{\hbar} S(n, n - 1) \right] \] (1.87)

where the difference \( \Delta t = t_n - t_{n-1} \) is assumed to be infinitesimally small, and \( S(n, n - 1) \) is evaluated in the limit \( \Delta t \to 0 \). The weight factor \( \frac{1}{\omega(\Delta t)} \) is assumed to depend only on the time interval \( t_n - t_{n-1} \), and is necessary since \( \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \) has the dimension of \( \frac{1}{\text{length}} \). Consider the exponent \( S(n, n - 1) \) in the limit \( \Delta t \to 0 \). Since \( \Delta t \) small, a straight-line approximation between \( (x_{n-1}, t_{n-1}) \) and \( (x_n, t_n) \) is justified.

\[
S(n, n - 1) = \int_{t_{n-1}}^{t_n} dt \left[ \frac{m \dot{x}^2}{2} - V(x) \right] \\
= \Delta t \left\{ \left( \frac{m}{2} \right) \left[ \frac{x_n - x_{n-1}}{\Delta t} \right]^2 - V \left( \frac{x_n + x_{n-1}}{2} \right) \right\} .
\] (1.88)

Consider the free motion case, \( V = 0 \), where (1.87) becomes

\[
\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \frac{1}{\omega(\Delta t)} \exp \left[ \frac{i}{\hbar} \frac{m}{2} \frac{(x_n - x_{n-1})^2}{\Delta t} \right] .
\] (1.89)

This expression is equivalent to the one for free particle propagation given in (1.69).

The weight form \( \frac{1}{\omega(\Delta t)} \) is assumed to be independent of \( V(x) \), so it may well be evaluated for the free propagation. Because of the normalization \( \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \delta(x_n - x_{n-1}) \), we obtain with

\[
\int_{-\infty}^{\infty} d\xi \exp \left( \frac{im \xi^2}{2\hbar \Delta t} \right) = \sqrt{\frac{2\pi i \hbar \Delta t}{m}}
\] (1.90)

for \( \frac{1}{\omega(\Delta t)} \)

\[
\frac{1}{\omega(\Delta t)} = \sqrt{\frac{m}{2\pi i \hbar \Delta t}}
\] (1.91)

and

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\[
\lim_{\Delta t \to 0} \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \exp \left( \frac{im \xi^2}{2\hbar \Delta t} \right) = \delta(\xi). 
\] (1.92)

In summary, as \( \Delta t \to 0 \) one obtains

\[
\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \exp \left[ \frac{i}{\hbar} S(n, n - 1) \right]. 
\] (1.93)

Thus, the final expression for the transition amplitude, where \( t_n - t_1 \) is finite, is given as

\[
\langle x_N, t_N | x_1, t_1 \rangle = \lim_{N \to \infty} \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \prod_{n=2}^{N} \exp \left[ \frac{i}{\hbar} S(n, n - 1) \right] 
\] (1.94)

where the limit \( N \to \infty \) is taken with \( x_N \) and \( t_N \) fixed. It is customary to define the functional

\[
\int_{x_n}^{x_N} D[x(t)] \equiv \lim_{N \to \infty} \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 
\] (1.95)

and

\[
\langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} D[x(t)] \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_N} dt \ L_{\text{classical}}(x, \dot{x}) \right]. 
\] (1.96)

This expression is known as **Feynman’s path integral**.

The above was not meant to be a shift derivation. The ideas borrowed from the conventional quantum mechanics are:

1. the superposition principle, used in summing up the conditions from various alternate paths
2. the composition property of the transition amplitude
3. the classical correspondence in the limit \( \hbar \to 0 \).
Now we need to show that Feynman’s expression for \( \langle x_N, t_N|x_1, t_1 \rangle \) satisfies the time-dependent Schrödinger equation in the variables \( x_N, t_N \). We show with

\[
\langle x_N, t_N|x_1, t_1 \rangle &= \int dx_{N-1} \langle x_N, t_N|x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1}|x_1, t_1 \rangle \\
&= \int_{-\infty}^{\infty} dx_{N-1} \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \exp \left[ i m \frac{(x_N - x_{N-1})^2}{2\hbar \Delta t} - \frac{i}{\hbar} V \Delta t \right] \langle x_{N-1}, t_{N-1}|x_1, t_1 \rangle
\] (1.97)

where \( t_N - t_{N-1} = \Delta t \) is assumed to be infinitesimal. Further introduce \( \xi \equiv x_N - x_{N-1} \) and let \( x_N \to X \), and \( t_N = t + \Delta t \). Then (1.97) becomes

\[
\langle x, t + \Delta t|x_1, t_1 \rangle = \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \int_{-\infty}^{\infty} d\xi \exp \left[ i m \frac{\xi^2}{2\hbar \Delta t} - \frac{i}{\hbar} V \Delta t \right] \langle x - \xi, t|x_1, t_1 \rangle .
\] (1.98)

From (1.92) it is obvious that in the \( \lim \delta t \to 0 \) the major contributions to the integral come from the \( \xi \approx 0 \) region. Thus, we expand \( \langle x - \xi, t|x_1, t_1 \rangle \) in powers of \( \xi \), and \( \langle x, t + \Delta t|x_1, t_1 \rangle \) and \( \exp \left[ - \frac{i}{\hbar} V \Delta t \right] \) in powers of \( \Delta t \).

\[
\langle x, t|x_1, t_1 \rangle + \Delta t \frac{\partial}{\partial t} \langle x, t|x_1, t_1 \rangle \\
= \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \int_{-\infty}^{\infty} d\xi \exp \left[ i m \frac{\xi^2}{2\hbar \Delta t} \right] \left[ 1 - \frac{i}{\hbar} V \Delta t + \cdots \right] \\
\times \left[ \langle x, t|x_1, t_1 \rangle + \left( \frac{\xi^2}{2} \right) \frac{\partial^2}{\partial \xi^2} \langle x, t|x_1, t_1 \rangle + \cdots \right]
\] (1.99)

where we dropped the term linear in \( \xi \), since it vanishes when integrating with respect to \( \xi \).

The first term on the right-hand side just integrates to \( \langle x, t|x_1, t_1 \rangle \) since the integral cancels the factor due to (1.91). In collecting the terms of first order in \( \Delta t \) gives

\[
\Delta t \frac{\partial}{\partial t} \langle x, t|x_1, t_1 \rangle = - \left( \frac{i}{\hbar} \right) \Delta t V \langle x, t|x_1, t_1 \rangle
\] (1.100)
\[
+ \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \sqrt{2\pi} \left( \frac{i \hbar \Delta t}{m} \right)^{3/2} \frac{1}{2} \frac{\partial^2}{\partial \xi^2} \langle x|t|t_1, t_1 \rangle
\]

where we have used

\[
\int_{-\infty}^{\infty} d\xi \frac{\xi^2}{2\hbar} \exp \left[ \frac{im \xi^2}{2\hbar} \Delta t \right] = \sqrt{2\pi} \left( \frac{i\hbar \Delta t}{m} \right)^{3/2}.
\] (1.101)

Thus

\[
i\hbar \frac{\partial}{\partial t} \langle x, t|x_1, t_1 \rangle = - \left( \frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \langle x, t|x_1, t_1 \rangle + V \langle x, t|x_1, t_1 \rangle
\] (1.102)

which corresponds to the time-dependent Schrödinger equation for the quantity \( \langle x, t|x_1, t_1 \rangle \)
Chapter 2

Lorentz Transformations

2.1 Elementary Considerations

We assume we have two coordinate systems $S$ and $S'$ with coordinates $x, y, z, t$ and $x', y', z', t'$, respectively. Physical events can be measured in either system, and the Lorentz transformation give the relation between the coordinates $x', y', z', t'$ and $x, y, z, t$. The transformation has to fulfill the following requirements:

1. The transformation should be linear. Otherwise a specific system $S$, or a point in space or time would be distinct. (For a linear transformation, the inverse has the same form.)

2. Each point in $\mathbb{R}^3$ given by $x', y', z'$ in $S'$ moves with constant velocity $\vec{v}$ with respect to a point $x, y, z$ in $S$.

3. A measurement of the speed of light should give $C$ in both systems.

We assume the uniform motion is in $z$–direction. Then

$$x' = x, \quad y' = y.$$  \hfill (2.1)

From (1) follows

$$z' = a_1z + a_2t \quad \hfill (2.2)$$

$$t' = b_1t + b_2z.$$