

# 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

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

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 unitarity 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  $t$

$$|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t) |a'\rangle . \quad (1.4)$$

In general

$$|c_{a'}(t)| \neq |c_{a'}(t_0)| \quad (1.5)$$

(unless  $A$  commutes with  $H$ ). Probability conservation requires

$$\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2 . \quad (1.6)$$

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

$$u \implies U^\dagger(t, t_0) U(t, t_0) = \mathbf{1} . \quad (1.7)$$

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

$$U(t_2, t_0) = U(t_2, t_1) U(t_1, t_0) ; \quad t_2 > t_1 > t_0 . \quad (1.8)$$

Consider an infinitesimal time-evolution at

$$|\alpha, t_0; t_0 + dt\rangle = U(t_0 + dt, t_0) |\alpha, t_0\rangle . \quad (1.9)$$

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

$$\lim_{dt \rightarrow 0} U(t_0 + dt, t_0) = \mathbf{1} . \quad (1.10)$$

We expect the difference between  $U(t_0 + dt, t_0)$  and  $\mathbf{1}$  to be of first order in  $dt$ .

$$U(t_0 + dt, t_0) = \mathbf{1} - i\Omega dt \quad (1.11)$$

where  $\Omega$  is a Hermitian operator,  $\Omega^\dagger \Omega = \mathbf{1}$ . Unitarity property can be checked as follows:

$$U^\dagger(t_0 + dt, t_0) U(t_0 + dt, t_0) = (1 + i\Omega dt)(1 - i\Omega dt) = 1 \quad (1.12)$$

to the extent that terms  $\approx (dt)^2$  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  $H$

$$\Omega = \frac{H}{\hbar} . \quad (1.13)$$

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

$$U(t + dt, t_0) = \mathbf{1} - \frac{i}{\hbar} H dt . \quad (1.14)$$

Exploit the composition property to derive an equation of  $U$  and consider

$$U(t + dt, t_0) = U(t + dt, t) U(t, t_0) = \left( \mathbf{1} - \frac{i}{\hbar} H dt \right) U(t, t_0) \quad (1.15)$$

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

$$U(t + dt, t_0) - U(t, t_0) = -\frac{i}{\hbar} H dt U(t, t_0) \quad (1.16)$$

or equivalently

$$i \hbar \frac{\partial}{\partial t} U(t, t_0) = H U(t, t_0) . \quad (1.17)$$

This is the **Schrödinger equation for the time-evolution operator**.

Applying (1.17) to a state  $Ket$  leads immediately to the Schrödinger equation for the state  $Ket$

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

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  $U(t, t_0)$  acts on the initial state  $|\alpha, t_0\rangle$  it is not necessary to bother with the Schrödinger equation for the state  $Ket$  (1.19). All one has to do is apply  $U(t, t_0)$  to  $|\alpha, t_0\rangle$  and obtain the state  $Ket$  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 prove this expand the potential

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

The derivation is given by

$$\frac{\partial}{\partial t} \exp \left[ - \frac{i}{\hbar} H(t - t_0) \right] = - \frac{i}{\hbar} H + \frac{1}{2} \cdot 2 \left( - \frac{i}{\hbar} \right)^2 H^2 (t - t_0) + \dots \quad (1.22)$$

Comparison with (1.17) shows that (1.20) fulfills the differential equation. For  $t \rightarrow t_0$  (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

$$U(t, t_0) = \exp \left[ -\frac{i}{\hbar} \int_{t_0}^t dt' H(t') \right]. \quad (1.23)$$

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

$$U(t, t_0) = \mathbf{1} + \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1) H(t_2) \cdots H(t_n) \quad (1.24)$$

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

$$[A, H] = 0 \quad (1.25)$$

such that the eigenstates of  $A$  are also eigenstates of  $H$  with

$$H |a'\rangle = E_{a'} |a'\rangle. \quad (1.26)$$

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

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

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

$$|\alpha, t_0 = 0\rangle = \sum_{a'} |a'\rangle \langle a'|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle. \quad (1.28)$$

We then have

$$|\alpha, t_0 = 0; t\rangle = \exp\left(-\frac{i}{\hbar} H t\right) |\alpha, t_0 = 0\rangle = \sum_{a'} |a'\rangle \langle a'|\alpha\rangle \exp\left(-\frac{i}{\hbar} E_{a'} t\right). \quad (1.29)$$

In other words, the expansion coefficient changes with time as

$$c_{a'}(t = 0) \longrightarrow c_{a'}(t) = c_{a'}(t = 0) \exp\left(-\frac{i}{\hbar} E_{a'} t\right). \quad (1.30)$$

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

$$|\alpha, t_0 = 0; t\rangle = |a'\rangle \exp\left(-\frac{i}{\hbar} E_{a'} t\right), \quad (1.31)$$

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  $|a', t_0 = 0; t\rangle = U(t, 0) |a'\rangle$  we have

$$\begin{aligned} \langle B \rangle &\equiv \langle a' | U^\dagger(t, 0) B U(t, 0) | a' \rangle \\ &= \langle a' | \exp\left(\frac{i}{\hbar} E' t\right) B \exp\left(-\frac{i}{\hbar} E_{a'} t\right) | a' \rangle \\ &= \langle a' | B | a' \rangle \end{aligned} \quad (1.32)$$

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

$$|\alpha, t = 0\rangle = \sum_{a'} c_{a'} |a'\rangle. \quad (1.33)$$

Then

$$\begin{aligned} \langle B \rangle &= \left[ \sum_{a'} c_a^* \langle a' | \exp\left(\frac{i}{\hbar} E_{a'} t\right) \right] B \left[ \sum_{a''} c_{a''} \exp\left(-\frac{i}{\hbar} E_{a''} t\right) | a'' \rangle \right] \\ &= \sum_{a'} \sum_{a''} c_{a'}^* c_{a''} \langle a' | B | a'' \rangle \exp\left(-\frac{i}{\hbar} (E_{a''} - E_{a'}) t\right). \end{aligned} \quad (1.34)$$

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

$$\omega_{a'' a'} = \frac{(E_{a''} - E_{a'})}{\hbar}. \quad (1.35)$$

## 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

$$\psi(\vec{x}', t) = \langle \vec{x}' | \alpha, t_0; t \rangle \quad (1.36)$$

as function of time. The Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(\vec{x}) \quad (1.37)$$

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

$$i \hbar \frac{\partial}{\partial t} \langle \vec{x}' | \alpha, t_0; t \rangle = \langle \vec{x}' | H | \alpha, t_0; t \rangle. \quad (1.38)$$

Inserting the Hamiltonian (1.37) leads to

$$i \hbar \frac{\partial}{\partial t} \langle \vec{x}' | \alpha, t_0; t \rangle = - \frac{\hbar^2}{2m} \nabla'^2 \langle \vec{x}' | \alpha, t_0; t \rangle + V(\vec{x}') \langle \vec{x}' | \alpha, t_0; t \rangle. \quad (1.39)$$

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),

$$\langle \vec{x}' | a', t_0; t \rangle = \langle \vec{x}' | a' \rangle \exp\left(-\frac{i}{\hbar} E_{a'} t\right), \quad (1.40)$$

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

$$- \frac{\hbar^2}{2m} \nabla'^2 \langle \vec{x}' | a' \rangle + V(\vec{x}') \langle \vec{x}' | a' \rangle = E_{a'} \langle \vec{x}' | a' \rangle. \quad (1.41)$$



This partial differential equation is satisfied by the energy eigenfunctions  $\langle \vec{x}' | a' \rangle$  with energy eigenvalues  $E_{a'}$ .

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

$$\rho(\vec{x}', t) \equiv |\psi(\vec{x}', t)|^2 = |\langle \vec{x}' | \alpha, t_0; t \rangle|^2 \quad (1.42)$$

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*  $\vec{j}(\vec{x}, t)$  by

$$\begin{aligned} \vec{j}(\vec{x}, t) &= - \left( \frac{i\hbar}{2m} \right) [\psi^* \nabla \psi - (\nabla \psi^*) \psi] \\ &= \frac{\hbar}{m} \Im(\psi^* \nabla \psi) \end{aligned} \quad (1.43)$$

we can derive the continuity equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0. \quad (1.44)$$

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

$$\psi(\vec{x}, t) = \sqrt{\rho(\vec{x}, t)} \exp\left(\frac{i}{\hbar} S(\vec{x}, t)\right) \quad (1.45)$$

with  $S$  real and  $\rho > 0$ . Any complex function of  $\vec{x}$  and  $t$  can be represented this way. Consider

$$\begin{aligned}
\psi^* \nabla \psi &= \sqrt{\rho} \exp\left(-\frac{i}{\hbar} S\right) \left[ \nabla \sqrt{\rho} \exp\left(\frac{i}{\hbar} S\right) + \sqrt{\rho} \frac{i}{\hbar} \nabla S \exp\left(\frac{i}{\hbar} S\right) \right] \\
&= \sqrt{\rho} \nabla \sqrt{\rho} + \frac{i}{\hbar} \rho \nabla S
\end{aligned} \tag{1.46}$$

and

$$\psi \nabla \psi^* = \sqrt{\rho} \nabla \sqrt{\rho} - \frac{i}{\hbar} \rho \nabla S \tag{1.47}$$

follows from (1.44)

$$\vec{j}(\vec{x}, t) = \frac{\rho(\vec{x}, t)}{m} \vec{\nabla} S(\vec{x}, t) . \tag{1.48}$$

Thus, the gradient of the phase  $S$ , i.e., the *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

$$\psi(\vec{x}, t) \approx \exp\left(\frac{i}{\hbar} \vec{p} \cdot \vec{x} - \frac{i}{\hbar} E t\right) . \tag{1.49}$$

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

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0 \tag{1.50}$$

as in fluid dynamics. But caution!

## 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  $H$ .

$$\begin{aligned} |\alpha, t_0; t\rangle &= \exp\left[-\frac{i}{\hbar} H (t - t_0)\right] |\alpha, t_0\rangle \\ &= \sum_{a'} |a'\rangle \langle a' | \alpha, t_0\rangle \exp\left[-\frac{i}{\hbar} E_{a'} (t - t_0)\right] \end{aligned} \quad (1.51)$$

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

$$\langle \vec{x}' | \alpha, t_0; t\rangle = \sum_{a'} \langle \vec{x}' | a'\rangle \langle a' | \alpha, t_0\rangle \exp\left[-\frac{i}{\hbar} E_{a'} (t - t_0)\right] \quad (1.52)$$

which is of the form

$$\psi(\vec{x}, t) = \sum_{a'} c_{a'}(t_0) u_{a'}(\vec{x}') \exp\left[-\frac{i}{\hbar} E_{a'} (t - t_0)\right], \quad (1.53)$$

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

$$\langle a' | \alpha, t_0\rangle = \int d^3 x' \langle a' | \vec{x}'\rangle \langle \vec{x}' | \alpha, t_0\rangle \quad (1.54)$$

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

$$c_{a'}(t_0) = \int d^3 \vec{x}' u_{a'}^*(\vec{x}') \psi(\vec{x}', t_0). \quad (1.55)$$

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:

$$\psi (\vec{x}'', t) = \int d^3 \vec{x} \mathbf{K} (\vec{x}'', t ; \vec{x}', t_0) \psi (\vec{x}', t_0) \quad (1.56)$$

where the kernel of the integral operator is given by

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

and is known as **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  $\mathbf{K} (\vec{x}'', t; \vec{x}', t_0)$  is known and  $\psi (\vec{x}', t_0)$  is given. In this sense, the Schrödinger theory is a *perfectly causal theory*. The time development of a wave function subjected to some potential is as deterministic as classical mechanics *provided the system is left undisturbed*. If a measurement intervenes, the wave function changes abruptly.

Properties of the propagator:

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

$$\lim_{t \rightarrow t_0} \mathbf{K} (\vec{x}'', t; \vec{x}', t_0) = \delta^3 (\vec{x}'' - \vec{x}') \quad (1.58)$$

because of the completeness of  $\{|a'\rangle\}$

In fact, (1.57) can be written as

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

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 multiplies  $\psi (\vec{x}', t_0)$  with  $\mathbf{K}$  and integrates over the entire space.

The propagator is the Green's function for the time-dependent Schrödinger equation satisfying

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

with the boundary condition

$$\mathbf{K}(\vec{x}'', t; \vec{x}', t_0) = 0 \quad \text{for } t < t_0. \quad (1.61)$$

The  $\delta$ -function  $\delta(t - t_0)$  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

$$\begin{aligned} \mathbf{K}(\vec{x}'', t; \vec{x}', 0) &= \langle \vec{x}'' | \exp\left[-\frac{i}{\hbar} H_0 t\right] | \vec{x}' \rangle \\ &= \int d^3 p' \langle \vec{x}'' | \exp\left[-\frac{i}{\hbar} \frac{p'^2}{2m} t\right] | \vec{p}' \rangle \langle \vec{p}' | \vec{x}' \rangle \\ &= \int d^3 p' \langle \vec{x}'' | \vec{p}' \rangle \langle \vec{p}' | \vec{x}' \rangle \exp\left[-\frac{i}{\hbar} \frac{p'^2}{2m} t\right] \\ &= \int d^3 p' \frac{1}{(2\pi \hbar)^3} e^{\frac{i}{\hbar} \vec{p}' \cdot (\vec{x}'' - \vec{x}')} e^{-\frac{i}{\hbar} \frac{p'^2}{2m} t} \\ &= \frac{1}{(2\pi \hbar)^3} \int d^3 p' e^{\frac{i}{\hbar} \left[ \vec{p}' \cdot (\vec{x}'' - \vec{x}') - \frac{p'^2}{2m} t \right]}. \end{aligned} \quad (1.63)$$

Splitting up the integral into  $\int d p'_1 \cdots \int d p'_2 \cdots \int d p'_3 \cdots$ , one has to solve

$$\int d p e^{\frac{i}{\hbar} \left( p x - \frac{p^2}{2m} t \right)}. \quad (1.64)$$

Consider exponent

$$\begin{aligned}
\left(-\frac{p^2}{2m}t + px\right) &= -\frac{t}{2m} \left(+p^2 - \frac{2m}{t}px + \frac{x^2m^2}{t^2}\right) + \frac{x^2m}{2t} \\
&= -\frac{t}{2m} \left(+p - \frac{mx}{t}\right)^2 + \frac{x^2m}{2t} \\
&= -\left(\frac{x}{2} \sqrt{\frac{2m}{t}} - \sqrt{\frac{t}{2m}}p\right)^2 + \frac{x^2m}{2t}.
\end{aligned} \tag{1.65}$$

Thus

$$\begin{aligned}
\int dp e^{\frac{i}{\hbar} \left(px - \frac{p^2}{2m}t\right)} &= \int d\left(p \cdot \sqrt{\frac{t}{2m\hbar}}\right) e^{\frac{i}{\hbar} \frac{mx^2}{2t}} \sqrt{\frac{2m\hbar}{t}} e^{-\frac{i}{\hbar} \left(\frac{x}{2} \sqrt{\frac{2m}{t}} - p \sqrt{\frac{t}{2m}}\right)^2} \\
&= e^{\frac{i}{\hbar} \frac{mx^2}{2t}} \sqrt{\frac{2m\hbar}{t}} \int d\left(p \sqrt{\frac{t}{2m\hbar}} - \frac{x}{2} \sqrt{\frac{2m}{t\hbar}}\right) e^{-\frac{i}{\hbar} \left(\frac{x}{2} \sqrt{\frac{2m}{t}} - p \sqrt{\frac{t}{2m}}\right)^2} \\
&= e^{\frac{i}{\hbar} \frac{mx^2}{2t}} \sqrt{\frac{2m\hbar}{t}} \int d\xi e^{-i\xi^2} \\
&= e^{\frac{i}{\hbar} \frac{mx^2}{2t}} \sqrt{\frac{2m\hbar}{t}} \sqrt{\frac{\pi}{i}} \\
&= e^{\frac{i}{\hbar} \frac{mx^2}{2t}} \sqrt{\frac{2m\pi\hbar}{it}}.
\end{aligned} \tag{1.66}$$

Thus

$$\frac{1}{2\pi\hbar} \int dp e^{\frac{i}{\hbar} \left(px - \frac{p^2}{2m}t\right)} = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{i}{\hbar} \frac{mx^2}{2t}}. \tag{1.67}$$

Thus for (1.64) one obtains

$$\begin{aligned}
\mathbf{K}(\vec{x}'', t, \vec{x}', 0) &= \frac{1}{(2\pi\hbar)^3} \int d^3p' e^{\frac{i}{\hbar} \vec{p}' \cdot (\vec{x}'' - \vec{x}')} e^{-\frac{i}{\hbar} \frac{p'^2}{2m} t} \\
&= \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} e^{\frac{i}{\hbar} \frac{m}{2t} (\vec{x}'' - \vec{x}')^2}
\end{aligned} \tag{1.68}$$

This expression can be used to study the spreading of a Gaussian wave packet over time.

Certain space and time integrals derivable from  $\mathbf{K}(\vec{x}''t; \vec{x}', t_0)$  are of special interest. Set again  $t_0 = 0$  and consider  $\vec{x}'' = \vec{x}'$  and integrate over space, i.e.,

$$\begin{aligned}
G(t) &= \int d^3 x' \mathbf{K}(\vec{x}', t, \vec{x}', 0) \\
&= \int d^3 x' \sum_{a'} |\langle \vec{x}' | a' \rangle|^2 \exp \left[ -\frac{i}{\hbar} E_{a'} t \right] \\
&= \sum_{a'} \exp \left[ -\frac{i}{\hbar} E_{a'} t \right].
\end{aligned} \tag{1.69}$$

Notice that setting  $\vec{x}'' = \vec{x}'$  is equivalent to taking the trace of the time-evolution operator in the  $\vec{x}$  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

$$\beta = \frac{it}{\hbar} \tag{1.70}$$

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

$$Z = \sum_{a'} \exp(-\beta E_{a'}) . \tag{1.71}$$

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  $G(t)$

$$\begin{aligned}
\tilde{G}(E) &= -\frac{-i}{\hbar} \int_0^\infty dt G(t) \exp \left( \frac{i}{\hbar} Et \right) \\
&= -\frac{i}{\hbar} \int_0^\infty dt \sum_{a'} \exp \left( -\frac{i}{\hbar} E_{a'} t \right) \exp \left( \frac{i}{\hbar} Et \right) .
\end{aligned} \tag{1.72}$$

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

$$\tilde{G}(E) = \sum_{a'} \frac{1}{E - E_{a'}}. \quad (1.73)$$

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

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

$$\begin{aligned} \mathbf{K}(\vec{x}'', t; \vec{x}', t_0) &= \langle \vec{x}'' | \exp \left[ -\frac{i}{\hbar} H (t - t_0) \right] | \vec{x}' \rangle \\ &= \sum_{a'} \langle \vec{x}'' | \exp \left[ -\frac{i}{\hbar} H t \right] | a' \rangle \langle a' | \exp \left[ \frac{i}{\hbar} H t_0 \right] | \vec{x}' \rangle \\ &= \langle \vec{x}'' | t | \vec{x}', t_0 \rangle. \end{aligned} \quad (1.74)$$

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

In this notation  $\langle \vec{x}'', t | \vec{x}', t_0 \rangle$  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,  $\langle \vec{x}'', t | \vec{x}', t_0 \rangle$  is the **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  $\langle \vec{x}'' | t | \vec{x}' t_0 \rangle$  is to view  $|\vec{x}' t_0\rangle$  as position *Ket* at  $t_0$  with eigenvalue  $\vec{x}'$ . Thus  $\langle \vec{x}'' | t | \vec{x}' t_0 \rangle$  is a transformation function that connects two sets of base *Kets* at different times, i.e., the time-evolution can be viewed as unitary transformation that connects one set of basis *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

$$\int d^3 x'' |\vec{x}'', t''\rangle \langle \vec{x}'', t''| = \mathbf{1}. \quad (1.75)$$



Thus the time-evolution from  $t'$  to  $t'''$  can be divided into two intervals:  
 $(t', t''') \rightarrow (t', t'') \cup (t'', t''')$  with  $t''' > t'' > t'$  as

$$\langle \vec{x}''', t''' | \vec{x}', t' \rangle = \int d^3 x'' \langle \vec{x}''', t''' | \vec{x}'', t'' \rangle \langle \vec{x}'', t'' | \vec{x}', t' \rangle \quad (1.76)$$

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

$$\begin{aligned} \langle \vec{x}''', t''' | \vec{x}', t' \rangle &= \int d^3 x''' \int d^3 x'' \langle \vec{x}''', t''' | \vec{x}''', t'' \rangle \\ &\quad \langle \vec{x}''', t'' | \vec{x}'', t'' \rangle \langle \vec{x}'', t'' | \vec{x}', t' \rangle \end{aligned} \quad (1.77)$$

## 1.4 Feynman Path Integral Formulation

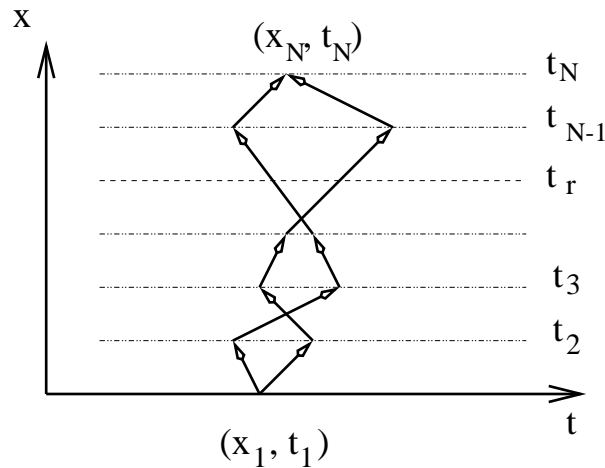
Without loss of generality, consider here only one-dimensional problems. Consider the transition amplitude for a particle going from an initial space time point  $(x_1, t_1)$  to a final space time point  $(x_N, t_N)$ . The entire time interval between  $t_1$  and  $t_N$  is divided into  $N - 1$  equal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

$$t_j - t_{j-1} \equiv \Delta t = \frac{(t_N - t_1)}{N - 1} \quad (1.78)$$

Exploiting the composition property gives

$$\begin{aligned} \langle x_N, t_N | x_1, t_1 \rangle &= \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle \quad (1.79) \\ &\quad \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_2, t_2 | x_1, t_1 \rangle . \end{aligned}$$

To visualize, consider the  $x - t$  plane in Fig. 1.1.



**Fig.**

**1.1** Paths in the x-t-plane

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  $x_2, x_3, \dots, x_{N-1}$ . 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

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

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

$$\begin{aligned} V(x) &= mgx \\ (x_1, t_1) &= (h, 0) \\ (x_N, t_N) &= \left(0, \sqrt{\frac{2h}{g}}\right) \end{aligned} \quad (1.81)$$

the classical path in the  $x - t$ -plane can **only** be

$$x = h - \frac{gt^2}{2} . \quad (1.82)$$

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

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

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  $\hbar \rightarrow 0$ .

Introduce the notation

$$S(n, n-1) \equiv \int_{t_{n-1}}^{t_n} dt L_{classical}(x, \dot{x}) . \quad (1.84)$$

Because  $L_{classical}$  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:

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

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  $x_2, x_3, \dots, x_{N-1}$ . At the same time, let time interval  $\Delta t$  be infinitesimally small. Thus, in a loose sense we may write

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

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

Qualitative remarks:

As  $\hbar \rightarrow 0$  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  $\hbar \rightarrow 0$  the major contributions must arise from a very narrow stripe containing the classical paths.

To formulate Feynman's conjecture more precisely, write

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \frac{1}{\omega(\delta t)} \exp \left[ \frac{i}{\hbar} S(n, n-1) \right] \quad (1.87)$$

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  $\delta t \rightarrow 0$ . 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  $\delta t \rightarrow 0$ . Since  $\delta t$  small, a straight-line approximation between  $(x_{n-1}, t_{n-1})$  and  $(x_n, t_n)$  is justified.

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

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

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

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

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

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

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

and

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

In summary, as  $\Delta t \rightarrow 0$  one obtains

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

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

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

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

$$\int_{x_1}^{x_N} \mathbf{D}[x(t)] \equiv \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \quad (1.95)$$

and

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

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  $\hbar \rightarrow 0$ .

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

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

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

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

From (1.92) it is obvious that in the lim  $\delta t \rightarrow 0$  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  $\Delta t$ .

$$\begin{aligned} \langle x, t | x_1, t_1 \rangle &+ \Delta t \frac{\partial}{\partial t} \langle x, t | x_1, t_1 \rangle \\ &= \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \int_{-\infty}^{\infty} d\xi \exp \left[ \frac{im}{2\hbar} \frac{\xi^2}{\Delta t} \right] \left[ \mathbf{1} - \frac{i}{\hbar} V \Delta t + \dots \right] \\ &\times \left[ \langle x, t | x_1, t_1 \rangle + \left( \frac{\xi^2}{2} \right) \frac{\partial^2}{\partial \xi^2} \langle x, t | x_1, t_1 \rangle + \dots \right] \end{aligned} \quad (1.99)$$

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

$$\Delta t \frac{\partial}{\partial t} \langle x, t | x_1, t_1 \rangle = - \left( \frac{i}{\hbar} \right) \Delta t V \langle x, t | x_1, t_1 \rangle \quad (1.100)$$

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

where we have used

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

Thus

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

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  $\mathbf{R}^3$  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

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

From (1) follows

$$\begin{aligned} z' &= a_1 z + a_2 t \\ t' &= b_1 t + b_2 z \end{aligned} \quad (2.2)$$