5. Dynamics: Schrödinger Equation

5.1 Basic Postulate and Schrödinger Picture

Dynamics: Schrödinger Equation

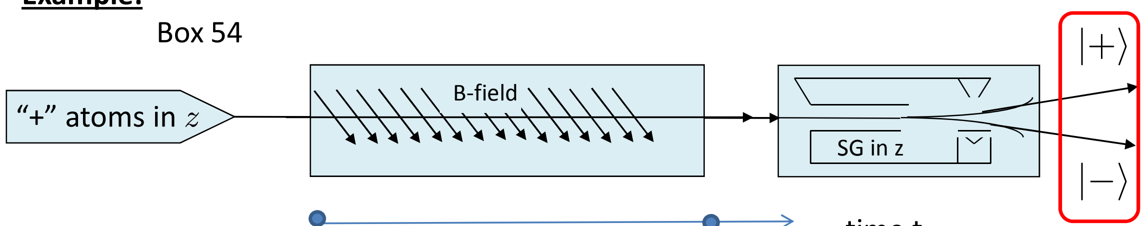
Postulate 6

The time evolution of a quantum system is determined by the *Hamiltonian* or total energy operator *H(t)* through the *Schrödinger Equation*

$$i\,\hbar\,\frac{d}{dt}\,|\Psi(t)\rangle = H(t)\,|\Psi(t)\rangle$$

Example:

Box 54



$|\Psi(0)\rangle = |+\rangle$ $\qquad$ $|\Psi(\Delta t)\rangle = |-\rangle$

measurement kets are time independent!

system kets are time dependent!

$$|\Psi(t)\rangle = c_+(t)\,|+\rangle + c_-(t)\,|-\rangle$$

Schrödinger picture

The time dependence of the ket that describes the physical system sits in the time dependence of the coefficients.

If we say that the system is in the state |+> at some specific time, then it means that it would always give the spin up measurement result in a Stern-Gerlach device performed on the system at the given time.

Hamilton Operator (Hamiltonian)

The operator H defines the dynamics of our system. The units of this operators are that of energy.

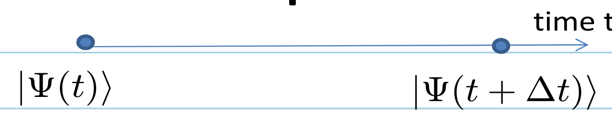
In this course we will not deal with the situation how to find the right Hamilton Operator, but we will deal with finding the solutions of the dynamics for our system for given Hamiltonians!

5.2 Derivation of Schrödinger Equation

Why we shouldn't be surprised ...

Step 1: $|\Psi(t+\Delta t)\rangle = U(t,\Delta t)|\Psi(t)\rangle$

unitary:operator: $U(t,\Delta t)$



The time evolution maps unit-vectors to unit vectors (preserving the norm), which is the same type of requirements as we used in section 4.6 when we studied unitary transformations. So the states at time t and at time t + Δt must be connected by a unitary transformation $U(t, \Delta t)$ which in principle can be different for any initial time t, and any time difference Δt.

Step 2: for small time advances Δ t:

$$U(t,\Delta t) = 1 + M(t)\ \Delta t + O(\Delta t^2)$$

operator M(t)

$$\frac{|\Psi(t+\Delta t)\rangle - |\Psi(t)\rangle}{\Delta t} = M(t)\ |\Psi(t)\rangle + O(\Delta t)$$

In this step we assume that the unitary operators depend smoothly on the time difference Δt so that we can perform a Taylor Expansion of the unitary around its value at time $\Delta t = 0$

Taylor expansion: To do a Taylor expansion of an operator (or actually for any other object) just think about the coordinate representation

$$U(\Delta t) \doteq \begin{pmatrix} u_{11}(\Delta t) & \cdots & u_{1n}(\Delta t) \\ \vdots & & \\ u_{n1}(\Delta t) & \cdots & u_{nn}(\Delta t) \end{pmatrix}$$

a) (the variable t is not relevant here)
b) Expand now each matrix entry in the variable Δt in a Taylor expansion.
c) Note that the first terms should be

$$u_{ij}\Big|_{\Delta t=0} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

because we expect

$$\mathcal{U}(\delta t = 0) = \mathbb{1} \quad \text{identity operator}$$

(after all, the state not change if the time does not change!)

d) collect the Taylor expansion term belonging to the same order in δt in one matrix (using linearity)

$$\mathcal{U}(\delta t) \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \\ 0 & & \ddots & \\ 0 & 0 & & 1 \end{pmatrix} + \underbrace{\begin{pmatrix} \frac{d}{d\delta t} \mathcal{U}_{11}(\delta t)\big|_{\delta t = 0} & \cdots & \cdot \\ \vdots & & \vdots \\ \vdots & & \vdots \end{pmatrix}}_{\doteq M} \delta t + O(\delta t^2)$$

Illustration: When discussing the Zeno effect (section 4.7) , we looked at a unitary

$$\mathcal{U}_\ell \leftrightarrow \begin{pmatrix} \cos\left(\frac{\ell}{L}\frac{\pi}{2}\right) & \sin\left(\frac{\ell}{L}\frac{\pi}{2}\right) \\ -\sin\left(\frac{\ell}{L}\frac{\pi}{2}\right) & \cos\left(\frac{\ell}{L}\frac{\pi}{2}\right) \end{pmatrix}$$

The distance l can be connected to time as l = v t with some velocity v.
Then we find

$$\mathcal{U}(t_0, t_0 + t) \leftrightarrow \begin{pmatrix} \cos(\alpha t) & \sin(\alpha t) \\ -\sin(\alpha t) & \cos(\alpha t) \end{pmatrix}$$

with $\alpha t = \frac{v}{L}\frac{\pi}{2} t \,, \quad \alpha \in \mathbb{R}$

Note that this operator is independent of t_0 .We can now expand this operator for infinitesimal t , denoted as dt.

$$\mathcal{U}(t_0, t_0 + dt) \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} dt + O(dt^2)$$

Rearrangement:

$$|\psi(t+\Delta t)\rangle = \left(\mathbb{1} + M(t)\Delta t + O(\Delta t^2)\right)|\psi(t)\rangle$$
$$= |\psi(t)\rangle + \Delta t\, M(t)|\psi(t)\rangle + O(\Delta t^2)$$

$$\Rightarrow \frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = M(t)|\psi(t)\rangle + O(\Delta t)$$

Step 3: unitarity condition on U:

$$M(t) + M^{\dagger}(t) = 0$$

➔ M(t) = - i H(t)/ $\hbar$

H(t) hermitian operator "Hamiltonian"

factors are pure convention!

$$U = \mathbb{1} + M\Delta t + O(\Delta t^2)$$
$$U^{\dagger} = \mathbb{1} + M^{\dagger}\Delta t + O(\Delta t^2)$$

$$UU^{\dagger} = \mathbb{1} + M\Delta t + M^{\dagger}\Delta t + O(\Delta t^2)$$
$$\overset{!}{=} \mathbb{1} \qquad \forall \Delta t$$

$$\Rightarrow M + M^{\dagger} = 0$$

We now reparameterize M to introduce the operator H, which now satisfies

$$H = H^{\dagger}$$

Note that all the pre-factors in the assignment $M(t) = -i\frac{H(t)}{\hbar}$

are pure convention that make our life easier!

The term Hamiltonian is coming from classical mechanics, where in the Hamiltonian formalism of classical mechanics the dynamics is governed by the expression of the total energy of the system. (See also Lecutre 5, section 2.1!)

Step 4: $\Delta t \to 0$

$$i\,\hbar\,\frac{d}{dt}\,|\Psi(t)\rangle = H(t)\,|\Psi(t)\rangle$$

The structure of Schrödinger's equation is not quantum mechanical, but just a true statement about smoothly changing time dependent vectors!

$$\lim_{\Delta t \to 0} \frac{|\Psi(t+\Delta t)\rangle - |\Psi(t)\rangle}{\Delta t} = \frac{d}{dt}\,|\Psi(t)\rangle$$

$$|\Psi(t)\rangle = \sum_n c_n(t)\,|\phi_n\rangle$$

$$\Rightarrow \left(\lim_{\Delta t \to 0} \sum_n \frac{c_n(t+\Delta t) - c_n(t)}{\Delta t}\,|\phi_n\rangle\right)$$

$$= \sum_n \left(\frac{d}{dt}\,c_n(t)\right)|\phi_n\rangle$$

This expression makes clear what the meaning of a derivative of a vector as function of time is!

Overall, note that our derivation used only the fact that our system is described by elements of a complex vector space, which develops smoothly over time in a way that conserves the norm of the vector.

So the secret of quantum mechanics is the use of complex vector spaces to describes systems, and not the appearance of $\hbar$ in the formulas!

Definition:
A Hamiltonian that does not depend on time is called time-independent.

From now on, we concentrate only on time-independent Hamiltonians!

Example of a time independent Hamiltonian is a situation where an atom sits in a time-independent homogeneous magnetic field.
This situation would become time dependent if we were to change the amplitude of that magnetic field as a function of time.

5.3 Solving Schrödinger's equation using the Energy eigenbasis
We learn now a basic approach to solve Schrödinger's equation. We assume that a Hamilton Operator (time-independent) is given to us. So the problem is described by

1) Dynamical equation:

Schrödinger Equation

$$i\,\hbar\,\frac{d}{dt}\,|\Psi(t)\rangle = H\,|\Psi(t)\rangle$$

2) Initial value:
we are given $|\Psi(t=0)\rangle = |\Psi(0)\rangle$

Let the Hamilton operator have
eigenvalues E_n
eigenvectors $|E_n\rangle$ (the eigenvectors form the energy eigenbasis!)

then we can expand the time dependent state vector as

$$|\Psi(t)\rangle = \sum_n c_n(t)\,|E_n\rangle$$

with some probability amplitudes $c_n(t)$

We insert this expansion into the Schrödinger equation and find

Left hand side:

$$i\hbar\frac{d}{dt}\,|\Psi(t)\rangle = \sum_n i\hbar\left(\frac{d}{dt}c_n(t)\right)|E_n\rangle$$

right hand side:

$$H\,|\Psi(t)\rangle = \sum_n c_n(t)H|E_n\rangle = \sum_n E_n c_n(t)|E_n\rangle$$

As both sides have to agree, and the expansion of a state in a orthonormal basis is unique, we have that the probability amplitudes of the Hamiltonian Eigenstates have to agree

$$i\hbar \frac{d}{dt} c_n(t) = E_n c_n(t)$$

So the probability amplitudes $c_n(t)$
have to satisfy a first order differential equation.
To determine the unique solution to this differential equation, we also need to have one intial value. This is given by the expansion of the given initial state as

$$|\psi(0)\rangle = \sum_n c_n \, |E_n\rangle$$

so $\quad c_n(t=0) = c_n(0) = c_n$

The solution to

$$\boxed{\begin{aligned} i\hbar \frac{d}{dt} c_n(t) &= E_n c_n(t) \\ c_n(0) &= c_n \end{aligned}}$$

is an exponential function

$$c_n(t) = c_n \, e^{-i\frac{E_n t}{\hbar}}$$

We can then reinsert these probability amplitudes into the expansion

$$|\Psi(t)\rangle = \sum_n c_n(t) \, |E_n\rangle$$

to find the state vector describing our system for an arbitrary time t:

$$|\Psi(t)\rangle = \sum_n c_n \, e^{-i\frac{E_n t}{\hbar}} \, |E_n\rangle$$

This approach can be summaries as follows

Solution:

Step 1: find eigenvectors $|E_n\rangle$ and eigenvalue E_n of H

Step 2: Expand initial state in eigenbasis

$$|\Psi(0)\rangle = \sum_n c_n \, |E_n\rangle$$

(finds coefficients c_n)

$$c_n = \langle E_n | \psi(0) \rangle$$

Step 3: Write down solution

$$|\Psi(t)\rangle = \sum_n c_n \, e^{-i\frac{E_n t}{\hbar}} \, |E_n\rangle$$

5. 4 Example

Given the Hamilton Operator

$$H = \hbar\omega\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$$

$$\doteq \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and the initial state

$$|\psi(0)\rangle = |+\rangle_x \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Step 1:

One can actually directly read-off

eigenvalues $\quad \hbar\omega \qquad -\hbar\omega$

corresponding eigenvectors $\quad |+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Step 2:

Expand initial state

$$|\psi(0)\rangle = |+\rangle_x = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$$

$$\doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Step 3:

Write down solution

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-i\frac{\hbar\omega}{\hbar}t}|+\rangle + \frac{1}{\sqrt{2}} e^{+\frac{\hbar\omega}{\hbar}t}|-\rangle$$

$$= \frac{1}{\sqrt{2}} e^{-i\omega t}|+\rangle + \frac{1}{\sqrt{2}} e^{+i\omega t}|-\rangle$$

$$\doteq \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\omega t} \\ e^{+i\omega t} \end{pmatrix}$$

note that we use the coordinate representation with respect to the z-basis (standard basis) since this turns out to the eigenbasis of H!

The result of our calculation can now be used to predict what a SG-Experiment oriented in the x-direction would give if we were to perform it at time t:

$$Pr(+ \text{ in } x \text{ at time } t)$$

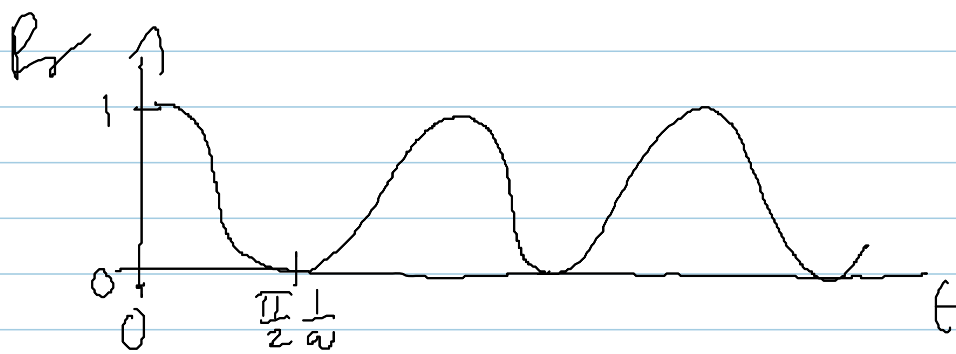
$$= \left| {}_x\langle +|\psi(t)\rangle \right|^2$$

$$= \left| \frac{1}{\sqrt{2}} (1, 1) \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{+i\omega t} \end{pmatrix} \right|^2$$

$$= \left| \frac{1}{2} \left(e^{-i\omega t} + e^{-i\omega t} \right) \right|^2$$

$$= \left| \cos(\omega t) \right|^2$$

So we find



at time t= $\frac{\pi}{2}\frac{1}{\omega}$

we find

$$Pr\left(+ \text{ in } x \text{ at time } t = \frac{\pi}{2}\frac{1}{\omega}\right) = 0$$

consistent with

$$|\psi(\tfrac{\pi}{2}\tfrac{1}{\omega})\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \doteq |-\rangle_x$$

while at time

$t = 0$

$$P_z(+ \text{ in } x \text{ at time } t=0) = 1$$

consistent with

$$|\psi(0)\rangle = |+\rangle_x \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$