# Quantum Physics 1 2015-2016

Lecture of 8 September 2015 (and used in several later lectures)

## **Question in the previous lecture?**

## **Question on the book Chapter 1?**

Additional announcements on how to do the course:

Guidelines for a good approach to solving problems

# Homework for week 2 of the course

Study: Chapter 2, up to and including 2.3 (part of 2.3 is reading material) The handout from the Feynman lectures

See http://www.quantumdevices.nl/teaching/

**Problems:** 

To be made <u>before</u> the tutorial Chapter 2 - 2.1, 2.3, 2.4, 2.8, and 2.9

# Systematic approach for solving problems:

- for homework and class
- for exam problems

## Advantages:

- It is more likely that you will succeed in solving the problem.
- You get to the solution faster.
- You get better help and guidance from the teachers.
- Better grade for the exam.

#### Systematic approach $\Rightarrow$ Solve in three steps:

#### 1) Analyze the problem:

What do they actually ask?

What other information is relevant and mentioned.

#### Make a sketch.

Are there hints mentioned? List the relevant symbols and formula's, theory.

#### 2) Start solving the problem:

- **2A)** Outline the approach to actual solving first (complete route from begin to end)
- **2B)** Work out the algebra in **symbols not in numbers**.

#### 3) Evaluate the outcome:

Does the answer make sense, is the sign right?

Finding that the mass of the electron is -25 kg, should cause some alarm and start some feedback.

#### Answer wrong? Still points for evaluating remarks on exam.

# **This lecture:**

Postulates of quantum physics

Formally constructing quantum theory.

Today and the next lecture: -Postulates about operators -Postulates about time evolution -Postulates about measurement

# **Next lecture also:**

Discuss double-slit quantum interference to re-visit the postulates in an example.

For this week's problem set, already introduce double-slit interference today??

Formally construct a theory from postulates:

<u>Postulates</u>: a minimal set of rules, which cannot derived any further, and for which it can only be checked by experiments whether they are correct.

From these postulates, all other laws of a theory can be derived.

A suitable set of postulates is not a unique basis for a theory.

**Quantum mechanical theory:** 

- can be based on postulates of today.
- can be based on "Feynman path integrals".

(see for example short discussion in Liboff book)

Formally construct a theory from postulates: Also for classical theories:

For example, classical mechanics is based on 4 postulates about a point particle P with mass m:

State of a system: a certain position and momentum.
 Influences on P are additive force vectors F.
 F = m-a
 F<sub>action</sub> = - F<sub>reaction</sub>

Based on this, for a many particle system, you can derive:

- Law of conservation of energy
- Law of conservation of linear momentum
- Law of conservation of angular momentum
- .....everything

# Quantum theory with respect to other theories

Mostly: Large, friction, warm, environment

Mostly: Small, isolated, cold

But NOT only about atoms and quarks!

Also, for example, for explaining superconductivity.

V< <c< th=""><th>V≈C</th></c<>	V≈C
Classical F=m·a Daily life, planets	General relativistic Special relativistic $E = mc^2 = \sqrt{p^2c^2 + (m_0c^2)^2}$
Quantum Schrödinger eq. ¥	Quantum-relativistic Dirac eq. Klein-Gordon eq.

Where are thermodynamics, diffusion equation, etc.?

Can be derived from the above, but deriving the second law of thermodynamics is still not fully clear.

#### **Postulates for quantum theory**

State 1) State at time t is described by a complex wave function Ψ(t). Ψ(t)\*Ψ(t) has the meaning probability density.
 2) All physical properties are described by an operator. Property A by an operator Â, an observable.

Time evolution 3) Schrödinger equation  $i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H} \Psi(x,t)$ 

Measurement of property A gives always an eigenvalue of Â, Is the result a, then the state after the measurement is the associated eigenfunction φ<sub>a</sub>.
 5) Probability density for measurement outcome is |∫ Ψ(x,t)\* φ<sub>a</sub> dx |<sup>2</sup>

Postulates about measurements form the basis of an IMPORTANT and handy model about measurements, but we do not need them if we can make a detailed description of the measurement process as an interaction between a meter and the system that is measured.

# **Central example these first weeks:**

# Point particle with mass m in 1 dimension x.

# But do not forget:

Quantum physics is about all systems and degrees of freedom!

# 

**Postulate 1 (see previous lectures)** 

State at time t is described by a complex wave function  $\Psi(x,t)$ .

 $\Psi(x,t)^*\Psi(x,t)$  has the meaning probability density.

The probability P for x to be in the small range around  $x_o$  of width dx is  $P(x_o < x < x_o + dx) = |\Psi(x_o, t)|^2 dx$ 

So, there is a **probability density**  $W(x) = |\Psi(x,t)|^2$ 

Ψ(x,t)\*Ψ(x,t)

 $=|\Psi(\mathbf{x},\mathbf{t})|^2$ 



#### **Postulate 1 (see previous lectures)**

State at time t is described by a complex wave function  $\Psi(x,t)$ .

 $\Psi(x,t)^*\Psi(x,t)$  has the meaning probability density.

Additional example for the case of discrete (rather than continuous) superposition of states. Say a system is in the state

$$\Psi(x) = c_1 \cdot \varphi_1(x) + c_2 \cdot \varphi_2(x)$$

Here  $c_1$  and  $c_2$  are called <u>probability amplitudes</u>. Then, the <u>probability</u> (not probability density) for the system to be in state

$$\varphi_1(x)$$
 is  $c_1^* c_1 = |c_1|^2$ 

and the probability for the system to be in state

$$\varphi_2(x)$$
 is  $c_2^* c_2 = |c_2|^2$ 

#### **Postulate 1 (see previous lectures)**

State at time t is described by a complex wave function  $\Psi(x,t)$ .

 $\Psi(x,t)^*\Psi(x,t)$  has the meaning probability density.

The example of the previous slide continued, for the relation with measurement (fully treated in postulate 4 and 5):

If you would measure whether the system is in state  $\varphi_1$  or state  $\varphi_2$ , these probabilities  $c_1^*c_1$  and  $c_2^*c_2$  also are the probabilities of the two possible measurement outcomes.

If the measurement result is state  $\phi_1$ , the system is purely in state  $\phi_1$  directly after the measurement.

If the measurement result is state  $\phi_2$ , the system is purely in state  $\phi_2$  directly after the measurement.



All physical properties are described by an operator. For property A, there is an operator Â. If A can be measured, the operator is an <u>observable</u>. An operator is an observable if its eigenvalues are real.

$$\hat{A} \varphi_n(x) = a_n \varphi_n(x) \quad \text{Eigenvalue equation}$$

$$a_n \quad \text{Eigenvalue}$$

$$\varphi_n(x) \quad \text{Eigenfunction}$$

A can be: energy, momentum, electrical dipole, .....

can have continuous (1D position of a particle) or discrete (energy of electron in an atom) spectrum of eigenvalues.

Link to LINEAR ALGEBRA – see also section 3.2 and Appendix A1-A6 in the Griffiths book (Griffiths already introduces operators in section 2.1)

# Note on the previous slides for students that use the Griffiths book (2<sup>nd</sup> ed.)

The eigenvalue problem/equation is really very fundamental to the physical and mathematical properties of all operators, and operators are very fundamental in the way quantum mechanics describes all physical properties of a system.

So, in this sense it is a weak point of the Griffiths book that it does not mention the eigenvalue equation till around Eq. [3.22].

At the same time, the book already uses it earlier, and it then may seem some randomly introduced example that comes out of nothing.

#### For example:

Operators are already mentioned around Eq. [1.35] (see also the footnotes below Eq. [1.35] and Eq. [2.11]). Eq. [2.12] is in fact the eigenvalue problem for total energy. Below Eq. [2.6] the book mentions *stationary states*, and *states with definite total energy* without mentioning that these are the energy eigenstates of the system (like the ground state and excited state of an atom).

Below Eq. [2.73] the book talks about *the "allowed" values of K*, which is again some vague language for finding the energy eigenvalues and energy eigenstates.

The whole analysis of getting Eq, [2.27], or [2.129] or [2.171] is in fact the mathematics of finding the energy eigenvalues (and on the pages around it also the energy eigenstates).

# **Example of how we already used this:**

Quantify a physical property of a system given its wave function

<u>Expectation value</u> for property A op  $t = t_0$ 

Say system is in state  $\Psi(x,t_0)$ 

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi(x, t_0) \hat{A} \Psi(x, t_0) dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi(x, t_0) * \hat{x} \Psi(x, t_0) dx$$

# Why operators?

First examples of operators used for a classical state.

With operators you can for example:

- 1. Describe how physical property can be calculated, give a certain state for the system.
- 2. Describe how a state B of a system evolves from a state A.

Notation for the state of a particle with mass m, moving in 1 dimension (here a classical state with precise values for X and P):

**X**<sub>1</sub>,**P**<sub>1</sub>

This blue box means "in de state" with the particle at position  $X_1$  and momentum  $P_1$ .

Describe how the final state of a system evolves from an initial state with an operator for time evolution.

Define an operator for time evolution of a state

(here for the case of a free particle):

$$\hat{U}(t_{START}, t_{END})$$
Hat on the U shows that it is an operator.  
The result of this operator working on a state  $X_1, P_1$  is

$$\hat{U}(t_{START}, t_{END}) \quad X_1, P_1 = \left(X_1 + \frac{P_1}{m} \cdot (t_{END} - t_{START})\right), P_1$$

Describe how a physical property can be calculated, given a system in

a certain state. The example here is for kinetic energy.

Define an operator for kinetic energy:

 $\hat{T}$  Hat on the T shows that it is an operator.

The result of this operator working an the state

$$\hat{T} \mathbf{X}_{1}, \mathbf{P}_{1} = \frac{P_{1}^{2}}{2m}$$

However, in quantum mechanics a system can be in multiple classical states at the same time. For example, this state:

$$c_a X_1,P_1 + c_b X_2,P_2$$
  
"+" means here "and simultaneously also in this state"  
 $c_a$  gives the weight for being in that state.

This state is then also possible!

$$\mathbf{c}_{a} \mathbf{X}_{1}, \mathbf{P}_{1} + \mathbf{c}_{b} \mathbf{X}_{2}, \mathbf{P}_{2} + \mathbf{c}_{c} \mathbf{X}_{1}, \mathbf{P}_{2}$$

What is now an easy approach for describe the value(s) for kinetic energy?

$$\hat{T}(\mathbf{c_a} \ \mathbf{X_1, P_1} + \mathbf{c_b} \ \mathbf{X_2, P_2} + \mathbf{c_c} \ \mathbf{X_1, P_2} ) = c_a \frac{P_1^2}{2m} + c_b \frac{P_2^2}{2m} + c_c \frac{P_2^2}{2m}$$

N.B., the pure state  $X_1, P_1$  is quantum mechanically not allowed by the Heisenberg uncertainty relation. This is neglected for these examples on operators for classical states.

# **Operators and the eigenvalue equation**

- How to look at this?
- What properties?
- See your course on linear algebra for background on the eigenvalue problem.

$$\hat{A}\varphi_n(x) = a_n\varphi_n(x)$$

Operator: a mathematical operation on a wave function, that works for any state of the system, which can have the meaning:

- Physical property of a system calculated for the state (wave function) of the system.
- Description of how state B of the system evolves from a state A .

# The previous slide in Dirac notation:

(for use later than the 2<sup>nd</sup> week of the course)

 $\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$ 

# **Example:**

Physical property of a system calculated for the state (wave function) of the system.

<u>Expectation value</u> for property A at  $t = t_0$ 

Say system is in state  $\Psi(x, t_0)$ 

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi(x, t_0) * \hat{A} \Psi(x, t_0) dx$$

# **Example (comes back later):**

Describe how a state B of a system evolves from a state A. Time evolution (for a system with a stationary Hamiltonian  $\hat{H}$  )

$$\hat{U} = e^{-\frac{it\hat{H}}{\hbar}}$$
$$\hat{U} \Psi(x, t_0) = \Psi(x, t_0 + t)$$

Note:  $\hat{U}$  is an operator but not an observable.

Other example: Operator that shifts the full wave function over a certain distance in space (add this to a homework problem?)\_ **Orthogonality of eigenfunctions** (for Operators in Griffiths section 3.2) Note: the expressions on this slide are only valid for the case that is an observable!

$$\hat{A} \varphi_n(x) = a_n \varphi_n(x)$$
 Eigenvalue equation  

$$a_n$$
 Eigenvalue (a real number for the case of an observable)  

$$\varphi_n(x)$$
 Eigenfunction

$$\int_{-\infty}^{\infty} \varphi_n^*(x) \varphi_m(x) dx = \begin{cases} 1 , \text{ for } n = m \\ 0 , \text{ for } n \neq m \end{cases} \implies$$
$$\int_{-\infty}^{\infty} \varphi_n^*(x) \hat{A} \varphi_m(x) dx = \begin{cases} a_n , \text{ for } n = m \\ 0 , \text{ for } n \neq m \end{cases} \implies \begin{cases} \text{Notel} \\ \text{This rule is only valid if } \varphi_n \text{ and } \varphi_m \\ \text{ are eigenfunctions of } \hat{A}. \end{cases}$$

# Kronecker delta

(Eq. [2.31] in Griffiths book)



#### Assume A is a scalar physical property

What is....?

$$\int \Psi(x,t_0) * \hat{A} \Psi(x,t_0) dx \Rightarrow A$$
 scalar quantity (that is, a number)

 $\hat{A}\Psi(x,t_0)$   $\Rightarrow$  Again a wave function (not always normalized)

$$\Psi(x,t_0)^*\hat{A}$$

⇒ Again a wave function (not always normalized)

Think about:

- wave functions as column-vectors
- (wave functions)\* as row-vectors
- Operators as matrices

Also for keeping the order correct in formulas and expressions!

#### Think about:

- wave functions as column-vectors
- (wave functions)\* as row-vectors
- Operators as matrices

Also for keeping the order correct in formulas and expressions!

#### For a scalar physical property A (observable Â)

$$\int \Psi(x,t_0)^* \hat{A} \Psi(x,t_0) dx \qquad \Rightarrow \qquad a \text{ real} \begin{pmatrix} c_1^* & c_2^* & c_3^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \sum_{i=1}^3 \sum_{j=1}^3 c_i^* c_j A_{ij} = \begin{array}{c} \text{ scalar} \\ \text{ number} \end{array}$$



For example: position of a particle

Discrete



31

 $\sum \Psi^*(n) \Psi(n) = 1$  $n = -\infty$ 

For example: number of electrons on a small conductor

# **Functions of operators**

#### Say

$$\hat{A}\varphi_n(x) = a_n\varphi_n(x)$$
$$a_n$$
$$\varphi_n(x)$$

**Eigenvalue equation** 

Eigenvalue

Eigenfunction

Then the operator  $f(\hat{A})$  has the following properties:

$$f(\hat{A})\varphi_n(x) = f(a_n)\varphi_n(x)$$
$$f(a_n)$$
$$\varphi_n(x)$$

**Eigenvalue equation** 

Eigenvalue

Eigenfunction

Operator for momentum  $\hat{p}_x$ 

$$\hat{p}_x \varphi_k(x) = p_x \varphi_k(x)$$

·--- ·--

$$\hat{p}_x \leftrightarrow -i\hbar \frac{\partial}{\partial x}$$

# For the case that we represent the state as a function of x. Follows from Hamiltonian mechanics.

See the extra reading material (link on the web, appendices Cohen Tannoudji book) or Chapter 1 in the Liboff book.

## Solutions for this eigenvalue problem:

$$\varphi_k = Ae^{\frac{ip_x x}{\hbar}} = Ae^{ikx}$$
 with  $k = \frac{p_x}{\hbar}$  of  $p_x = \hbar k$ 

### What is k?

$$k = \frac{2\pi}{\lambda}$$
 gives De Broglie  $\lambda = \frac{h}{p_x}$ 

Operator for position  $\hat{X}$ 

$$\hat{X}\delta(x-x_n) = x_n\delta(x-x_n)$$
$$\hat{X} \leftrightarrow x \qquad \text{for the case that we represe}$$

^

or the case that we represent a state as a function of.



Operator for total energy H

#### (Hamiltonian)

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

#### Solution for a free particle

$$\frac{\hat{p}_x^2}{2m}\varphi_n(x) = E_n\varphi_n(x)$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_n(x) = E_n\varphi_n(x)$$

$$\frac{\partial^2}{\partial x^2}\varphi_n(x) + k^2\varphi_n(x) = 0 \qquad \qquad k^2 = \frac{2mE_n}{\hbar^2}$$

Λ

$$\varphi(x) = Ae^{ikx} + Be^{-ikx}$$

Plane wave solutions, same as for  $p_x$ -operator Why should this have been expected?

#### **Time-independent Schrödinger equation**

(see a few slides further how this can also be derived from the time-dependent Schrödinger eq.)

# **Expectation value:**

Calculate a physical property for a system given a certain state (wave function)

<u>Expectation value</u> for property A at  $t = t_0$ 

Say, the system is in state  $\Psi(x)$ 

$$\Psi(x,t_0)$$

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi(x,t_0)^* \hat{A} \Psi(x,t_0) dx$$

#### **Example expectation value: position x**



$$\left\langle \hat{X} \right\rangle = \int_{-\infty}^{\infty} \Psi(x)^* \hat{X} \Psi(x) dx$$

$$\left\langle \hat{X} \right\rangle = \int_{0}^{a} \left(\frac{1}{\sqrt{a}}\right)^{*} x \left(\frac{1}{\sqrt{a}}\right) dx = \frac{a}{2}$$

$$\begin{cases} \hat{X} \frac{1}{\sqrt{a}} = x \frac{1}{\sqrt{a}} \\ \hat{X} 0 = 0 \end{cases}$$

#### **Example expectation value:** $\Delta x$



$$\Delta X = \sqrt{\left\langle \hat{X}^2 \right\rangle} - \left\langle \hat{X} \right\rangle^2$$
$$\left\langle \hat{X}^2 \right\rangle = \int_0^a \left(\frac{1}{\sqrt{a}}\right)^* x^2 \left(\frac{1}{\sqrt{a}}\right) dx = \frac{a^2}{3}$$
$$\Delta X = \sqrt{\frac{a^2}{3} - \frac{a^2}{4}} = \frac{a}{\sqrt{12}} \approx 0.29 a$$



The Hamiltonian of a system determines the time evolution of that system, according to the *time-dependent* Schrödinger equation.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H} \Psi(x,t)$$

In physics research of this approach:

First solve the *time-independent* Schrödinger equation for a situation for the system that makes that it has a time-independent Hamiltonian. In a next step, look into

- time evolution of that system with a stationary Hamiltonian
- influence of non-stationary terms in the Hamiltonian (later in this course and in the course Quantum Physics 2)

VERSION IN DIRAC NOTATION, FOR USE LATER THAN THE 2<sup>nd</sup> WEEK OF THE COURSE 41

Postulate 3

The Hamiltonian of a system determines the time evolution of that system, according to the *time-dependent* Schrödinger equation.

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

In physics research of this approach:

First solve the <u>time-independent</u> Schrödinger equation for a situation for the system that makes that it has a time-independent Hamiltonian. In a next step, look into

- time evolution of that system with a stationary Hamiltonian
- influence of non-stationary terms in the Hamiltonian (later in this course and in the course Quantum Physics 2)

#### What do we mean with a stationary Hamiltonian?



p changes in time, but the operator (expression) for p does not



#### Deriving the time-independent Schrödinger equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}_0 \Psi(x,t)$$
 Say  $\Psi(x,t) = \varphi(x)\chi(t)$ 

Separation of variables

$$\frac{i\hbar}{\chi(t)}\frac{\partial\chi(t)}{\partial t} = \frac{\hat{H}_0\varphi(x)}{\varphi(x)} = E \quad \text{(constant)} \quad \Rightarrow$$

$$\hat{H}_0\varphi(x) = E\varphi(x)$$

⇒ Time-independent Schrödinger equation, eigenvalue problem for energy

$$i\hbar \frac{\mathrm{d}\chi(t)}{\chi(t)} = E \,\mathrm{d}t \quad \Rightarrow$$

Time evolution of the energy eigenstates

# **Time-evolution operator:**

For system with time-independent Hamiltonian  $\,H_{
m o}$ 

Solve: 
$$i\hbar \frac{\mathrm{d}\chi(t)}{\chi(t)} = E \,\mathrm{d}t \implies \chi(t) = A \, e^{\frac{-iEt}{\hbar}}$$

Holds for all values of *E*, probability is conserved (*A*=1), used to define  $\hat{U} = e^{\frac{-i\hat{H}_0 t}{\hbar}} \implies \hat{U}\Psi(x,t_0) = \Psi(x,t_0+t)$ 

For system at *t*=0 in an energy eigenstate  $\varphi_n(x)$  with eigenvalue  $E_n$  $\Psi(x,t) = \hat{U} \varphi_n(x) = e^{\frac{-i\hat{H}_0 t}{\hbar}} \varphi_n(x) = e^{\frac{-iE_n t}{\hbar}} \varphi_n(x)$ 

Note that you apply here the rules of the earlier slide on "function of operators"

# Note on the previous slides for students that use the Griffiths book (2<sup>nd</sup> ed.)

Note that describing the time evolution for a system with a stationary Hamiltonian using

$$\hat{U} = e^{\frac{-iH_0t}{\hbar}} \implies \hat{U}\Psi(x,t_0) = \Psi(x,t_0+t)$$

^

is a slightly more fundamental and compact way of describing this than how it is introduced in the book.

The book presents this in Eq. [2.15], and introduces the values and without mentioning that these are in fact the energy eigenvalues, and that it is in fact the result of how the Hamiltonian operator acts on a state.

Taylor expansion of 
$$\hat{U} = e^{rac{-i\hat{H}_0t}{\hbar}}$$
 (on board),

See also problem W3.5j.

# **Stationary states – <u>nothing</u> moves:**

For system with time-independent Hamiltonian  ${\hat H}_0$  in energy eigenstate  ${\,}^{arphi}{n}$ 

at t = 0, how does an arbitrary property A depend on time?

Use: 
$$\hat{U}\Psi(x,t=0)=\Psi(x,t)$$
  $\hat{U}=e^{\frac{-i\hat{H}_0t}{\hbar}}$ 

$$\langle \hat{A} \rangle (t) = \int_{-\infty}^{\infty} \Psi(x,t)^* \hat{A} \Psi(x,t) dx$$

$$\left\langle \hat{A} \right\rangle (t) = \int_{-\infty}^{\infty} e^{\frac{+iE_nt}{\hbar}} \varphi_n(x)^* \hat{A} e^{\frac{-iE_nt}{\hbar}} \varphi_n(x) dx$$

$$\langle \hat{A} \rangle (t) = \int_{-\infty}^{\infty} \varphi_n(x)^* \hat{A} \varphi_n(x) dx$$
 Is co

s constant in time!

# **Arbitrary phase factor:**

For example:

For system with time-independent Hamiltonian  $H_0$  in energy eigenstate  $\varphi_n$ 

at t = 0, how does its wave function evolve in time?

$$\Psi(x,t) = \hat{U} \Psi(x,t=0) = e^{\frac{-iE_nt}{\hbar}} \varphi_n$$

What are the consequences of this evolving "global" phase factor?

Nothing that can be observed.

You can add any constant to all the E<sub>n</sub>.

# **Dynamics of the system** *I*

For system with time-independent Hamiltonian  $\hat{H}_0$  in a state

$$\Psi(x,t=0) = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$

$$\hat{H}_0\varphi_n(x) = E_n\varphi_n(x)$$

$$\left\langle \hat{H}_{0} \right\rangle (0) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2}} \left( \varphi_{1} + \varphi_{2} \right)^{*} \hat{H}_{0} \frac{1}{\sqrt{2}} \left( \varphi_{1} + \varphi_{2} \right) dx \left\langle \hat{H}_{0} \right\rangle (t) = \frac{1}{2} \int_{-\infty}^{\infty} \left[ e^{\frac{+iE_{1}t}{\hbar}} \varphi_{1}(x)^{*} + e^{\frac{+iE_{2}t}{\hbar}} \varphi_{2}(x)^{*} \right] \hat{H}_{0} \left[ e^{\frac{-iE_{1}t}{\hbar}} \varphi_{1}(x) + e^{\frac{-iE_{2}t}{\hbar}} \varphi_{2}(x) \right] dx$$

 $\langle \hat{H}_0 \rangle (t) = \frac{E_1 + E_2}{2}$  Is constant in time!

# **Dynamics of the system** *I***I**

So, is there any physical property A that can depend on time, for system with time-independent Hamiltonian  $\hat{H}_0$  ?

Assume again state  $\Psi(x, t=0) = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$ , A is some arbitrary property

$$\begin{split} &\langle \hat{A} \rangle(0) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2}} \left( \varphi_1 + \varphi_2 \right)^* \hat{A} \frac{1}{\sqrt{2}} \left( \varphi_1 + \varphi_2 \right) dx \\ &\langle \hat{A} \rangle(t) = \frac{1}{2} \int_{-\infty}^{\infty} \left[ e^{\frac{+iE_1t}{\hbar}} \varphi_1(x)^* + e^{\frac{+iE_2t}{\hbar}} \varphi_2(x)^* \right] \hat{A} \left[ e^{\frac{-iE_1t}{\hbar}} \varphi_1(x) + e^{\frac{-iE_2t}{\hbar}} \varphi_2(x) \right] dx \\ &\langle \hat{A} \rangle(t) = \frac{\langle \hat{A} \rangle_{11}}{2} + \frac{\langle \hat{A} \rangle_{22}}{2} + \langle \hat{A} \rangle_{12} \cos\left(\frac{E_2 - E_1}{\hbar}t\right) \qquad \left( \text{used here } \langle \hat{A} \rangle_{12} = \langle \hat{A} \rangle_{21} \right) \end{split}$$

(not always the case)

System with time-independent Hamiltonian  $\hat{H}_0$  has only time dependence of physical properties in the form of oscillations  $e^{i\omega t}$ ,

with  $\hbar\omega = E_n - E_m$  .



Measurement of property A always gives an eigenvalue of  $\hat{A}$  as outcome. Is the result a, then the state after the measurement is the associated eigenfunction  $\phi_a$ .



#### Measurement of property A always gives an eigenvalue of $\hat{A}$ as outcome. Is the result a, then the state after the measurement is the associated eigenfunction $\varphi_a$ .



VERSION IN DIRAC NOTATION 53



# **Postulate 5 – General formulation using Dirac notation** (not treated very well in the book)

<u>Probability</u>  $P_a$  for a measurement outcome with result a

$$P_{a} = \left| \left\langle \varphi_{a} \left| \Psi \right\rangle \right|^{2}$$



Study this by doing problem W4.1 !!

**Postulate 5 - Discrete** (little attention for it in the book)

**Probability** for a measurement outcome is  $|\Sigma \Psi(n,t)^* \varphi_a(n)|^2$ 

#### Same example A=N<sup>2</sup>

inner product  $\Psi(n,t)^*$  and  $\varphi_a(n)$  2

Note: in this example (previous slide), the eigenvectors  $\varphi_a(n)$  coincide with the basis vectors that belong to the coordinates n. The more general case is presented on later slides (see also problem W4.1 in week 4 for an exercise on this with a concrete example).

#### Say before the measurement

$$\Psi(n) = 0 \varphi_0(n) + c_1 \varphi_1(n) + c_2 \varphi_2(n) + 0 \varphi_3(n) + c_4 \varphi_4(n) + 0 \varphi_5(n)$$
  
$$\Psi(n) = \sum_n c_n \varphi_n(n) \quad \text{met} \quad \sum_n c_n^* c_n = 1$$

Then, the probability for outcome 16 is

$$\sum_{n} \Psi(n)^* \varphi_4(n) \bigg|^2 = \bigg| \sum_{n} c_n^* \varphi_n^*(n) \cdot \varphi_4(n) \bigg|^2 = \big| c_4 \big|^2$$

Previous slide written as vectors (here over the range n=0..4, outside this range all  $c_n$ =0):

$$\Psi(n)^* = \begin{pmatrix} 0 & c_1^* & c_2^* & 0 & c_4^* \end{pmatrix} \qquad \varphi_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\left|\sum_{n} \Psi(n)^{*} \varphi_{4}\right|^{2} = \left|\begin{pmatrix}0 & c_{1}^{*} & c_{2}^{*} & 0 & c_{4}^{*}\end{pmatrix} \begin{pmatrix}0\\0\\0\\0\\1\end{pmatrix}\right|^{2} = \left|c_{4}\right|^{2}$$

#### **Version in Dirac notation**

 $\langle \Psi$ 

Previous slide written as vectors (here over the range n=0..4, outside this range all  $c_n$ =0):

$$\left| \leftrightarrow \left( \begin{array}{ccc} c_{1}^{*} & c_{2}^{*} & 0 & c_{4}^{*} \right) & \left| \varphi_{4} \right\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right|$$
$$\left| \left\langle \Psi \left| \varphi_{4} \right\rangle \right|^{2} \leftrightarrow \left| \left( \begin{array}{ccc} c_{1}^{*} & c_{2}^{*} & 0 & c_{4}^{*} \right) \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right|^{2} = \left| c_{4} \right|^{2}$$

Note: in the example on this slide (see also previous slides), the eigenvectors  $\varphi_a(n)$  coincide with the basis vectors that belong to the coordinates n.

#### Postulate 5 continued – discrete case

In het general, the eigenvectors  $\varphi_a(n)$  do not coincide with the basis vectors that are used in the summation over the coordinates n. Study the example below for getting insight in how it is formulated for the continuous case (next slides)

(see also problem W4.1 in week 4 for an exercise on this with a concrete example).

#### Say before the measurement

$$\Psi(n) = 0 \varphi_0(n) + c_1 \varphi_1(n) + c_2 \varphi_2(n) + 0 \varphi_3(n) + c_4 \varphi_4(n) + 0 \varphi_5(n)$$

$$\Psi(n) = \sum_{m} c_{m} \varphi_{m}(n) \quad \text{met} \quad \sum_{m} c_{m}^{*} c_{m} = 1$$

Then, the probability for the measurement outcome that belongs to eigenvector  $\varphi_4(n)$  is

$$\left|\sum_{n} \Psi(n)^{*} \varphi_{4}(n)\right|^{2} = \left|\sum_{n} \left(\sum_{m} c_{m}^{*} \varphi_{m}^{*}(n)\right) \cdot \varphi_{4}(n)\right|^{2} = 0 + \left|\sum_{n} c_{1}^{*} \varphi_{1}^{*}(n) \cdot \varphi_{4}(n)\right|^{2} + \left|\sum_{n} c_{2}^{*} \varphi_{2}^{*}(n) \cdot \varphi_{4}(n)\right|^{2} + 0 + \left|\sum_{n} c_{4}^{*} \varphi_{4}^{*}(n) \cdot \varphi_{4}(n)\right|^{2} + 0 = 0 + 0 + 0 + \left|c_{4}^{*}\right|^{2} + 0 = \left|c_{4}\right|^{2}$$

#### Version in Dirac notation <sup>60</sup>

**Postulate 5 - Discrete** (little attention for it in the book) <u>Probability</u> for a measurement outcome is  $\left|\left\langle \Psi(t)\right|\varphi_{a}\right\rangle\right|^{2}$ 

Same example A=N<sup>2</sup>

inner product  $\Psi(n,t)^*$  and  $\varphi_a(n)$  2

Say before measuring

$$|\Psi\rangle = c_1 |\varphi_1\rangle + c_2 |\varphi_2\rangle + c_4 |\varphi_4\rangle$$
$$\sum_m c_m^* c_m = 1$$

<u>Probability</u> for measurement outcome 16 is  $\left|\left\langle \Psi \middle| \varphi_4 \right\rangle\right|^2$ 

$$\left|\left\langle \Psi\left|\varphi_{4}\right\rangle\right|^{2}=\left|c_{1}^{*}\left\langle\varphi_{1}\left|\varphi_{4}\right\rangle\right|^{2}+\left|c_{2}^{*}\left\langle\varphi_{2}\left|\varphi_{4}\right\rangle\right|^{2}+\left|c_{4}^{*}\left\langle\varphi_{4}\left|\varphi_{4}\right\rangle\right|^{2}=\left|c_{4}\right|^{2}$$

To determine the  $c_m$  for an arbitrary  $\Psi(m)$ :  $c_m = \langle \varphi_m | \Psi \rangle$ 

 $\Rightarrow$  Spectral decomposition

Postulate 5 – continuous case (little attention for it in the book) The probability density for measurement outcome a is  $|\int \Psi(x,t)^* \phi_a(x) dx|^2$ inner product  $\Psi(x,t)^*$  and  $\phi_a(x)$ <sup>2</sup>

The probability for a measurement outcome between  $a_1$  and  $a_2$  is:

$$\int_{a_1}^{a_2} \left| \int_{-\infty}^{\infty} \Psi(x,t)^* \varphi_a(x) dx \right|^2 da$$

See also problem W4.1 in week 4 for an exercise on this with a concrete example

(drawings of wave functions were made on the blackboard to graphically explain the integrals)

#### 61

The calculation of the probabilities in the previous slide with  $P_a = |\langle \varphi_a | \Psi \rangle|^2$  is more general that how it was presented earlier in the course.

You can now also make a calculation for the case where you describe your states in a certain basis, while both  $|\Psi\rangle$  and the eigenfunctions  $|\varphi_a\rangle$  are not aligned with those basis states. The following simple case (for a system that can be described as a superposition of two states only) was done on the blackboard in week 4. Here  $\hat{A}$  and  $\hat{B}$  are observables with two orthonormal eigenstates.

$$\begin{cases} \hat{A}|\varphi_1\rangle = a_1|\varphi_1\rangle & \left\{ \hat{B}|\chi_1\rangle = b_1|\chi_1\rangle & \left\langle \varphi_1|\varphi_1\rangle = 1, \quad \left\langle \varphi_1|\varphi_2\rangle = 0, \quad etc. \\ \hat{A}|\varphi_2\rangle = a_2|\varphi_2\rangle & \left\{ \hat{B}|\chi_2\rangle = b_2|\chi_2\rangle \end{cases} \end{cases}$$

 $|\Psi\rangle = \alpha |\varphi_1\rangle + \beta |\varphi_2\rangle$ 

Measure 
$$\hat{A}$$
, then (for example)  
 $P(a_1) = |\langle \varphi_1 | \Psi \rangle|^2 = |\alpha|^2$ 



Measure 
$$\hat{B}$$
, while you also know 
$$\begin{cases} |\chi_1\rangle = \delta |\varphi_1\rangle + \varepsilon |\varphi_2\rangle \\ |\chi_2\rangle = \varepsilon |\varphi_1\rangle - \delta |\varphi_2\rangle \end{cases}$$

then (for example)  $P(b_1) = |\langle \chi_1 | \Psi \rangle|^2$   $= | \left( \delta^* \langle \varphi_1 | + \varepsilon^* \langle \varphi_2 | \right) \left( \alpha | \varphi_1 \rangle + \beta | \varphi_2 \rangle \right) |^2$   $= | \delta^* \alpha + \varepsilon^* \beta |^2$ 

# Schrödinger's cat paradox

(Erwin Schrödinger, 1935, details done on the board)



"HONESTLY, ERWIN. CAN'T YOU JUST FLIP A COIN?"

#### Postulate 4 and 5 are about measurements – a few remarks:

Good model for thinking about what the effects are when doing a measurement in the following extreme limit (ideal measurement):

- measurements with a very strong interaction between the meter and the quantum system.
- The measurement only takes a very short time.
- There is no interaction with the meter before and after the measurement.

The language used for this case are "*reduction*" or "*collapse*" of the wave function.

In practice, measurements do not always work like this!

The postulates, with the probabilistic interpretation of the wave function and the simple rules for measurement on the previous slides, form the most widely used interpretation of quantum mechanics, and is called the <u>Copenhagen interpretation</u>.

# **Time evolution and measurement**



# **Summary:**

- 1. Postulates
- 2. Operators
- 3. Everything, for example De Broglie

and 
$$\hbar\omega = E_n - E_m$$
 ,

can be derived from the postulates.

# Homework for week 3 of the course

 Study:
 Chapters 2 and 3,

 emphasis on sections 2.4, 3.1, 3.2, 3.6

 and Eqs. [2.111]-[2.113] (Dirac delta function in Sec. 2.5, )

 (2.1, 2.2, 2.3 was last week)

See http://www.quantumdevices.nl/teaching/

**Problems:** 

To be made <u>before</u> the tutorial session Chapter 2 - 2.18, 2.19, and 2.21 Chapter 3 - 3.1, 3.3, and 3.22