## VU Quantum Computing

WS 2023/24

Hans Tompits

Institut für Logic and Computation Forschungsbereich Wissensbasierte Systeme

www.kr.tuwien.ac.at

# §2 Principles of Quantum Mechanics

2.1 Brief History of Quantum Mechanics

### Max Planck

- ➤ The origin of quantum mechanics lies in the year 1900.
- ➤ Max Planck proposed an interpolation formula to fill the discrepancy between the Rayleigh-Jeans law and the Wien approximation of the spectral radiance of the electromagnetic radiation of a black body as a function of the wavelength at a given temperature.

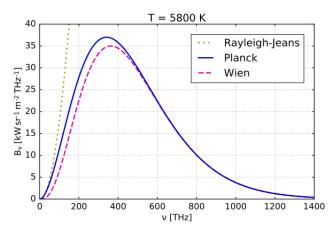


Max Planck (1901)

# Max Planck (ctd.)

- ➤ The Rayleigh-Jeans law agrees with experimental results at large wavelengths (low frequencies) but disagrees at short wavelengths (high frequencies).
  - This inconsistency between observations and the predictions of classical physics is referred to as the *ultraviolet catastrophe*.
- ➤ The Wien law describes accurately the short wavelength (high frequency) spectrum of thermal emission from objects, but it fails to accurately describe the experimental observations for long wavelengths (low frequency) emission.

## Max Planck (ctd.)



Rayleigh-Jeans law vs. Wien approximation and Planck's law, for a body of 5800K.

### From Planck to Bohr

- Planck's interpolation formula can be derived from the assumption (the "quantum hypothesis") that energy states can only be multiples of  $h\nu$ , where h is Planck's constant (h = "Hilfsgröße") and  $\nu$  is the frequency.
- ➤ In 1905, on the basis of the quantum hypothesis, Albert Einstein was able to describe the photoelectric effect (by which is understood the emission of electrons when light shines on a material).
  - Einstein was awarded the Nobel Prize in 1921 for this work.

6. Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt; von A. Einstein.

Zwischen den theoretischen Vorstellungen, welche sich die Physiker über die Gise und andere ponderable Köprer gebildet haben, und der Maxwellschen Theorie der elektromagnetischen Prozesse im togenannten leeren Raume besteht ein teigereidere formaler Unterschied. Während wir uns nämlich den Zustand eines Körpers durch die Lagen und Geschwindigkeiten einer swar sehr großen, jedoch endlichen Anzahl von Atonen und Elektronen für vollkommen bestimmt ansehen, bedienen wir uns zur Bestimmung des elektromagnetischen Zustandes eines Raumes kontinuierlicher räumlicher Funktionen, so daß alto eine endliche Anzahl von Größen nicht als genügend anzusehen ist zur vollständigen Festlegung des elektromagnenstiehen Zustandes eines Raumes. Nach der

Beginning part of Einstein's 1905 paper (the paper has 17 pages).

# From Planck to Bohr (ctd.)

- ▶ In 1912, Niels Bohr proposed a model of the atom which is founded on the assumption that the angular momentum of electrons can only be integer multiples of  $\hbar = \frac{h}{2\pi}$ .
  - Until 1923, Bohr's theory was developed into the so-called "old quantum mechanics", which was, however, rather ad hoc and unsatisfying from a theoretical point of view.
  - Bohr was awarded the Nobel Prize in 1922 for his contributions to the understanding of the structure of atoms.



Niels Bohr in 1922.

### Heisenberg and de Broglie

- By 1925, Louis de Broglie proposed the wave properties of matter and Werner Heisenberg developed the so-called "matrix mechanics".
  - de Broglie was awarded in 1929 the Nobel Prize for his wave mechanics and Heisenberg was awarded it in 1932 for his development of quantum mechanics.





Heisenberg in 1933 (left) and de Broglie (right).

### Erwin Schrödinger

➤ In 1926, Erwin Schrödinger introduced his "wave mechanics" and showed it to be equivalent to the matrix mechanics of Heisenberg.

He received the Nobel Prize in 1933 (together with Paul Dirac).



Schrödinger in 1933.

## Erwin Schrödinger (ctd.)



Old Austrian Schilling bill with Schrödinger and his wave function  $\psi$  on the front side and the University of Vienna on the back side.

## Wolfgang Pauli and John von Neumann

- ➤ In 1927, Wolfgang Pauli developed the formal theory of the electron spin (he was awarded the Nobel Prize in 1945).
- ➤ The modern form of quantum mechanics, based on the Hilbert-space formalism, was first presented in comprehensive form by John von Neumann in his book "Die mathematischen Grundlagen der Quantenmechanik" in 1932 (he was 29 then).





Pauli in 1945 (left) and von Neumann in 1932 (right).

### 2.2 Mathematical Foundations

2.2.1 Vector Spaces

## Complex Numbers

#### Notation:

- ➤ N = set of natural numbers;
- $ightharpoonup \mathbb{R}$  = set of real numbers.

#### Definition

A *complex number* is an expression of form z = x + iy, where  $x, y \in \mathbb{R}$  and  $i = \sqrt{-1}$ .

- $\triangleright$  x is the *real part* of z, denoted by Re(z);
- $\triangleright$  y is the *imaginary part* of z, denoted by Im(z);
- ➤ *i* is the *indeterminate*, or, as referred to by Descartes, *imaginary number*.

#### It holds:

- $ightharpoonup z_1=z_2\Leftrightarrow Re(z_1)=Re(z_2) ext{ and } Im(z_1)=Im(z_2).$
- ightharpoonup The complex number z = x + iy corresponds to the tuple (x, y).

# Complex Numbers (ctd.)

> Addition and multiplication of complex numbers:

$$(x_1 + iy_1) + (x_2 + iy_2) := (x_1 + x_2) + i(y_1 + y_2)$$
  
 $(x_1 + iy_1) \cdot (x_2 + iy_2) := (x_1x_2 - y_1y_2) + i(x_1y_2 + x_2y_1)$ 

- ➤ The set of all complex numbers is denoted by C.
- $\blacktriangleright$  ( $\mathbb{C},+,\cdot$ ) forms a *field*.

### Complex-Valued Functions

- Similarly to real-valued functions, one can define functions of form f : C → C.
  - The area of mathematics which deals with the study of such functions is called *complex analysis* ("Funktionentheorie" in German).
- ▶ Important for our purposes are complex-valued generalisations of the functions sine, cosine, and the exponential function, defined as follows (for  $z \in \mathbb{C}$ ):

$$\sin(z) := \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n+1}}{(2n+1)!}$$

$$\cos(z) := \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n}}{(2n)!}$$

$$e^z := \sum_{n=0}^{\infty} \frac{z^n}{n!}$$

# Complex-Valued Functions (ctd.)

### Properties:

- 1.  $e^{iz} = cos(z) + i sin(z)$   $\forall z \in \mathbb{C}$ ; ("Euler's formula")
- 2.  $e^{z_1+z_2}=e^{z_1}\cdot e^{z_2} \quad \forall z_1,z_2\in\mathbb{C};$
- 3.  $e^{z+2\pi i}=e^z \quad \forall z\in\mathbb{C}$ , i.e.,  $e^z$  is periodic with period  $2\pi i$ .

#### Definition

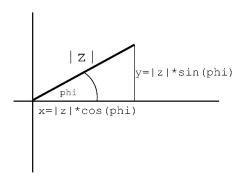
- 1. For z = x + iy, we call  $\overline{z} := x iy$  the *complex conjungate* number.
- 2. The absolute value of z = x + iy is given by

$$|z| = \sqrt{x^2 + y^2} = \sqrt{z \cdot \overline{z}}.$$

### Polar Representation

Every complex number z = x + iy can be represented in the following manner:

$$z = |z| \cdot e^{i\varphi}$$
 (polar representation)



### Vector Spaces

**Definition**: Let  $K = \mathbb{R}$  or  $\mathbb{C}$ . A set V is called *vector space over* K if operations

- $\triangleright$  + :  $V \times V \rightarrow V$  (vector addition) and
- $\triangleright$  :  $K \times V \rightarrow V$  (scalar multiplication)

are defined, which satisfy the following properties  $(\forall x, y, z \in V; \forall \lambda, \mu \in K)$ :

- 1. x + y = y + x; ("commutativity")
- 2. x + (y + z) = (x + y) + z; ("associativity")
- 3. there is a *neutral element* 0 ("zero vector") such that x + 0 = x;
- 4. for all x, there is an *inverse element* (-x) such that x + (-x) = 0;
- 5.  $1 \cdot x = x$ :
- 6.  $\lambda \cdot (\mu \cdot x) = (\lambda \cdot \mu) \cdot x$ ;
- 7.  $(\lambda + \mu) \cdot x = \lambda \cdot x + \mu \cdot x$ ;
- 8.  $\lambda \cdot (x + y) = \lambda \cdot x + \lambda \cdot y$ .

## **Examples**

1. Let  $K = \mathbb{R}$  or  $\mathbb{C}$ . The set

$$K^n := \left\{ \left( \begin{array}{c} x_1 \\ \vdots \\ x_n \end{array} \right) \middle| x_i \in K \right\}$$

is a vector space over K in view of the following operations:

$$\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} := \begin{pmatrix} x_1 + y_1 \\ \vdots \\ x_n + y_n \end{pmatrix};$$

$$\lambda \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} := \begin{pmatrix} \lambda \cdot x_1 \\ \vdots \\ \lambda \cdot x_n \end{pmatrix}, \quad \lambda \in K$$

## Examples (ctd.)

2. For  $a, b \in \mathbb{R}$ , let

$$L^{2}[a,b]:=\left\{f\left|f:[a,b]\to\mathbb{C},\int_{a}^{b}\left|f(x)\right|^{2}dx<\infty\right.\right\}$$

where (i) the integral is understood in the sense of *Lebesgue* (the Lebesgue integral is a generalisation of the Riemann integral) and (ii) functions which agree almost everywhere are identified.

- Two functions agree *almost everywhere* iff the set they disagree on has measure zero, i.e.,
  - it can be covered by a finite or denumerable sequence of intervals whose total length is arbitrarily small.
  - The set  $L^2[a, b]$  is called the space of *square-integrable* functions over [a, b].
  - It is a vector space over  $\mathbb{C}$  in view of the following operations:

$$(f+g)(x) := f(x) + g(x) \quad \forall x \in [a,b];$$

$$(\lambda \cdot f)(x) := \lambda \cdot f(x) \quad \forall x \in [a,b], \forall \lambda \in \mathbb{C}.$$

### Norms

#### Definition

Let V be a vector space over  $K = \mathbb{R}$  or  $\mathbb{C}$ . A *norm* is a function

$$\|\cdot\|:V\to\mathbb{R}$$

satisfying the following properties:

$$\begin{array}{lll} (\textit{N}_1) & \|x\| \geq 0, \text{ and } \|x\| = 0 \Leftrightarrow x = 0 & \forall x \in \textit{V} \\ (\textit{N}_2) & \|\lambda \cdot x\| = |\lambda| \cdot \|x\| & \forall \lambda \in \textit{K}, \forall x \in \textit{V} \\ (\textit{N}_3) & \|x + y\| \leq \|x\| + \|y\| & \forall x, y \in \textit{V} & \text{("triangle inequality")} \\ \end{array}$$

A vector space is *normed* if a norm is defined on V.

### Banach Spaces

#### Definition

Let V be a normed vector space over  $K = \mathbb{R}$  or  $\mathbb{C}$  with norm  $\|\cdot\|$  and  $(x_n)_{n\geq 0}$  a sequence of elements  $x_n\in V, \forall n\geq 0$ .

- 1.  $(x_n)_{n\geq 0}$  is a Cauchy sequence if
  - $\forall \varepsilon > 0 \ \exists N > 0 \ \text{such that} \ \forall m, n > N, \ \|x_m x_n\| < \varepsilon.$
- 2.  $(x_n)_{n\geq 0}$  is *convergent* if there is a  $x\in V$  such that

$$\forall \varepsilon > 0 \; \exists N > 0 \; \text{and} \; \forall n > N \; \text{it holds that} \; ||x_n - x|| < \varepsilon.$$

The element x is called the *limit* of  $(x_n)_{n\geq 0}$ .

3. A series  $\sum_{n\geq 0} x_n$  is convergent if the sequence  $\left(\sum_{n=0}^k x_n\right)_{k\geq 0}$  of its partial sums is convergent.

# Banach Spaces (ctd.)

#### Note:

➤ Every convergent sequence is a Cauchy sequence but not vice versa!

#### Definition

- ➤ A normed vector space is *complete* if every Cauchy sequence converges.
- ➤ Such a vector space is called a *Banach space* (after the Polish mathematician Stefan Banach [1892–1945]).
- In what follows, we only consider vector spaces over  $\mathbb{C}$ .

### Inner Product

#### Definition

Let V be a vector space over  $\mathbb{C}$ . A function  $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C}$  is an *inner product* if the following conditions hold  $(\forall \lambda, \mu \in \mathbb{C}, \forall x, y \in V)$ :

$$\begin{array}{ll} (I_1) & \langle x, \lambda y + \mu z \rangle = \lambda \, \langle x, y \rangle + \mu \, \langle x, z \rangle; \\ (I_2) & \langle x, y \rangle = \overline{\langle y, x \rangle}; \\ (I_3) & \langle x, x \rangle \geq 0, \text{ and } \langle x, x \rangle = 0 \Leftrightarrow x = 0. \end{array}$$

#### Remarks:

 $\triangleright$  ( $I_1$ ) and ( $I_2$ ) imply the following property:

- This definition of the inner product is the one as standard in physics
  - in mathematics, it is often defined as linear in the first argument and semilinear in the second.

An inner product defines canonically a norm as follows:

$$||x|| := \sqrt{\langle x, x \rangle}.$$

### Hilbert Space

#### Definition

A vector space with an inner product  $\langle \cdot, \cdot \rangle$  which is with the induced norm  $\|x\| = \sqrt{\langle x, x \rangle}$  complete is a *Hilbert space*.

### Examples:

1.  $\mathbb{C}^n$  with the inner product  $\langle x,y\rangle:=\sum_{i=1}^n \overline{x_i}\cdot y_i$  for

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \qquad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

is a Hilbert space.

$$\Rightarrow \|x\| = \sqrt{\langle x, x \rangle} = \sqrt{\sum_{i=1}^{n} |x_i|^2}$$
 ("Euclidian norm")

2.  $L^2[a,b]$  with  $\langle f,g\rangle:=\int_a^b\overline{f(x)}g(x)dx$  is a Hilbert space.

### Orthonormal Basis

- 1. An element  $x \in V$  of a normed vector space (V, ||.||) is *normed* or a *unit vector*, if ||x|| = 1.
- 2. A finite or denumberable sequence  $(e_n)$  of elements of a vector space V with inner product  $\langle \cdot, \cdot \rangle$  is an *orthonormal system* if:

$$\langle e_i, e_j \rangle = \left\{ egin{array}{ll} 1 & \quad ext{if } i = j; \\ 0 & \quad ext{otherwise} \end{array} \right.$$

3. An orthonormal system  $(e_n)$  is an *orthonormal basis* (or simply a *basis*) of a Hilbert space  $(V, \|.\|)$  if

$$x = \sum_{n} \lambda_n e_n$$

for each  $x \in V$ , where  $\lambda_n \in \mathbb{C}$ .

- The convergence of this series is in the sense of the Hilbert-space norm!
- It holds that if  $(e_n)$  is a basis and  $x = \sum_n \lambda_n e_n$ , then  $\lambda_n = \langle e_n, x \rangle$ , i.e.,  $x = \sum_n \langle e_n, x \rangle e_n$ .

### Examples

- 1. The sequence  $e_1 = (1, 0, 0, \dots, 0)$ ,  $e_2 = (0, 1, 0, \dots, 0)$ ,...,  $e_n = (0, 0, 0, \dots, 1)$  is a basis for  $\mathbb{C}^n$ .
- 2. In the Hilbert space  $L^2[-\pi,\pi]$  with  $\langle f,g\rangle:=\int_{-\pi}^{\pi}\overline{f(x)}g(x)dx$ , the sequence  $(\frac{1}{\sqrt{2\pi}}e^{inx})_{n=-\infty}^{\infty}$  is a basis.
  - ▶ For each  $f \in L^2[-\pi, \pi]$  we have:

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \lambda_n e^{inx}, \quad x \in [-\pi, \pi]$$

where

$$\lambda_n = \langle e_n, f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-inx} f(x) dx.$$

The series  $\frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \lambda_n e^{inx}$  is generally referred to as a *Fourier series*, and the  $\lambda_n$  are the *Fourier coefficients*.

2.2.2 Linear Operators

### **Linear Operators**

#### Definition

Let V, W be vector spaces. A mapping  $T: V \to W$  is a *linear operator* if:

$$T(\lambda x + \mu y) = \lambda T(x) + \mu T(y)$$
  $\forall \lambda, \mu \in \mathbb{C}, \forall x, y \in V.$ 

For operators, usually one writes Tx for T(x).

## Examples

1.  $T: \mathbb{C}^n \to \mathbb{C}^m$  defined by

$$\begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} \mapsto T \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} := \begin{pmatrix} \sum_{j=1}^n a_{1j} z_j \\ \vdots \\ \sum_{j=1}^n a_{mj} z_j \end{pmatrix} \qquad (a_{ij} \in \mathbb{C})$$

is a linear operator.

We write

$$\begin{pmatrix} \sum_{j=1}^{n} a_{1j} z_{j} \\ \vdots \\ \sum_{j=1}^{n} a_{mj} z_{j} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix} \begin{pmatrix} z_{1} \\ \vdots \\ z_{n} \end{pmatrix}$$

and call  $A = (a_{ij})$  an  $m \times n$ -matrix.

2. Let V be a vector space. The operator  $I: V \to V$  defined by I(x) = x,  $\forall x \in V$ , is clearly linear and is called *identity operator*.

### Classes of Operators

We distinguish the following sorts of operators:

#### Definition

Let  $T: V \to V$  be a linear operator.

1. The operator  $T^*: V \to V$ , defined by the condition

$$\langle x, Ty \rangle = \langle T^*x, y \rangle \quad \forall x, y \in V$$

is called adjoined.

- 2. *T* is *hermitian*, or *self adjoined*, if  $T = T^*$  (i.e., if  $Tx = T^*x$ ,  $\forall x \in V$ , holds).
- 3. T is *unitary*, if  $TT^* = T^*T = I$  (i.e., if  $TT^*x = T^*Tx = x$ ,  $\forall x \in V$ , holds).
- 4. T is an orthogonal projection (or simply projection), if T is self adjoined and  $T = T^2$  holds.

### Remark

For unitary operators it holds that  $T^* = T^{-1}$  and furthermore  $\langle x, y \rangle = \langle Ix, y \rangle = \langle T^* Tx, y \rangle = \langle Tx, Ty \rangle$ .

▶ I.e., unitary operators preserve the inner product.

## Examples

- 1. Let  $V = \mathbb{C}^n$  and T a linear operator on V, defined in terms of an  $n \times n$ -matrix  $A = (a_{ij})$ .
  - The operator  $T^*$  adjoined to T is obtained as follows:
    - For each  $n \times n$ -matrix  $B = (b_{ij})$ , the transposed matrix  $B^T = (b_{ji})$  is that which is obtained by exchanging rows with columns of B.
    - Moreover, let  $\overline{B} = (\overline{b_{ij}})$  be the result of replacing all elements of B by their complex conjugate ones.
    - $\rightarrow$   $T^*$  is given in terms of the matrix  $A^* = (\overline{A})^T = (\overline{a_{ii}})$ .
  - For instance, for

$$A = \left(\begin{array}{cc} 1+3i & 2i \\ 1+i & 1-4i \end{array}\right)$$

we have

$$A^* = \left(\begin{array}{cc} 1 - 3i & 1 - i \\ -2i & 1 + 4i \end{array}\right).$$

# Examples (ctd.)

2. The operator  $T: \mathbb{C}^2 \to \mathbb{C}^2$ , given by the matrix

$$A = \left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right)$$

is a projection.

• In particular, *T* corresponds to the projection to the first component:

$$T\left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) = \left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right) \left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) = \left(\begin{array}{c} x_1 \\ 0 \end{array}\right).$$

### Eigenvectors

**Definition:** Let  $T: V \to V$  be a linear operator on V.

- ▶ An element x in V is an eigenvector of T if  $x \neq 0$  and there is some  $\lambda \in \mathbb{C}$  such that  $Tx = \lambda x$ .
- $\triangleright \lambda$  is called *eigenvalue* to the eigenvector x.

### Important Properies

- 1. Eigenvalues of self-adjoined operators are always real valued.
- 2. Unitary operators are *isometric*, i.e., for all unitary operators  $T: V \rightarrow V$  it holds that

$$||Tx|| = ||x||, \quad \forall x \in V.$$

- Eigenvalues of a unitary operator T are *unimodular*, i.e., it holds that  $|\lambda| = 1$ , for every eigenvalue  $\lambda$  of T.
- 3. Projection operators always have eigenvalue 0 or 1.
- 4. For each self-adjoined operator T one can define an operator of form  $e^{i\lambda T}$  ( $\lambda \geq 0$ ).
  - It holds:  $e^{i\lambda T}$  is unitary and  $(e^{i\lambda T})^* = e^{-i\lambda T}$ .
  - One can show:
    - The function  $\Psi(t) := e^{itT}(\psi_0)$  satisfies the differential equation

$$\frac{d}{dt}\Psi(t)=iT\Psi(t),$$

together with the initial condition  $\Psi(0) = \psi_0$ .

## Important Properies (ctd.)

Moreover, for a self-adjoined operator T, the following properties can be shown (given certain technical provisos which are assumed in our setting):

- 1. The set of the eigenvectors associated with the different eigenvalues of  ${\cal T}$  yield an orthonormal basis.
- 2. T has a spectral representation of form  $T = \sum_{i>0} \lambda_i P_i$ , where
  - the  $\lambda_i$  are the (real valued) eigenvalues of T and the  $P_i$  are orthogonal projections.
  - Note that the convergence of these series is in the sense of the Hilbert-space norm, i.e., it holds that  $\left\| \mathit{Tx} \sum_{i=0}^k \lambda_i P_i x \right\| \to 0$  for  $k \to \infty$ , for all x.
- 3.  $e^{i\lambda T}$  can be represented as series:

$$e^{i\lambda T} = \sum_{n>0} \frac{(i\lambda T)^n}{n!}.$$

### Tensor Product

**Definition:** Let  $A = (a_{ij})$  be an  $m \times n$ -matrix and  $B = (b_{kl})$  a  $p \times q$ -matrix. Then, the *tensor product*,  $A \otimes B$ , is the following  $m \cdot p \times n \cdot q$ -matrix:

$$\begin{pmatrix}
a_{11}B & a_{12}B & \dots & a_{1n}B \\
\vdots & \vdots & \vdots & \vdots \\
a_{m1}B & a_{m2}B & \dots & a_{mn}B
\end{pmatrix}$$

$$m \cdot p \text{ rows}$$

$$n \cdot q \text{ columns}$$

where the expressions  $a_{ij}B$  stand for

$$a_{ij}b_{11}$$
 ...  $a_{ij}b_{1q}$   
 $\vdots$   $\vdots$   $\vdots$   
 $a_{ij}b_{p1}$  ...  $a_{ij}b_{pq}$ .

## Tensor Product (ctd.)

For the case m=n=p=q=2,  $A\otimes B$  looks therefore as follows:

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}.$$

➤ Since vectors in  $\mathbb{C}^n$  can be seen as  $n \times 1$ -matrices, we have, e.g., that:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \otimes \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} x_1 y_1 \\ x_1 y_2 \\ x_2 y_1 \\ x_2 y_2 \end{pmatrix}.$$

Accordingly, we can define the tensor product  $V \otimes W$  of two vector spaces V, W, which is "spanned" by tensors  $v \otimes w$ , where  $v \in V$ ,  $w \in W$ .

### Bra- and Ket-Notation

- ➤ In physics, following Paul Dirac, the so-called *bra* and *ket-notation* ("bra-ket") for vectors is customary (the name "bra" and "ket" is derived from "bracket").
- The basic idea of this notation is that the inner product  $\langle x,y\rangle$  of two vectors x,y can be seen as the application of the "bra-vector"  $\langle x|$  to the "ket-vector"  $|y\rangle$ , i.e., one writes  $\langle x|y\rangle$  for  $\langle x,y\rangle$ .
  - Accordingly, for an operator T, one thus writes  $\langle x|T|y\rangle$  for  $\langle x,Ty\rangle$ .
- ➤ Ket-vectors correspond to the usual vectors, whilst bra-vectors are seen as elements of a "dual space".
  - For finite dimensional spaces it holds that

$$|x\rangle = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$
 and  $\langle x| = (\overline{x_1}, \dots, \overline{x_n}).$ 

### Bra- and Ket-Notation (ctd.)

➤ One can define the *outer product*  $|x\rangle\langle y|$  between a ket-vector  $|x\rangle$  and a bra-vector  $\langle y|$  as a linear operator as follows:

$$(|x\rangle\langle y|)(|z\rangle) := \langle y|z\rangle|x\rangle, \quad \forall z.$$

➤ E.g., for an orthonormal basis  $(|e_i\rangle)_{i>0}$ , we obtain:

$$|x\rangle = \sum_{i>0} \lambda_i |e_i\rangle = \sum_{i>0} \langle e_i | x \rangle |e_i\rangle = \sum_{i>0} (|e_i\rangle \langle e_i|) (|x\rangle).$$

 $\blacktriangleright$  It must hold that  $I = \sum_{i>0} |e_i\rangle \langle e_i|$  ("completeness relation").

**N.B.**:  $P_i := |e_i\rangle \langle e_i|$  represents the projection to  $|e_i\rangle$ .