# 2. Introduction to quantum mechanics

## 2.1 Linear algebra

## **Dirac notation**

Complex conjugate	$z^*$
Vector/ket	$ \psi angle$
Dual vector/bra	$ \langle arphi $
Inner product/bracket	$\langle arphi   \psi  angle$
Tensor product	$ \varphi\rangle\otimes \psi\rangle\equiv \varphi\rangle \psi\rangle$
Complex conj. matrix	$A^*$
Transpose of matrix	$A^T$
Hermitian conj/ adjoint of matrix	$A^{\dagger} = (A^T)^*$
Inner product	$\langle \varphi   A   \psi \rangle$

## Basis, vector representation

For a set of vectors  $|v_1\rangle,...,|v_n\rangle$  spanning  $\mathbf{C}^n$ 

$$|v\rangle = \sum_{i} a_{i} |v_{i}\rangle \equiv \begin{bmatrix} a_{1} \\ a_{2} \\ \vdots \\ a_{n} \end{bmatrix}$$

The set  $|v_1\rangle,...,|v_n\rangle$  constitutes a *basis* for  $\mathbb{C}^n$ 

## Linear operators

A linear operator A means

$$A\left(\sum_{i} a_{i}|v_{i}\rangle\right) = \sum_{i} a_{i}A(|v_{i}\rangle)$$

**Notation** 

$$A|v\rangle \equiv A(|v\rangle)$$
  $BA|v\rangle \equiv B(A(|v\rangle))$ 

## Matrix representation

For  $|v_1\rangle,...,|v_n\rangle$  spanning  ${f C}^n$  ,  $|w_1\rangle,...,|w_m\rangle$  spanning  ${f C}^m$  ,

a *matrix representation* of  $A: \mathbf{C}^n \to \mathbf{C}^m$  means

$$A|v_j\rangle = \sum_i A_{ij}|w_i\rangle$$

Numbers  $A_{ij}$  form matrix  $A \Rightarrow$ 

Linear operator (basis given) ⇔ matrix representation (to be used interchangeably...)

#### Pauli matrices

$$\sigma_0 \equiv I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
  $\sigma_1 \equiv \sigma_x \equiv X \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ 

$$\sigma_2 \equiv \sigma_y \equiv Y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
  $\sigma_3 \equiv \sigma_z \equiv Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ 

#### Inner vector product

A inner product on  $\mathbb{C}^n$  is

$$((a_1,...,a_n),(b_1,...,b_n)) = \sum_{i=1}^n a_i^* b_i$$

We use notation

$$\langle w|v\rangle \equiv (|w\rangle, |v\rangle)$$

*Hilbert space* = inner product space

The vectors  $|v\rangle, |w\rangle$  are *orthogonal* if

$$\langle w|v\rangle = 0$$

The *norm* of a vector is

$$|||v\rangle|| = \sqrt{\langle v|v\rangle}$$

An *orthonormal set* of vectors  $|i\rangle$  obey

$$\langle j|i\rangle = \delta_{ij}$$

#### **Vector representation**

With respect to an orthonormal basis  $|i\rangle$  for  ${f C}^n$ 

$$|v\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \qquad |w\rangle = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

the inner product is

$$\langle w|v\rangle = [b_1^*, b_2^*, ...., b_n^*] \begin{bmatrix} a_1 \\ a_2 \\ ... \\ a_n \end{bmatrix}$$

We thus have

$$\langle w | = \sum_{i} b_{i}^{*} \langle i | \equiv [b_{1}^{*}, b_{2}^{*}, .., b_{n}^{*}]$$

(an orthonormal basis will be used unless otherwise stated)

## Outer vector product

The *outer product* 

$$|\varphi\rangle\langle\psi|$$

is a linear operator

$$|\varphi\rangle\langle\psi|\left(|\psi'\rangle\right) = |\varphi\rangle\langle\psi|\psi'\rangle = \langle\psi|\psi'\rangle|\varphi\rangle$$

### Cauchy-Schwartz inequality

For two vectors  $|v\rangle, |w\rangle$ 

$$\langle v|v\rangle\langle w|w\rangle \ge |\langle v|w\rangle|^2$$

## Completeness relation

For vectors  $|i\rangle$  forming an orthonormal basis  $\langle j|i\rangle=\delta_{ij}$  for  ${\bf C}^n$ 

$$\sum_{i=1}^{n} |i\rangle\langle i| = I$$

### Eigenvectors and eigenvalues

The *eigenvector*  $|v\rangle$  to A obeys

$$A|v\rangle = v|v\rangle$$

with v the eigenvalue.

The *diagonal representation* of A is (for diagonalizable A)

$$A = \sum_{i} \lambda_{i} |i\rangle\langle i|$$

in terms of eigenvalues  $\lambda_i$  and orthonormal eigenvectors |i
angle of A

## Hermitian operators

The *Hermitian conjugate*/adjoint of A is  $A^{\dagger}$ 

We have 
$$(AB)^\dagger=B^\dagger A^\dagger$$
 and  $|v\rangle^\dagger=\langle v|$ ,  $(|v\rangle\langle w|)^\dagger=|w\rangle\langle v|$ 

An Hermitian operator obeys

$$A^{\dagger} = A$$

### Projection operator

The operator

$$P = \sum_{i=1}^{m} |i\rangle\langle i|$$

is a *projection* operator  $P: \mathbb{C}^n \to \mathbb{C}^m, \ m < n$ 

**Properties** 

$$P^2 = P$$
  $P^{\dagger} = P$ 

Orthogonal complement Q = I - P

### Normal operator

An operator A is *normal* if

$$A^{\dagger}A = AA^{\dagger}$$

An operator is normal if and only if it is diagonalizable. An Hermitian operator is normal.

### **Unitary matrix**

A matrix/operator U is *unitary* if

$$U^{\dagger}U = UU^{\dagger} = I$$

### Positive operator

An operator A is *positive* if

$$\langle v|A|v\rangle \ge 0$$

and real for any vector  $|v\rangle$  .

Any positive operator is Hermitian ⇒
Any positive operator has real, positive eigenvalues and a *spectral decomposition* 

$$A = \sum_{i} \lambda_{i} |i\rangle\langle i|$$

in terms of eigenvalues  $\;\lambda_i$  and orthonormal eigenvectors  $\;|i
angle\;$  of  $\;A$ 

### Tensor product

A *tensor product* between vectors  $|v\rangle, |w\rangle$  in  $\mathbb{C}^n, \mathbb{C}^m$ 

$$|v\rangle \otimes |w\rangle \equiv |v\rangle |w\rangle \equiv |vw\rangle$$

is a vector in  $\mathbf{C}^{n \times m}$ 

#### **Example:**

$$\left[\begin{array}{c} v_1 \\ v_2 \end{array}\right] \otimes \left[\begin{array}{c} w_1 \\ w_2 \end{array}\right] = \left[\begin{array}{c} v_1 w_1 \\ v_1 w_2 \\ v_2 w_1 \\ v_2 w_2 \end{array}\right]$$

A tensor product between operators/matrices A, B is denoted

$$A \otimes B$$

Operation

$$A \otimes B(|v\rangle \otimes |w\rangle) = A|v\rangle \otimes B|w\rangle$$

## **Properties**

$$(A \otimes B)^{\dagger} = A^{\dagger} \otimes B^{\dagger}$$

#### Matrix representation

## **Example:**

For matrices

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \qquad B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

we have the tensor product

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{bmatrix}$$

$$= \begin{bmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{bmatrix}$$

## **Operator functions**

For a normal operator A, written in the spectral decomposition

$$A = \sum_{a} a |a\rangle\langle a|$$

we define the/operator matrix function

$$f(A) = \sum_{a} f(a)|a\rangle\langle a|$$

#### **Trace**

The *trace* of a matrix A is

$$tr(A) = \sum_{i} A_{ii}$$

Cyclic property

$$tr(ABC) = tr(CAB) = tr(BCA)$$

Outer product formulation

$$tr(A|\psi\rangle\langle\psi|) = \langle\psi|A|\psi\rangle$$

#### Commutators

The *commutator* between two operators/matrices A,B is

$$[A, B] = AB - BA$$

The *anti-commutator* between two operators/matrices A, B is

$$\{A, B\} = AB + BA$$

### Matrix decompositions

*Polar decomposition*: For a linear operator A there exists a unitary operator U and positive operators J,K so that

$$A = UJ = KU$$

Singular value decomposition: For a square matrix A there exists unitary matrices U,V and a diagonal matrix D with non-negative elements (singular values), such that

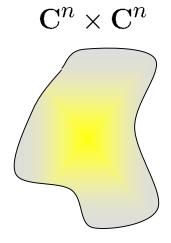
$$A = UDV$$

## 2.2 Postulates of quantum mechanics

### State space

#### Postulate 1:

Associated to any isolated physical system is a Hilbert space, known as the *state space* of the system. The system is completely described by its *state vector*, a unit vector in the state space



#### **Definitions/names**

A two-level,  $\mathit{qubit}$  state  $|\psi\rangle$  can generally be written as

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

This is a *superposition* of the two basis states  $|0\rangle$  and  $|1\rangle$ , with *amplitudes* a and b

The normalization condition gives

$$\langle \psi | \psi \rangle = |a|^2 + |b|^2 = 1$$

#### **Evolution**

#### Postulate 2:

The evolution of a quantum system is described by a *unitary transformation*. That is, the state  $|\psi\rangle$  of the system at time t is related to the state  $|\psi'\rangle$  of the system at time t' by a unitary operator U as

$$|\psi'\rangle = U|\psi\rangle$$

#### Postulate 2':

The evolution of state  $|\psi\rangle$  of a quantum system is described by the Schrödinger equation

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

where  $\mathcal{T}_{l}$  is Plancks constant and H the Hamiltonian, a Hermitian operator.

### **Closed system**

For a closed system the Hamiltonian H is independent on time and the system state  $|\psi(t)\rangle$  is

$$|\psi(t_2)\rangle = \exp\left[\frac{-iH(t_2-t_1)}{\hbar}\right]|\psi(t_1)\rangle = U(t_2,t_1)|\psi(t_1)\rangle$$

where we define the unitary time evolution operator

$$U(t_2, t_1) = \exp\left[\frac{-iH(t_2 - t_1)}{\hbar}\right]$$

The Hamiltonian has the spectral decomposition

$$H = \sum_{E} E|E\rangle\langle E|$$

where  $|E\rangle$  are the *energy eigenstates* and E the *energy*.

#### Effective Hamiltonian for open systems

For many open systems we have an effective time dependent Hamiltonian acting on the system  $\Rightarrow$  The solution to the Schrödinger equation is non-trivial

#### Measurement

#### **Projection measurement postulate**

A projective measurement is described by an observable, M, an Hermitian operator on the state space of the system. The observable has the spectral decomposition

$$M = \sum_{m} m P_m = \sum_{m} m |m\rangle\langle m|$$

 $M=\sum_m m P_m = \sum_m m |m\rangle\langle m|$  The possible outcomes correspond to the eigenvalues  $\ m$  of  $\ M.$ 

Upon measuring the state  $|\psi\rangle$  the probability of getting the result mis given by

$$p(m) = \langle \psi | P_m | \psi \rangle$$

Given that m has occured, the state immediately after the measurement is (wavefunction collapse)

$$rac{P_m|\psi
angle}{\sqrt{p(m)}}$$

#### Average and fluctuations

The *average* measured value (over an ensemble of identical states  $|\psi\rangle$  )

$$\sum_{m} mp(m) = \sum_{m} \langle \psi | P_{m} | \psi \rangle = \langle \psi | \left( \sum_{m} m P_{m} \right) | \psi \rangle = \langle \psi | M | \psi \rangle \equiv \langle M \rangle$$

The magnitude of the quantum *fluctuations* are

$$\langle (\Delta M)^2 \rangle = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2$$

**Derivation:** Heisenbergs uncertainty principle is

$$\Delta(C)\Delta(D) \equiv \sqrt{\langle (\Delta C)^2 \rangle \langle (\Delta D)^2 \rangle} \ge \frac{1}{2} |\langle [C, D] \rangle|$$

#### General measurement

#### Postulate 3:

Quantum measurements are described by a collection  $\{M_m\}$  of measurement operators, acting on the state space of the system. The index m refers to the possible measurement outcomes. Upon measuring the state  $|\psi\rangle$ , the probability of getting the result m is given by

$$p(m) = \langle \psi | M_m^{\dagger} M_m | \psi \rangle$$

and the state after the measurement is

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M_m^{\dagger}M_m|\psi\rangle}}$$

Generally

 $M_m M_{m'} \neq \delta_{mm'} M_m$ 

projection

$$M_m = P_m$$

The measurement operators satisfy the completeness relation

$$\sum_{m} M_{m}^{\dagger} M_{m} = I$$

Probabilities sum to one

$$\sum_{m} p(m) = \sum_{m} \langle \psi | M_{m}^{\dagger} M_{m} | \psi \rangle = 1$$

### Composite systems

#### Postulate 4:

The state space of a composite system is the tensor product of the state spaces of the component systems.

If we have systems numbered 1through n, and system i is prepared in state  $|\psi_i\rangle$ , the state of the total system is

$$|\psi_1\rangle\otimes|\psi_2\rangle\otimes...\otimes|\psi_n\rangle$$

### General measurement and projection II

**Derivation:** Given projection measurements and an *ancilla* system, derive the general measurement principles.

#### POVM measurement

General measurement postulate (post-measurement state not important).

A measurement is described by measurement operators  $\,M_m$  . The probability to get the outcome m is given by

$$p(m) = \langle \psi | M_m^{\dagger} M_m | \psi \rangle$$

We define the positive operator

$$E_m = M_m^{\dagger} M_m$$

which has the properties

$$\sum_{m} E_m = I \qquad p(m) = \langle \psi | E_m | \psi \rangle$$

We call  $E_m$  the *POVM-elements* and the set  $\{E_m\}$  a *POVM.* 

### Distinghuishing quantum states

Given a single copy of one of two non-orthogonal states  $|\psi_1\rangle, |\psi_2\rangle$ , it is not possible to determine which state by any measurement.

**Derivation:** The example with  $\{E_1, E_2, E_3\}$ 

#### **Entanglement of two qubits**

A composite state  $|\psi\rangle$  of two qubits that can not be written as a tensor product of the states  $|a\rangle,|b\rangle$  of the two qubits is *entangled*, that is

$$|\psi\rangle \neq |a\rangle|b\rangle$$

**Derivation:** Show that the Bell state

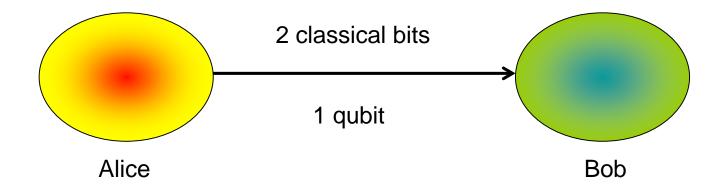
$$|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |11\rangle]$$

is entangled

Entanglement is the "energy" for quantum information processing

## 2.3 Superdense coding

Suppose that Alice wants to send two bits of classical information to Bob by only sending one qubit. Can she do it?



**Derivation:** Superdense coding