# Notes of Quantum Mechanics

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# Preface

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# Contents

# List of Figures

# List of Tables

# Listings

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## Chapter 1

# Mathematical Formalism

## 1.1 Introduction

The formalism of quantum mechanics (QM) involves symbols and methods for denoting and determining the time dependent state of a physical system along with a mathematical structure for evaluating the possible outcomes and associated proabailities of measurements.

**State**

A **state** is evything knowable about the dynamical aspects of a system at a certain time.

A particle has associated a **wavefunction** $\psi(\boldsymbol{r},t)$ whose probability interpretation resides on $|\psi(\boldsymbol{r},t)|^2$: it represents the probabilifty density function which serves a a probability finder in space and time. The probability of finding the particle somewhere in space is thus equal to 1:

$$\int_{\text{all space}} d^3r\ |\psi(\boldsymbol{r},t)|^2 = 1. \tag{1.1}$$

Thus, in order that this integral converges, we must deal with a set of square-integrable functions, called $L^2$. We can only retain the functions $\psi(\boldsymbol{r},t)$ which are everywhere defined, continuous, and infinitely differenciable $C^\infty$. Also, we confine to wavefunctions that have a bounded domain (we can find the particle in a finite region of space).

We list the formal definition of a vector space which is used to define particular vector spaces.

**Vector space**

A **vector space** over a field $F$ (set defined with addition and multiplication) is a non-empty set $V$ together with a *vector addition* and a *scalar multiplication* that satisfies eight axioms. The elements of $V$ are called vectors and the elements of $F$ are caleld scalars.

| | |
|---|---|
| Commutativity of vector addition | $\boldsymbol{u}+\boldsymbol{v}=\boldsymbol{v}+\boldsymbol{u}$ |
| Associativity of vector addition | $(\boldsymbol{u}+\boldsymbol{v})+\boldsymbol{w}=\boldsymbol{u}+(\boldsymbol{v}+\boldsymbol{w})$ |
| Identity element of vector addition | $\exists \boldsymbol{0}, \boldsymbol{v}\in V: \quad \boldsymbol{v}+\boldsymbol{0}=\boldsymbol{v}$ |
| Inverse element of vector addition | $\forall \boldsymbol{v}\in V,\ \exists -\boldsymbol{v}\in V: \quad \boldsymbol{v}+(-\boldsymbol{v})=\boldsymbol{0}$ |
| Associativity of scalar multiplication | $\alpha(\beta\boldsymbol{v})=(\alpha\beta)\boldsymbol{v}$ |
| Distributivity over vector addition | $\alpha(\boldsymbol{u}+\boldsymbol{v})=\alpha\boldsymbol{u}+\alpha\boldsymbol{v}$ |
| Distributivity over scalar addition | $(\alpha+\beta)\boldsymbol{v}=\alpha\boldsymbol{v}+\beta\boldsymbol{v}$ |
| Identity element of scalar multiplication | $\boldsymbol{1v}=\boldsymbol{v}$ |

(1.2)

When the scalar field is the real numbers, the vector space is called a real vector space, when the scalar field is the complex numbers, then is called a complex vector space.

**Vector space $\mathscr{F}$**

The set of wavefunctions $\mathscr{F}\in L^2$ is composed of sufficiently regular functions of $L^2$.

### 1.1.1 Scalar product

With each pair of orderer elements of $\mathscr{F}$, $(\varphi(\boldsymbol{r}),\psi(\boldsymbol{r}))$, we associate a *complex number*:

$$(\varphi,\psi)=\int d^3r\ \varphi^*(\boldsymbol{r})\psi(\boldsymbol{r})\in\mathbb{C}\,. \tag{1.3}$$

Its properties are listed below:

| Adjoint | Linear in the second term | Antilinear in the first term |
|---|---|---|
| $(\varphi,\psi)=(\psi,\varphi)^*$ | $(\varphi,\lambda_1\psi_1+\lambda_2\psi_2)=\lambda_1(\varphi,\psi_1)+\lambda_2(\varphi,\psi_2)$ | $(\lambda_1\varphi_1+\lambda_2\varphi_2,\psi)=\lambda_1^*(\varphi_2,\psi)+\lambda_2^*(\varphi_2,\psi)$ |

If $(\varphi,\psi)=0$, then $\varphi(\boldsymbol{r})$ and $\psi(\boldsymbol{r})$ are said to be **orthogonal**. In addition, the scalar product of a vector with itself return its *norm squared*:

$$\text{Parseval's theorem} \qquad (\varphi,\varphi)=\int d^3r\ |\psi(\boldsymbol{r})|^2\geq 0\in\mathbb{R}. \tag{1.4}$$

We also have the Schwarz inequality defined with the norms:

$$|(\psi_1,\psi_2)|\leq\sqrt{(\psi_1,\psi_1)}\sqrt{(\psi_2,\psi_2)}. \tag{1.5}$$

### 1.1.2 Linear operators

A linear operator $A$ is a mathematical entity which associates with every function $\phi(\boldsymbol{r})\in\mathscr{F}$ another function $\phi'(\boldsymbol{r})$ linearly:

$$\begin{aligned}&\phi'(\boldsymbol{r})=A\phi(\boldsymbol{r})\\&A[\lambda_1\phi_1(\boldsymbol{r})+\lambda_2\phi_2(\boldsymbol{r})]=\lambda_1A\phi_1(\boldsymbol{r})+\lambda_2A\phi_2(\boldsymbol{r})\end{aligned} \tag{1.6}$$

Let $A,B$ be two linear operators, their product $AB$ on a vector corresponds to the application of $B$ first, and then A acts on the new vector $\varphi(\boldsymbol{r})=B\psi(\boldsymbol{r})$:

$$(AB)\psi(\boldsymbol{r})=A[B\psi(\boldsymbol{r})]. \tag{1.7}$$

In general, the order of application matter and a way to quantify it is through the **commutator**:

$$[A,B]=AB-BA\,. \tag{1.8}$$

### 1.1.3 Discrete orthonormal bases in $\mathscr{F}$ : $\{u_i(\boldsymbol{r})\}$

#### Definition of discrete orthonormal bases

Let be a countable set of function $\{u_1(\boldsymbol{r})\}\in\mathscr{F}$.

- This set is orthonormal if only the inner profuct of the same function returns a non-zero value:

$$\text{Orthonormalization relation} \qquad (u_i,u_j)=\int d^3r\ u_i^*(\boldsymbol{r})u_j(\boldsymbol{r})=\delta_{ij}\,, \tag{1.9}$$

  where $\delta_{ij}$ is the kronecker function:

$$\delta_{ij}=\begin{cases}1, & i=j\\0, & i\neq j\end{cases}. \tag{1.10}$$

- It constitutes a **basis** if every function $\psi(\boldsymbol{r})\in\mathscr{F}$ can be expanded in only **one way** in $\{u_i(\boldsymbol{r})\}$ as a linear combination:

$$\text{Expansion} \qquad \psi(\boldsymbol{r})=\sum_i c_iu_i(\boldsymbol{r})\,, \tag{1.11}$$

whose elements of projection $c_i$ are obtained computing the scalar product $(u_j, \psi(x))$:

$$(u_j, \psi) = \left( u_j, \sum_i c_i u_i(\boldsymbol{r}) \right) = \sum_i c_i (u_j, u_i) = \sum_i c_i \delta_{ij} = c_j.$$

Thus,

$$\text{Coefficient expansion} \qquad c_i = (u_i, \psi) = \int d^3r \; u_i^*(\boldsymbol{r}) \psi(\boldsymbol{r}) \,. \tag{1.12}$$

Once projected in $\{u_i(\boldsymbol{r})\}$ it is equivalent to specify $\psi(\boldsymbol{r})$ or the set of $c_i$, which represent $\psi(\boldsymbol{r})$ in the $\{u_i(\boldsymbol{r})\}$ basis. The 3D generalization is given in A-22-A-24.

The scalar product of two wavefunctions can also be expressed in terms of the coefficients of projection. Let be $\varphi(\boldsymbol{r}), \psi(\boldsymbol{r})$,

$$(\varphi, \psi) = \left[ \sum_i b_i u_i, \sum_j c_j u_j \right] = \sum_{i,j} b_i^* c_j (u_i, u_j) = \sum_{i,j} b_i^* c_j \delta_{ij}. \tag{1.13}$$

Therefore, the scalar product is:

$$\text{Scalar product} \qquad (\varphi, \psi) = \sum_i b_i^* c_i \tag{1.14}$$

Its generalization for 3D is given in A-28.

### Closure relation

Equation (1.9) is called *orthonormalization relation* over the set $\{u_i(\boldsymbol{r})\}$. There is another condition called *Closure relation*, which express the fact that this set constitutes a basis.

If $\{u_i(\boldsymbol{r})\} \in \mathscr{F}$, the any function $\psi(\boldsymbol{r}) \in \mathscr{F}$ is decomposed using equation (1.11):

$$\psi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r}) = \sum_i (u_i, \psi) u_i(\boldsymbol{r}) = \sum_i \left[ \int d^3r' \; u_i^*(\boldsymbol{r}') \psi(\boldsymbol{r}') \right] u_i(\boldsymbol{r}) = \int d^3r' \; \psi(\boldsymbol{r}') \left[ \sum_i u_i(\boldsymbol{r}) u_i^*(\boldsymbol{r}') \right]$$

This integration with sum will be $\psi(\boldsymbol{r})$ only when $\boldsymbol{r} = \boldsymbol{r}'$, which is characteristic of a delta function centered at $\boldsymbol{r} = \boldsymbol{r}'$. Thus, the only way to achieve that is that the sum must be a delta function $\delta(\boldsymbol{r} - \boldsymbol{r}')$ and we have

$$\text{Closure relation} \qquad \sum_i u_i(\boldsymbol{r}) u_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \,. \tag{1.15}$$

If an orthonormal set $\{u_i(\boldsymbol{r})\}$ satisfies the closure relation then it constitutes a basis.

## 1.1.4 Bases not belonging to $\mathscr{F}$

The $\{u_i(\boldsymbol{r})\}$ bases are composed of square-integrable functions. It can also be convenient to introduce bases of functions **not belonging** to $\mathscr{F}$ or $L_2$, but in terms of which any wavefunction $\psi(\boldsymbol{r})$ can nevertheless be expanded. We will discuss two examples: 1D plane wave, and delta functions, after which we will study continuous bases.

### Plane waves

Consider a plane wave $v_p(x)$ with wave vector $p/\hbar$

$$v_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}. \tag{1.16}$$

The integral of $|v_p(x)|^2 = \frac{1}{2\pi\hbar}$ over $x \in \mathbb{R}$ diverges, therefore $v_p(x) \notin \mathscr{F}_x$. We shall designate $\{v_o(x)\}$ the set of all plane waves, with the continuous index $p \in (-\infty, \infty)$. The Fourier-pair equations

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) e^{ipx/\hbar}, \quad \text{and} \quad \bar{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\ \psi(x) e^{-ipx/\hbar},$$

can be rewritten with the definition of the plane wave:

$$\psi(x) = \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) v_p(x), \tag{1.17}$$

$$\bar{\psi}(p) = (v_p, \psi) = \int_{-\infty}^{\infty} dx\ v_p^*(x)\psi(x). \tag{1.18}$$

The two formulas can be compared to equations (1.11) and (1.12). In this case, every function $\psi(x) \in \mathscr{F}_x$ can be expanded in only one way as a continuous linear combination of planes waves, whose components are given by (1.18). The set of these components constitutes a function of $p$, $\bar{\psi}(p)$, the Fourier transform of $\psi(x)$.

$\bar{\psi}(p)$ is analogous to $c_i$, both represent the components of the same function $\psi(x)$ in two different bases: $\{v_p(x)\}$ and $\{u_i(x)\}$.

If we calculate the square of the norm of $\psi(x)$ we will get:

$$\text{Parseval's theorem} \qquad (\psi, \psi) = \int_{-\infty}^{\infty} dp\ |\bar{\psi}(p)|^2. \tag{1.19}$$

We can also show that $v_p(x)$ satisfy the closure relation:

$$\begin{aligned}\psi(x) &= \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) v_p(x) = \int_{-\infty}^{\infty} dp\ (v_p, \psi) v_p(x) = \int_{-\infty}^{\infty} dp\ \left[\int_{-\infty}^{\infty} dx'\ v_p^*(x')\psi(x')\right] v_p(x) \\ &= \int_{-\infty}^{\infty} dx'\ \psi(x') \left[\int_{-\infty}^{\infty} dp\ v_p(x) v_p^*(x')\right].\end{aligned}$$

The term inside the brackets corresponds to

$$\text{Closure relation} \qquad \int_{-\infty}^{\infty} dp\ v_p(x) v_p^*(x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dp}{\hbar} e^{i\frac{p}{\hbar}(x-x')} \overset{(a)}{=} \delta(x - x'). \tag{1.20}$$

In $(a)$ the following relation was used:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\ e^{iku} = \delta(u).$$

Equation (1.20) is analogous to (1.15). In the same way, we can derive the orthonormalization relation using $(a)$:

$$(v_p, v_{p'}) = \int_{-\infty}^{\infty} dx\ v_p^*(x) v_{p'}(x) = \frac{1}{2\pi} \int \frac{dx}{\hbar} e^{i\frac{x}{\hbar}(p'-p)} = \delta(p-p').$$

Therefore,

$$\text{Orthonormalization relation} \qquad (v_p, v_{p'}) = \delta(p-p')\,. \tag{1.21}$$

Now instead of a kronecker delta, we have a delta function. If $p = p'$, the scalar product **diverges**: we see again that $v_p(x) \notin \mathscr{F}_x$. It is also sait that $v_p(x)$ is "orthonormalized in the Dirac sense". The generalization to three dimension is given by

$$v_{\boldsymbol{p}}(\boldsymbol{r}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i\cdot\boldsymbol{p}/\hbar}. \tag{1.22}$$

The functions of $\{v_p(\boldsymbol{r})\}$ basis now depend on the thre continuous indices $p_x, p_y, p_z$ condensed in $\boldsymbol{p}$. In addition,

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d^3p\ \bar{\psi}(\boldsymbol{p}) v_{\boldsymbol{p}}(\boldsymbol{r}) \tag{1.23}$$

$$\text{Coefficient expansion} \qquad \bar{\psi}(\boldsymbol{p}) = (v_{\boldsymbol{p}}, \psi) = \int d^3r\ v_{\boldsymbol{p}}^*(\boldsymbol{r}) \psi(\boldsymbol{r}) \tag{1.24}$$

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d^3p\ \bar{\varphi}^*(\boldsymbol{p}) \bar{\psi}(\boldsymbol{p}) \tag{1.25}$$

$$\text{Closure relation} \qquad \int d^3p\ v_{\boldsymbol{p}}(\boldsymbol{r}) v_{\boldsymbol{p}}^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') \tag{1.26}$$

$$\text{Orthornormalization relation} \qquad (v_{\boldsymbol{p}}, v_{\boldsymbol{p}'}) = \delta(\boldsymbol{p}-\boldsymbol{p}') \tag{1.27}$$

The $v_p(\boldsymbol{r})$ can be considered to constitute a **continuous** basis.

### Delta function

We can also consider a set of functions of $\boldsymbol{r}$, $\{\xi_{\boldsymbol{r}_o}(\boldsymbol{r})\}$, labeled by the continuous index $\boldsymbol{r}_0 = (x_0, y_0, z_0)$ and defined by

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r}-\boldsymbol{r}_0). \tag{1.28}$$

Obviously, $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ is not square-integrable: $\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) \notin \mathscr{F}$.

Then, we can have the following

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d^3r_0\ \psi(\boldsymbol{r}_0) \xi_{\boldsymbol{r}_0}(\boldsymbol{r}), \quad \text{and} \tag{1.29}$$

$$\text{Coefficient expansion} \qquad \psi(\boldsymbol{r}_0) = (\xi_{\boldsymbol{r}_0}, \psi) = \int d^3r\ \xi_{\boldsymbol{r}_0}^*(\boldsymbol{r}) \psi(\boldsymbol{r}). \tag{1.30}$$

The equations are analogous to equations (1.11) and (1.12).

$\psi(\boldsymbol{r}_0)$ is the equivalent of $c_i$, which represent the components of the same function $\psi(\boldsymbol{r})$ in two different bases: $\{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$ and $\{u_i(\boldsymbol{r})\}$.

We also list, the other formulas:

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d^3r_0 \; \varphi^*(\boldsymbol{r}_0)\psi(\boldsymbol{r}_0) \tag{1.31}$$

$$\text{Closure relation} \qquad \int d^3r_0 \; \xi_{\boldsymbol{r}_0}(\boldsymbol{r})\xi^*_{\boldsymbol{r}_0}(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{1.32}$$

$$\text{Orthonormalization relation} \qquad (\xi_{\boldsymbol{r}_0}, \xi_{\boldsymbol{r}'_0}) = \delta(\boldsymbol{r}_0 - \boldsymbol{r}'_0) \tag{1.33}$$

The $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ can be considered to constitute a **continuous** basis.

A physical state must **always** correspond to a qaure-integrable wavefunction. In no case $v_p(\boldsymbol{r})$ and $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ can represent the state of a particle. They are nothing more than intermediaries, useful for calculations.

### Continuous orthonormal bases

We will denote a continuous orthonormal basis to a set of function of $\boldsymbol{r}$, $\{w_\alpha(\boldsymbol{r})\}$, labeled by a continuous index $\alpha$, which satisfy the closure and orthonormalization relations:

$$\text{Orthonormalization relation} \qquad (w_\alpha, w_{\alpha'}) = \int d^3r \; w^*_\alpha(\boldsymbol{r})w_{\alpha'}(\boldsymbol{r}) = \delta(\alpha - \alpha') \tag{1.34}$$

$$\text{Closure relation} \qquad \int d\alpha \; w_\alpha(\boldsymbol{r})w^*_\alpha(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.35}$$

When $\alpha = \alpha'$, $(w_\alpha, w_{\alpha'})$ **diverges**. Therefore, $\omega_\alpha(\boldsymbol{r}) \notin \mathscr{F}$. Recall that this is a generalized continuous basis, so it can represent the plane waves and delta functions by setting $\alpha = \boldsymbol{p}$ and $\alpha = \boldsymbol{r}_0$, respectively.

In the case of mixed (discrete and continuous) basis $\{u_i(\boldsymbol{r}), w_\alpha(\boldsymbol{r})\}$, the orthonormalization relations are

$$\text{Orthonormalization relation for mixed basis} \qquad \begin{array}{l} (u_i, u_j) = \delta_{ij} \\ (w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha') \\ (u_i, w_\alpha) = 0 \end{array} . \tag{1.36}$$

And the closure relation becomes:

$$\text{Closure relation for mixed basis} \qquad \sum_i u_i(\boldsymbol{r})u^*_i(\boldsymbol{r}') + \int d\alpha \; w_\alpha(\boldsymbol{r})w^*_\alpha(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.37}$$

We also list the expansion, coefficient of expansion and the scalar product for the continuous basis:

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d\alpha \; c(\alpha)w_\alpha(\boldsymbol{r}) \tag{1.38}$$

$$\text{Coefficient expansion} \qquad c(\alpha) = (w_\alpha, \psi) = \int d^3r' \; w^*_\alpha(\boldsymbol{r}')\psi(\boldsymbol{r}') \tag{1.39}$$

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d\alpha \; b^*(\alpha)c(\alpha) \tag{1.40}$$

The squared norm of the wavefunction with itself is then

$$\text{Parseval's theorem} \qquad (\psi,\psi) = \int d\alpha\, |c(\alpha)|^2. \tag{1.41}$$

Finally, all the formulas can thus be generalized from discrete basis of index $i$ and continuous basis with index $\alpha$ (which can consider the plane wave and delta functions) through the following change of variables:

$$\text{Transformation } \{u_i(\boldsymbol{r})\} \longleftrightarrow \{w_\alpha(\boldsymbol{r})\} \qquad \begin{array}{c} i \longleftrightarrow \alpha \\ \displaystyle\sum_i \longleftrightarrow \int d\alpha \\ \delta_{ij} \longleftrightarrow \delta(\alpha-\alpha') \end{array} \tag{1.42}$$

**Table 1.1** Fundamental formulas for discrete and continuous basis.

| Property | Discrete basis $\{u_i(\boldsymbol{r})\}$ | Continuous basis $\{w_\alpha(\boldsymbol{r})\}$ |
|---|---|---|
| Scalar product | $(\varphi,\psi) = \sum_i b_i^* c_i$ | $(\varphi,\psi) = \int d\alpha\, b^*(\alpha)c(\alpha)$ |
| Parseval | $(\psi,\psi) = \sum_i \lvert c_i\rvert^2$ | $(\psi,\psi) = \int d\alpha\, \lvert c(\alpha)\rvert^2$ |
| Orthonormalization relation | $(u_i,u_j) = \delta_{ij}$ | $(w_\alpha, w_{\alpha'}) = \delta(\alpha-\alpha')$ |
| Closure relation | $\sum_i u_i(\boldsymbol{r})u_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}')$ | $\int d\alpha\, w_\alpha(\boldsymbol{r})w_\alpha^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}')$ |
| Expansion | $\psi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r})$ | $\psi(\boldsymbol{r}) = \int d\alpha\, c(\alpha)w_\alpha(\boldsymbol{r})$ |
| Components | $c_i = (u_i,\psi)$ | $c(\alpha) = (w_\alpha,\psi)$ |

## 1.2 Dirac notation

Each quantum state of a particle will be characterized by a **state vector**, belonging to an abstract space $\mathscr{E}_{\boldsymbol{r}}$, called the **state space** of the particle. The fact that the space $\mathscr{F}$ is a subspace of $L^2$ means that $E_{\boldsymbol{r}}$ is a subspace of a Hilbert space.

The introduction of these quantities permits a generalization of the formalism. In fact, there exist physical systems whose quantum description cannot be given by a wavefunction.

**State vector**

The quantum state of any physical system is characterized by a state vector, belonging to a space $\mathscr{E}$ which is the state space of the system. The state space is the set of all of the possible states in which the system can exist.

### 1.2.1 Ket and Bra vectors

#### Ket vectors

Any element or vector of space $\mathscr{E}$ is called a **key vector** or ket, and is represented by the symbol $|\cdot\rangle$. We shall define the space $\mathscr{E}_{\boldsymbol{r}}$ of the states of a particle by associating with every square-integrable function $|psi(\boldsymbol{r})$ a ket vector $|\psi\rangle$ of $\mathscr{E}_{\boldsymbol{r}}$:

$$\psi(\boldsymbol{r}) \in \mathscr{F} \Longrightarrow |\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}. \tag{1.43}$$

Altough $\mathscr{F}$ and $\mathscr{E}_{\boldsymbol{r}}$ are **isomorphic**, we shal carefully distinguish between them. We see that the $\boldsymbol{r}$-dependence no longer appears in $|\psi\rangle$: only appears $\psi$ as an object that is used to extract information.

#### Dual space and bra vectors

A **linear function** $\chi$ is a linear operation which associantes a complex number with every ket $|\psi\rangle$:

$$\begin{aligned} &|\psi\rangle \in \mathscr{E} \xrightarrow{\chi} \chi(|\psi\rangle) \in \mathbb{C} \\ &\chi(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1\chi(|\psi_1\rangle) + \lambda_2\chi(|\psi_2\rangle). \end{aligned} \tag{1.44}$$

A linear functional is an operator that returns a complex number, while a linear operator returns another ket (vector).

The set of linear functionals defined on $|\psi\rangle \in \mathscr{E}$ constitutes a vector space, which is called **dual space** of $\mathscr{E}$ and which will be symbolized by $\mathscr{E}^*$.

Any element, or vector of the space $\mathscr{E}^*$ is called a **bra vector**, or bra and is denoted by $\langle\cdot|$.

The bra acts as a linear operator over the ket, which can be used to define the scalar product to return a complex number:

$$\text{Scalar product} \qquad \langle\varphi|\psi\rangle = (|\varphi\rangle, |\psi\rangle)\,. \tag{1.45}$$

We then have similar properties for the scalar product:

$$\begin{array}{lll} \text{Adjoint} & \text{Linear to the second vector} & \text{Antilinear to the first vector} \\ \langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^* & \langle\varphi|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\langle\varphi|\psi_1\rangle + \lambda_2\langle\varphi|\psi_2\rangle & \langle\lambda_1\varphi_1 + \lambda_2\varphi_2|\psi\rangle = \lambda_1^*\langle\varphi_1|\psi\rangle + \lambda_2^*\langle\varphi_2|\psi\rangle \end{array} \tag{1.46}$$

#### Relation bra-ket

There is an antilinear relation between a ket and its bra, so that we have the following multiplications by a scalar for the vectors

$$|\lambda\psi\rangle = \lambda|\psi\rangle \in \mathscr{E} \Longrightarrow \langle\lambda\psi| = \lambda^*\langle\psi| \in \mathscr{E}^*, \quad \lambda \in \mathbb{C}. \tag{1.47}$$

Although to every ket there corresponds a bra, it is possible to find bras that have no corresponding kets such as delta functions and plane waves spaces. This dissymetry of the correspondence bra-ket is related to the existence of continuous basis for $\mathscr{F}_x$. This happens when the norm of the functions blow up making them not belong to $\mathscr{F}_x$, so we cannot associate a ket of $\mathscr{E}_x$ with them. Nervertheless, their scalar pdouct with a function of $\mathscr{F}_x$ is defined, and this permits us to assicate with them a linear function of $\mathscr{E}_x$: the bra

belonging to $\mathscr{E}_x^*$. However, we can define **generalized kets**, defined using functions that are not $L^2$, but whose scalar product with every function of $\mathscr{F}_x$ exists.

When working with plane waves and delta functions, we assume the following approximation:

$$|\xi_{x_0}\rangle \overset{\text{Refers to}}{\longrightarrow} |\xi_{x_0}^{(\epsilon)}\rangle, \quad \text{and} \quad |v_{p_0}\rangle \overset{\text{Refers to}}{\longrightarrow} |v_{p_0}^{(L)}\rangle, \tag{1.48}$$

where $\epsilon$ is very small and $L$ very large compared to all other lengths of the problem, so we are always working in $\mathscr{E}_x$.

Note that

$$\begin{array}{l} \xi_{x_0}^{(\epsilon)}(x) \in \mathscr{F}_x \Longleftrightarrow |\xi_{x_0}^{(\epsilon)}\rangle \in \mathscr{E}_x \\ \lim\limits_{\epsilon\to 0} |\xi_{x_0}^{(\epsilon)}\rangle \notin \mathscr{E}_x \\ \lim\limits_{\epsilon\to 0} \langle\xi_{x_0}^{(\epsilon)}| = \langle\xi_{x_0}| \in \mathscr{E}_x^* \\ |\psi\rangle \in \mathscr{E}_x \Longrightarrow \langle\xi_{x_0}|\psi\rangle = \psi(x_0) \end{array} \quad , \quad \text{and} \quad \begin{array}{l} v_{p_0}^{(L)}(x) \in \mathscr{F}_x \Longleftrightarrow |v_{p_0}^{(L)}\rangle \in \mathscr{E}_x \\ \lim\limits_{L\to\infty} |v_{p_0}^{(L)}\rangle \notin \mathscr{E}_x \\ \lim\limits_{L\to\infty} \langle v_{p_0}^{(L)}| = \langle v_{p_0}| \in \mathscr{E}_x^* \\ |\psi\rangle \in \mathscr{E}_x \Longrightarrow \langle v_{p_0}|\psi\rangle = \bar{\psi}(p_0) \end{array} \tag{1.49}$$

In general, the dual space $\mathscr{E}^*$ and the stae space $\mathscr{E}$ are not isomorphic, exept that $\mathscr{E}$ is finite-dimensional. Although to each ket there corresponds a bra, the converse is not true. In addition to use vector of $\mathscr{E}$ (whose norm is finite), **generalized kets** with infinite norms but whose scalar product with every ket of $\mathscr{E}$ is finite. Thus, to each bra of $\mathscr{E}^*$ there will correpsond a ket. But generalized kets do not represent physical states of the system.

### 1.2.2 Linear operators

A linear operator $A$ associates with every ket $|\psi\rangle \in \mathscr{E}$ another ket $|\psi'\rangle \in \mathscr{E}$ linearly:

$$|\psi'\rangle = A|\psi\rangle \tag{1.50}$$

$$A(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1 A|\psi_1\rangle + \lambda_2 A|\psi_2\rangle. \tag{1.51}$$

The product of two linear operators $AB$ is defined by first acting $B$ in the ket $|\psi\rangle$, and then $A$:

$$(AB)|\psi\rangle = A(B|\psi\rangle). \tag{1.52}$$

The commutator express the degree of difference between the change of order of operation:

$$[A, B] = AB - BA\,. \tag{1.53}$$

We call the **matrix element** of $A$ between $|\varphi\rangle$ and $|\psi\rangle$, the scalar product that measure the collinearity between the action of the operator onto $|\varphi\rangle$:

$$\langle\varphi|A|\psi\rangle \in \mathbb{C}\,. \tag{1.54}$$

#### Projector

Lets assume that $\langle\psi|\psi\rangle = 1$ (normalized), we define the **projector** as an operator that projects a ket into another ket:

$$P_\psi = |\psi\rangle\langle\psi| \tag{1.55}$$

When it acts into a vector, it first compute the scalar product and the assign the value to the vector from which the product was computed:

$$P_\psi|\varphi\rangle = |\psi\rangle \underbrace{\langle\psi|\varphi\rangle}_{\text{number}}.$$

It is also *idempotent*, which means that

$$P_\psi^2 = P_\psi P_\psi = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = P_\psi. \tag{1.56}$$

The most generalized form is project a ket into a orthonormalized ($\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$) subespace $\{\varphi_q\} \in \mathscr{E}_q \subseteq \mathscr{E}$. Let $P_q$ be then the linear operator

$$P_q = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i|. \tag{1.57}$$

It then takes the ket, and compute the projection to every vector $|\varphi_i\rangle$ and the form a linear combination.

### 1.2.3 Hermitian conjugation (adjoint)

There is also possible to define actions of $A$ on bras as $\langle\chi|A$, whose order is important.

We can also link with every linear operator $A$ another linear operator $A^\dagger$, caled the adjoint operator (or Hermitian conjugate) of $A$. The operatoe $A$ associates with it another ket $|\psi'\rangle = A|\psi\rangle \in \mathscr{E}$. The correspondende between kets and bras permits us to define the action of operator $A^\dagger$ on the bras:

$$|\psi\rangle \text{ corresponds to } \langle\psi| \Longrightarrow |\psi'\rangle = A|\psi\rangle \text{ corresponds to } \langle\psi'| = \langle\psi|A^\dagger. \tag{1.58}$$

The relation $\langle\psi'| = \langle\psi|A^\dagger$ is **linear**, as

$$A(\lambda_1^*|\psi_1\rangle + \lambda_2^*|\psi_2\rangle) = \lambda_1^* A|\psi_1'\rangle + \lambda_2^* A|\psi_2'\rangle \text{ corresponds to } (\lambda_1\langle\psi_1| + \lambda_2\langle\psi_2|)A^\dagger = \lambda_2\langle\psi_1|A^\dagger + \lambda_2\langle\psi_2|A^\dagger.$$

Therefore, $A^\dagger$ is a linear operator defined by

$$|\psi'\rangle = A|\psi\rangle \Longleftrightarrow \langle\psi'| = \langle\psi|A^\dagger, \tag{1.59}$$

which also implies that

$$\langle\psi|A^\dagger|\varphi\rangle = \langle\varphi|A|\psi\rangle^*. \tag{1.60}$$

#### Properties

$$\begin{aligned}
&(A^\dagger)^\dagger = A \\
&(\lambda A)^\dagger = \lambda^* A^\dagger \\
&(A+B)^\dagger = A^\dagger + B^\dagger \\
&(AB)^\dagger = B^\dagger A^\dagger
\end{aligned}$$

#### Hermitian conjugation in Dirac notation

A ket $|\psi\rangle$ and its corresponding bra $\langle\psi|$ are said to be Hermitian conjugates of each other. In the same manner, $A^\dagger$ is also called Hermitian conjugate operator of $A$.

The operation of Hermitian conjugate is followed by a very simple rule:

**Rule of Hermitian conjugate**

To obtain the adjoint of any expression composed f constantes, kets, bras, and operators, one must:

$$\text{Replace} \quad \begin{cases} \text{the constants by their complex conjugates} \\ \text{the kets by the bras associated} \\ \text{the bras by the kets associated} \\ \text{the operators by their adjoints} \end{cases}$$

Reverse the order of the factors — Only constants can move around (commute)

As an example,

$$\left(\lambda\langle u|A|v\rangle|w\rangle\langle\psi|\right)^\dagger = |\psi\rangle\langle w|\langle v|A^\dagger|u\rangle \overbrace{\lambda^*}^{\text{can move around}}$$

### Hermitian operators

An operator $A$ is said to be Hermitian if $A = A^\dagger$, which stasify the following relations:

$$\langle\psi|A|\varphi\rangle = \langle\varphi|A|\psi\rangle^* \quad \text{and} | \quad \langle A\varphi|\psi\rangle = \langle\varphi|A\psi\rangle.$$

In addition, the projector $P_\psi$ is an Hermitian operator:

$$P_\psi^* = |\psi\rangle\langle\psi| = P_\psi. \tag{1.61}$$

The product of two Hermitian operators $A, B$ is Hermitian only if $[A, B] = 0$.

## 1.3 Representations in state space

Choosing a representation means choosing and orthonormal (discrete or continuous) basis in the state space $\mathscr{E}$. Vectors and operators are then represented in this basis by *numbers*: components for the vectors, matrix elements for the operators.

We now translate all properties such as orthonormaliation relation and closure relation to the Dirac notation.

### 1.3.1 Relations characteristic of an orthonormal basis

#### Orthonormalization relation

A set of kets, discrete $\{|u_i\rangle\}$ or continuous $\{|w_\alpha\rangle\}$ is said to be orthonotmal if they satisfy the following equation:

$$\text{Orthonormalization relation} \quad \begin{array}{l} \langle u_i|u_j\rangle = \delta_{ij} \\ \langle w_\alpha|w_{\alpha'}\rangle = \delta(\alpha - \alpha') \end{array}. \tag{1.62}$$

As can be seen, for a continuous set $\langle w_\alpha|w_\alpha\rangle$ **does not exists**: the $|w_\alpha\rangle$ have an infinite norm and therefore not belong to $\mathscr{E}$. Nevertheless, the vectors of $\mathscr{E}$ can be expanded on the $|w_\alpha\rangle$. It is useful then to accept $|w_\alpha\rangle$ as *generalized kets*.

### Closure relation

A discrete or continuous set constitutes a basis if every ket $|\psi\rangle \in \mathscr{E}$ has a **unique** expansion on $|u_i\rangle$ or $|w_\alpha\rangle$:

$$\text{Closure relation} \qquad \begin{array}{l} |\psi\rangle = \sum\limits_i c_i |u_i\rangle \\ |\psi\rangle = \int d\alpha \; c(\alpha)|w_\alpha\rangle \end{array}, \tag{1.63}$$

whose components are obtained multiplying $\langle u_j|$ ($\langle \omega_{\alpha'}|$) in the closure relation and using equation (1.62):

$$\text{Coefficient expansion} \qquad \begin{array}{l} \langle u_j|\psi\rangle = c_j \\ \langle w_{\alpha'}|\psi\rangle = c(\alpha') \end{array}. \tag{1.64}$$

We can reexpress the expansion employing the coefficient expansion equations:

$$|\psi\rangle = \sum_i c_i|u_i\rangle = \sum_i \langle u_i|\psi\rangle|u_i\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \left[\sum_i |u_i\rangle\langle u_i|\right]|\psi\rangle = P_{\{u_i\}}|\psi\rangle,$$
$$|\psi\rangle = \int d\alpha \; c(\alpha)|w_\alpha\rangle = \int d\alpha \; \langle w_\alpha|\psi\rangle|w_\alpha\rangle = \int d\alpha \; |w_\alpha\rangle\langle w_\alpha|\psi\rangle = \left[\int d\alpha \; |w_\alpha\rangle\langle w_\alpha|\right]|\psi\rangle = P_{\{w_\alpha\}}|\psi\rangle.$$

We then have the projector onto a discrete and continuous basis:

$$\text{Projectors} \qquad \begin{array}{l} P_{\{u_i\}} = \sum\limits_i |u_i\rangle\langle u_i| = \mathbb{1} \\ P_{\{w_\alpha\}} = \int d\alpha \; |w_\alpha\rangle\langle w_\alpha| = \mathbb{1} \end{array} \qquad \text{Closure relation,} \tag{1.65}$$

where $\mathbb{1}$ denotes the identiy operator in $\mathscr{E}$. These relations express the fact that $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ constitute bases.

**Table 1.2** Fundamental formulas for calculation in the $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ representations.

| $\{\|u_i\rangle\}$ representation | $\{\|w_\alpha\rangle\}$ representation |
|---|---|
| $\langle u_i\|u_j\rangle = \delta_{ij}$ | $\langle w_\alpha\|w_{\alpha'}\rangle = \delta(\alpha - \alpha')$ |
| $P_{\{u_i\}} = \sum\limits_i \|u_i\rangle\langle u_i\| = \mathbb{1}$ | $P_{\{w_\alpha\}} = \int d\alpha \; \|w_\alpha\rangle\langle w_\alpha\| = \mathbb{1}$ |

### 1.3.2 Representation of kets and bras

In the $\{|u_i\rangle\}$ basis, the ket $|\psi\rangle$ is represented by a set of its components $x_i\langle u_i|psi\rangle$. These numbers are arranged vertically to form a column matrix. On the other hand, for continuous basis $\{|w_\alpha\rangle\}$, the ket $|\psi\rangle$ is represented by a continuous **infinity** of numbers $c(\alpha) = \langle w_\alpha|\psi\rangle$: a function of $\alpha$. We then draw a vertical axis with the values of $c(\alpha)$:

$$|\psi\rangle_{\{|u_i\rangle\}} = \mathbb{1}|\psi\rangle = P_{\{|u_i\rangle\}}|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \sum_i c_i|u_i\rangle,$$
$$|\psi\rangle_{\{|w_\alpha\rangle\}} = \mathbb{1}|\psi\rangle = P_{\{|w_\alpha\rangle\}}|\psi\rangle = \int d\alpha \; |w_\alpha\rangle\langle w_\alpha|\psi\rangle = \int d\alpha \; c(\alpha)|\psi\rangle.$$

Then,

$$|\psi\rangle_{\{|u_i\rangle\}} = \begin{bmatrix} \langle u_1|\psi\rangle \\ \langle u_2|\psi\rangle \\ \vdots \\ \langle u_i|\psi\rangle \\ \vdots \end{bmatrix}, \quad \text{and} \quad |\psi\rangle_{\{|w_\alpha\rangle\}} = \begin{matrix} \\ \\ \alpha \downarrow \\ \\ \\ \end{matrix} \begin{bmatrix} \vdots \\ \vdots \\ \langle w_\alpha|\psi\rangle \\ \vdots \\ \vdots \end{bmatrix}. \tag{1.66}$$

Something similar happens to the respective bras:

$$\langle\varphi|_{\{|u_i\rangle\}} = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{|u_i\rangle\}} = \sum_i \langle\varphi|u_i\rangle\langle u_i| = \sum_i b_i^*\langle u_i|,$$
$$\langle\varphi|_{\{|w_\alpha\rangle\}} = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{|w_\alpha\rangle\}} = \int d\alpha\ \langle\varphi|w_\alpha\rangle\langle w_\alpha| = \int d\alpha\ b^*(\alpha)\langle\varphi|.$$

We can see that the components of the bra are the complex conjugates of the components $b_i = \langle u_i|\varphi\rangle$ and $b(\alpha) = \langle w_\alpha|\varphi\rangle$ of the ket $|\varphi\rangle$ associated with $\langle\varphi|$.

Let us then arrange them horizontally, to form a row matrix:

$$\langle\varphi|_{\{|u_i\rangle\}} = \begin{bmatrix} \langle\varphi|u_1\rangle & \langle\varphi|u_2\rangle & \cdots & \langle\varphi|u_i\rangle & \cdots \end{bmatrix}, \quad \text{and} \tag{1.67}$$

$$\langle\varphi|_{\{|w_\alpha\rangle\}} = \begin{matrix} \\ \alpha \\ \rightarrow \\ \end{matrix} \begin{bmatrix} \cdots & \cdots & \langle\varphi|w_\alpha\rangle & \cdots & \cdots \end{bmatrix}. \tag{1.68}$$

The scalar product is then given by a **matrix multiplication**:

$$\langle\varphi|\psi\rangle = \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{u_i\}}|\psi\rangle = \sum_i \langle\varphi|u_i\rangle\langle u_i|\varphi\rangle = \sum_i b_i^* c_i \tag{1.69}$$

$$\langle\varphi|\psi\rangle = \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{w_\alpha\}}|\psi\rangle = \int d\alpha\ \langle\varphi|w_\alpha\rangle\langle w_\alpha|\psi\rangle = \int d\alpha\ b^*(\alpha)c(\alpha). \tag{1.70}$$

### 1.3.3 Representation of operators

#### Representation of $A$ by a square matrix

Given a linear operator $A$, we can in $\{|u_i\rangle\}$ or $\{|w_\alpha\rangle\}$ basis, associate with it a series of numbers defined by

$$A_{ij} = \langle u_i|A|u_j\rangle, \quad \text{or} \quad A(\alpha,\alpha') = \langle w_\alpha|A|w_{\alpha'}\rangle. \tag{1.71}$$

They are arranged into a square matrix, as

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} & \cdots & A_{2j} & \cdots \\ \vdots & \vdots & & \vdots & \\ A_{i1} & A_{i2} & \cdots & A_{ij} & \cdots \\ \vdots & \vdots & & \vdots & \end{bmatrix}, \quad \text{or} \quad \begin{matrix} \\ \\ \alpha \downarrow \\ \\ \\ \end{matrix} \begin{matrix} \\ \\ \alpha' \\ \longrightarrow \\ \\ \end{matrix} \begin{bmatrix} & & \vdots & \\ & & \vdots & \\ \cdots & \cdots & A(\alpha,\alpha') & \cdots \\ & & \vdots & \end{bmatrix}. \tag{1.72}$$

For the case of the matrix representing the operator $AB$ in the $\{|u_i\rangle\}$ basis, we have:

$$\langle u_i|AB|u_j\rangle = \langle u_i|A\mathbb{1}B|u_j\rangle = \langle u_i|AP_{\{u_k\}}B|u_j\rangle = \sum_k \langle u_i|A|u_k\rangle\langle u_k|B|u_j\rangle = \sum_k A_{ik}B_{kj}.$$

### Representation of the ket $|\psi'\rangle = A|\psi\rangle$

Knowing the componetns of $|\psi\rangle$ and the matrix elements of $A$ in a given representation, how can we calculate the components of $|\psi'\rangle = S|\psi\rangle$ in the same representation?

We know that in the $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ basis, we have

$$c'_i = \langle u_i|\psi'\rangle = \langle u_i|A|\psi\rangle, \quad \text{and} \quad c'(\alpha) = \langle w_\alpha|\psi'\rangle.$$

Inserting the closure relation between $A$ and $|\psi\rangle$:

$$c'_i = \langle u_1|A\mathbb{1}|\psi\rangle = \langle u_i|AP_{\{u_j\}}|\psi\rangle = \sum_j \langle u_i|A|u_j\rangle\langle u_j|\psi\rangle = \sum_j A_{ij}c_j$$

$$c'(\alpha) = \langle w_\alpha|A\mathbb{1}|\psi\rangle = \int d\alpha'\ \langle w_\alpha|A|w_{\alpha'}\rangle\langle w_{\alpha'}|\psi\rangle = \int d\alpha'\ A(\alpha,\alpha')c(\alpha').$$

We see that the column matrix representing $|\psi'\rangle$ is equal to the matrix multiplication of the column matrix $|\psi\rangle$ and the square matrix $A$.

### Expression for the number $\langle\varphi|A|\psi\rangle$

On the other hand, we can derive an expression for $\langle\varphi|A|\psi\rangle$ for both basis:

$$\langle\varphi|A|\psi\rangle = \langle\varphi|P_{\{u_i\}}AP_{\{u_j\}}|\psi\rangle = \sum_{i,j}\langle\varphi|u_i\rangle\langle u_i|A|u_j\rangle\langle u_j|\psi\rangle = \sum_{i,j} b_i^* A_{ij}c_j,$$

$$\langle\varphi|P_{\{w_\alpha\}}AP_{\{w_{\alpha'}\}}|\psi\rangle = \iint d\alpha\ d\alpha'\ \langle\varphi|w_\alpha\rangle\langle w_\alpha|A|w_{\alpha'}\rangle\langle w_{\alpha'}|\psi\rangle = \iint d\alpha\ d\alpha'\ b^*(\alpha)A(\alpha,\alpha')c(\alpha').$$

Thus, the term $\langle\varphi|A|\psi\rangle$ which is a number, can be computed as a matrix multiplication of the column vector $|\psi\rangle$ by the matrix $A$, and then by the row vector $\langle\varphi|$.

### Matrix representation of $A^\dagger$

The adjoint of $A$ can also be written as:

$$\begin{aligned}(A^\dagger)_{ij} &= \langle u_i|A^\dagger|u_j\rangle = \langle u_j|A|u_i\rangle^* = A^*_{ji}\\ A^\dagger(\alpha,\alpha') &= \langle w_\alpha|A^\dagger|w_{\alpha'}\rangle = \langle w_{\alpha'}|A|w_\alpha\rangle^* = A^*(\alpha',\alpha).\end{aligned} \tag{1.73}$$

The matrices representing $A$ and $A^\dagger$ are then Hermitian conjugates of each other.

If $A$ is Hermitian, then $A_{ij} = A^*_{ji}$ and $A(\alpha,\alpha') = A^*(\alpha',\alpha)$. A hermitian operator is therefore represented by a Hermitian matrix. For $i = j$, $\alpha = \alpha'$ we see that $A_{ii} = A^*_{ii}$, $A(\alpha,\alpha) = A^*(\alpha,\alpha)$. Thus,

The diagonal elements of a Hermitian matrix are therefore always real numbers.

### 1.3.4 Change of representation

We can representate a ket $|\psi\rangle$ in different bases, similar to representing a point in space by cartesian and spherical coordinates. The relation of these two representation allow us to turn from one to the other easily.

If we assume an old discrete basis $\{|u_i\rangle\}$ to a new one $\{|t_k\rangle\}$, the change of basis is defined by specifying the components $S_{ik} = \langle u_i|t_k\rangle$ of each kets of the new basis in terms of the kets of the old one. The adjoint is: $(S^\dagger)_{ki} = (S_{ik})^* = \langle t_k|u_i\rangle$. This transformation matrix is **unitary**: $S^\dagger S = SS^\dagger = I$.

We will derive the transformation for a ket, a bra, and the matrix elements of an operator using the closure relation of each basis as explained in the derivation.

$$\langle t_k|\psi\rangle = \langle t_k|\mathbb{1}|\psi\rangle = \langle t_k|P_{\{u_i\}}|\psi\rangle = \sum_i \langle t_k|u_i\rangle\langle u_i|\psi\rangle = \sum_i S^\dagger_{ki}\langle u_i|\psi\rangle$$

$$\langle u_i|\psi\rangle = \langle u_i|\mathbb{1}|\psi\rangle = \langle u_i|P_{\{t_k\}}|\psi\rangle = \sum_k \langle u_i|t_k\rangle\langle t_k|\psi\rangle = \sum_i S_{ik}\langle t_k|\psi\rangle$$

$$\langle \psi|t_k\rangle = \langle \psi|\mathbb{1}|t_k\rangle = \langle \psi|P_{\{u_i\}}|t_k\rangle = \sum_i \langle \psi|u_i\rangle\langle u_i|t_k\rangle = \sum_i \langle \psi|u_i\rangle S_{ik}$$

$$\langle \psi|u_i\rangle = \langle \psi|\mathbb{1}|u_i\rangle = \langle \psi|P_{\{t_k\}}|u_i\rangle = \sum_k \langle \psi|t_k\rangle\langle t_k|u_i\rangle = \sum_k \langle \psi|t_k\rangle S^\dagger_{ki}$$

$$A_{kl} = \langle t_k|A|t_l\rangle = \langle t_k|\mathbb{1}A\mathbb{1}|t_l\rangle = \langle t_k|P_{\{u_i\}}AP_{\{u_j\}}|t_l\rangle = \sum_{i,j}\langle t_k|u_i\rangle\langle u_i|A|u_j\rangle\langle u_j|t_l\rangle = \sum_{i,j} S^\dagger_{ki}A_{ij}S_{jl}$$

$$A_{ij} = \langle u_i|A|u_j\rangle = \langle u_i|\mathbb{1}A\mathbb{1}|u_j\rangle = \langle u_i|P_{\{t_k\}}AP_{\{t_l\}}|u_j\rangle = \sum_{k,l}\langle u_i|t_k\rangle\langle t_k|A|t_l\rangle\langle t_l|u_j\rangle = \sum_{k,l} S_{ik}A_{kl}S^\dagger_{lj}.$$

The final results are shown in table

**Table 1.3** Transformation of a ket, bra, and matrix elements from one basis to another.

| Transformation | Expression |
|---|---|
| Ket components $\{u_i\} \longrightarrow \{t_k\}$ representation | $\langle t_k|\psi\rangle = \sum_i S^\dagger_{ki}\langle u_i|\psi\rangle$ |
| Ket components $\{t_k\} \longrightarrow \{u_i\}$ representation | $\langle u_i|\psi\rangle = \sum_i S_{ik}\langle t_k|\psi\rangle$ |
| Bra components $\{u_i\} \longrightarrow \{t_k\}$ representation | $\langle \psi|t_k\rangle = \sum_i \langle \psi|u_i\rangle S_{ik}$ |
| Bra components $\{t_k\} \longrightarrow \{u_i\}$ representation | $\langle \psi|u_i\rangle = \sum_k \langle \psi|t_k\rangle S^\dagger_{ki}$ |
| Matrix elements $\{u_{i,j}\} \longrightarrow \{t_{k,l}\}$ representation | $A_{kl} = \sum_{i,j} S^\dagger_{ki}A_{ij}S_{jl}$ |
| Matrix elements $\{t_{k,l}\} \longrightarrow \{u_{i,j}\}$ representation | $A_{ij} = \sum_{k,l} S_{ik}A_{kl}S^\dagger_{lj}$ |

## 1.4 Eigenvalue equations. Observables

### 1.4.1 Eigenket and eigenbra equations

$|\psi\rangle$ is said to be an **eigenvector** (or eigenket) of the linear operator $A$ if

$$\text{Eigenket equation of } A \qquad A|\psi\rangle = \lambda|\psi\rangle, \quad \lambda \in \mathbb{C}\,. \tag{1.74}$$

This eigenketequation possesses solutions only when $\lambda$ takes on certain values, called **eigenvalues** of $A$. The set of the eigenvalues is called **spectrum** of $A$.

**Collinear of an eigenvector is also an eigenvector**

If $|\psi\rangle$ is an eigenvector of $A$ with eigenvalue $\lambda$, then $\alpha|\psi\rangle,\ \alpha \in \mathbb{C}$ is also an eigenvector of $A$.

The eigenvalue $\lambda$ is called *non-degenerate* (or simple) when its corresponding eigenvector is **unique** to within a constant factor (collinear). On the other hand, if there exists at least two linearly independent eigenkets with the **same** eigenvalue, the eigenvalue is said to be *degenerate*. Its *degree of degeneracy* $g$ is then the number of linearly independent eigenvectors $|\psi^i\rangle,\ i = \{1, 2, \cdots, g\}$ associated with it.

The set of eigenkets associated with a degenerate eigenvalue constitutes a *g-dimensional vector space* called **eigensubspace** of $\lambda$.

Taking the adjoint of the eigeketnequation yields its corresponding form to eigenbraequation

$$\text{Eigenbra equation of } A^\dagger \qquad \langle\psi|A^\dagger = \lambda^*\langle\psi|\,. \tag{1.75}$$

If $|\psi\rangle$ is an eigenket of $A$ with $\lambda$, it can also be said that $\langle\psi|$ is an eigenbra of $A^\dagger$ with $\lambda^*$.

#### Finding the eigenvalues and eigenvector in an operator

Assuming the state space is of finite dimension $N$, granting the generalization to an infinite-dimensional state space.

Choosing $\{|u_i\rangle\}$, lets us project the vector (1.74) onto the various orthonormal basis vectors $|u_i\rangle$:

$$\langle u_i|A|\psi\rangle = \lambda\langle u_i|\psi\rangle. \tag{1.76}$$

Inserting the closure relation between $A$ and $|\psi\rangle$:

$$\langle u_i|A\mathbb{1}|\psi\rangle = \sum_j \underbrace{\langle u_i|A|u_j\rangle}_{A_{ij}}\underbrace{\langle u_j|\psi\rangle}_{c_j} = \lambda\underbrace{\langle u_i|\psi\rangle}_{c_i} \longrightarrow \sum_j [A_{ij} - \lambda\delta_{ij}]c_j = 0\,. \tag{1.77}$$

Equation (1.77) is a system of equations with $N$ equations and $N$ unknowns $c_j$. It has non-trivial solution iff its characteristic equation is zero:

$$\text{Characteristic equation of the eigenket equation} \qquad P(\lambda) = \det[A - \lambda I] = 0\,. \tag{1.78}$$

This expression enable us to determine the spectrum of $A$. The characteristic equation is **independent** of the representation chosen. Then,

The eigenvalues of an operator are the roots $\lambda$ of its $N$th order characteristic equation $P(\lambda)$.

### Determination of eigenvectors

Given a transformation $T(v) = Mv : \ V \in \mathbb{C}^{\mathbb{N}} \longrightarrow W \in \mathbb{C}^{N}$, the theorem says:

$$\dim(V) = \text{rank}(T) + \text{null}(T), \tag{1.79}$$

where

$$\begin{aligned} \dim(V) &= \text{Number of columns of V} \\ \text{rank}(T) &= \text{Number of independent equations (non zero rows)} \\ \text{null}(T) = \dim[\ker(T)] &= \text{Number of free variables, degree of freedom (dof).} \end{aligned}$$

In our case, $T(v) = Mv = (A - \lambda I)v$ and $\dim(V) = N$.

Based on the nature of the eigenvalue, we can have different eigenvalues but also repeated. Therefore, we define the following useful quantities:

- **Algebraic multiplicity ($AM$)** Number of repetition of the eigenvalue (degree of degeneracy $g$).
- **Geometric multiplicity ($GM$)** Dimension of the subspace that the eigenvalues generate (how many linearly independent eigenvectors exist for that eigenvalue).

We then can have the following three cases:

- $AM = GM = 1$ Only one eigenvector corresponds to the eigenvalue (within a constant factor). At the moment of substituting an eigenvalue $\lambda_0$ into equation (1.77) there will be $\text{rank}(M) = N - 1$ independent equations so one equation is redundant. When this happens, $\text{null}(M) = 1$ free variable (or degree of freedom, dof) $c_1$ is available which can be defined arbitrarily and from which all other variables can be expressed.

  If we fix $c_1$, then all $c_j$ are proportional to it:

  $$c_j = \alpha_j^0 c_1 \quad (\alpha_1^0 = 1). \tag{1.80}$$

  the $N - 1$ coefficients $\alpha_j^0, \ j \neq 1$ are determined from the matrix elements $A_{ij}$ and $\lambda_0$. The eigenvectors associated with $\lambda_0$ differ only by the value chosen for $c_1$. They are therefore all given by

  $$|\psi_0(c_1)\rangle = \sum_j \alpha_j^0 c_1 |u_j\rangle = c_1 |\psi_0\rangle, \quad \text{with} \quad |\psi_0\rangle = \sum_j \alpha_j^0 |u_j\rangle. \tag{1.81}$$

  When $\lambda_0$ is simple, only one eigenvector corresponds to it.

**Ejemplo 1.1** **Simple eigenvalues**

In the matrix

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

the eigenvalues are $\lambda \in \{1, 2, 3\}$. Lets make $\lambda_0 = 1$ and replace it into the eigenvalue problem:

$$(A - \lambda I)v = (A - I)v = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix} = 0$$

We see that there is no value in the first column, meaning that $x_1$ is free whereas $x_2 = x_3 = 0$. Therefore, the eigenvector is $v_1 = (1\ 0\ 0)$.

---

- $AM = GM > 1$ When evaluating $\lambda_0$, the system will have rank$(M) = N - p$ independent equations $(1 < p < q)$. To the eigenvalue $\lambda_0$ there corresponds an eigensubspace of dimension null$(M) = p$, and $\lambda_0$ is a p-fold degenerate eiganvalue.

  Assuming that for $\lambda = \lambda_0$ is composed of $N - 2$ linearly independent equations. These equations enable us to calculate the coefficients $c_j$ in terms of any of them, for example $c_1$ and $c_2$:

  $$c_j = \beta_j^0 c_1 + \gamma_j^0 c_2.$$

  Al the eigenvectors associated with $\lambda_0$ are then of the form

  $$|\psi_0(c_1, c_2)\rangle = c_1|\psi_0^1\rangle + c_2|\psi_0^2\rangle, \quad \text{with} \quad |\psi_0^1\rangle = \sum_j \beta_j^0 |u_j\rangle, \quad |\psi_0^2\rangle = \sum_j \gamma_j^0 |u_j\rangle. \tag{1.82}$$

  The vectors $|\psi_0(c_1, c_2)\rangle$ do indeed constitute a two-dimensional vector space, this beeing characteristic of a two-fold degenerate eigenvalue.

- $AM > GM > 1$ In this case, the subspace is less than the degree of degeneracy and therefore not all degenerate eigenvectors are linearly independent. This means that there is not enough information to create a basis. However, techniques such as Jordan canonical form helps to create generalized eigenvector and to span the whole space.

When an operator is Hermitian, it can be shown that the degree of degeneracy $p$ of an eigenvalue $\lambda$ is always equal to the muliplicity of the corresponding root in the characteristic equations. In a space of finite dimension $N$, a Hermitian operator always has $N$ linearly independent eigenvectors: this operator can therefore be diagonalized.

### 1.4.2 Observables

#### Properties of the eigenvalues and eigenvectors of a Hermitian operator

i) The eigenvalues of a Hermitian operator are real.

ii) Two eigenvectors of a Hermitian operator corresponding to two different eigenvalues are orthogonal.

#### Definition of a observable

Consider a Hermitian operator $A$ with discrete spectrum. The degree of degeneracy of the eigenvalue $a_n$ is denoted by $g_n$. We shall denote by $|\psi_n^i\rangle$ $g_n$ linearly independent vectors chosen in the eigensubspace $\mathscr{E}_n$ of $a_n$:

$$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle, \quad i = 1, 2, \cdots, g_n. \tag{1.83}$$

Every vector of $\mathscr{E}_n$ is orthogonal to every vector of another subspace $\mathscr{E}_{n'}$: $\langle\psi_n^i|\psi_{n'}^j\rangle = 0, \quad n \neq n'$.

Inside the subspace $\mathscr{E}_n$, the $|\psi_n^i\rangle$ can always be chosen orthonormal, such that

$$\langle\psi_n^i|\psi_n^j\rangle = \delta_{ij}. \tag{1.84}$$

If such a choise is made, the result is an orthonormal system of eigenvectors of $A$: the $|\psi_n^i\rangle$ satisfying the relations:

$$\langle\psi_n^i|\psi_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}. \tag{1.85}$$

**Observable**

The Hermitian operator $A$ is an **observable** if its eigenvectors **form a basis** in the state space:

Closure relation of an observable

$$\sum_{n=1}^{\infty}\sum_{i=1}^{g_n}|\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}\,. \tag{1.86}$$

The projector onto the subspace $\mathscr{E}_n$ is written as:

$$P_n = \sum_{i=1}^{g_n}|\psi_n^i\rangle\langle\psi_n^i|. \tag{1.87}$$

The observable $A$ is the ngiven by:

$$A = \sum_n a_n P_n\,. \tag{1.88}$$

Equation (1.86) can be generalized to include cases of continuous spectrum using the previous table of the first section.

If $A$ has a mixed spectrum, then it is an observable if this system form a basis, that is, if

$$\sum_n\sum_{i=1}^{g_n}|\psi_n^i\rangle\langle\psi_n^i| + \int_{\nu_1}^{\nu_2} d\nu\ |\psi_\nu\rangle\langle\psi_\nu| = \mathbb{1}. \tag{1.89}$$

**The projector $P_\psi$ is an observable**

The projector $P_\psi = |\psi\rangle\langle\psi|$ is an observable. We know that it is Hermitian, and that its eigenvalues are 1 and 0, the first one is simple and the other infinitely degenerate. It can be shown that any ket $|\psi\rangle$ can be expanded on these eigenkets, therefore $P_\psi$ is an observable.

### 1.4.3 Sets of commuting observables

#### Important theorems

**Theorem I**

If two operators $A$ and $B$ commute, and if $|\psi\rangle$ is an eigenvector of $A$, $B|\psi\rangle$ is aso an eigenvectr of $A$, with the same eigenvalue.

Another form:

If two operators $A$ and $B$ comute, every eigensubspace of $A$ is globaly invariant under the action of $B$ ($B|\psi\rangle$ belongs to the eigensubspace $\mathscr{E}_a$ of $A$, corresponding to the eigenvalue $a$).

**Theorem II (consequence of theorem I)**

If two observables $A$ and $B$ commute, and if $|\psi_1\rangle$ and $|\psi_2\rangle$ are two eigenvectors of $A$ with different eigenvalues, the matrix element $\langle\psi_1|B|\psi_2\rangle$ is zero.

**Theorem III**

If two observables $A$ and $B$ commute, one can construct an orthonormal basis of the state spce with eigenvectors common to $A$ and $B$.

Lets prove the theorem III. Consider two commuting observables $A$ and $B$, with discrete spectrum. Since $A$ is observable, there exists at least one orthonormal system of eigenvectors $|u_n^i\rangle$ which forms a basis in the state space:

$$A|u_n^i\rangle = a_n|u_n^i\rangle, \qquad \begin{matrix} n = 1, 2, \cdots \\ i = 1, 2, \cdots, g_n \end{matrix} \tag{1.90}$$

We also have $\langle u_n^i|u_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}$. What does the matrix look like which represent $B$ in the $\{|u_n^i\rangle\}$ basis? We know that the matrix elements $\langle u_n^i|B|u_{n'}^{i'}\rangle$ are zero when $n \neq n'$ (theorem II). Let us arrange the basis vectors $|u_n^i\rangle$ in the order:

$$|u_1^1\rangle, |u_1^2\rangle, \cdots, |u_1^{g_1}\rangle;\ |u_2^1\rangle, \cdots, |u_2^{g_2}\rangle;\ |u_3^1\rangle, \cdots$$

Whe then obtain for $B$ a block-diagonal matrix of the form:

$$\left[\begin{array}{cc|ccc|cc} & \mathscr{E}_1 & & \mathscr{E}_2 & & \mathscr{E}_3 & \cdots \\ \mathscr{E}_1 & \ddots \quad \ddots & & 0 & & 0 & 0 \\ & \ddots \quad \ddots & & & & & \\ \hline \mathscr{E}_2 & & & \ddots \quad \ddots \quad \ddots & & & \\ & 0 & & \ddots \quad \ddots \quad \ddots & & 0 & 0 \\ & & & \ddots \quad \ddots \quad \ddots & & & \\ \hline \mathscr{E}_3 & 0 & & 0 & & \ddots & 0 \\ \hline \vdots & 0 & & 0 & & 0 & \ddots \quad \ddots \\ & & & & & & \ddots \quad \ddots \end{array}\right] \tag{1.91}$$

Then the degeneracy of the eigenvalue is 1, then the block reduces to a $1 \times 1$ matrix. In the column associated with $|u_n\rangle$ all the other matrix elements are zero, this expresses the fact that $|u_n\rangle$ is an eigenvector common to $A$ and $B$. When $a_n$ is a $g_n$-degenerate eigenvalue of $A$, the block which represents $B$ in $\mathscr{E}_n$ is not, in general, diagonal: the $|u_n^i\rangle$ are not, in general, eigenvector of $B$. The action of $A$ in the $g_n$ eigenvectors $|u_n^i\rangle$ reduces to $a_n|u_n^i\rangle$, the matrix representing the restriction of $A$ wo within $\mathscr{E}_n$ is equal to $a_n I_{g_n \times g_n}$. The matrix representing the operator $A$ in $\mathscr{E}_n$ is always diagonal and equal to $a_n I_{g_n \times g_n}$.

We use this property to obtain a basis of $\mathscr{E}_n$ composed of vectors that are also eigenvectors of $B$. The matrix representing $B$ in $\mathscr{E}_n$ when the basis is chosen is

$$\{|u_n^i\rangle\ , \quad i = 1, 2, \cdots, g_n\}, \tag{1.92}$$

has for its elements:

$$\beta_{ij}^{(n)} = \langle u_n^i | B | u_n^j \rangle. \tag{1.93}$$

Thi matri is Hermitian, since $B$ is a Hermitian operator. It is therefore diagonizable: one can find a new basis $\{|v_n^i\rangle;\ i = 1, 2, \cdots, g_n\}$ in which $B$ is represented by a diagonal matrix:

$$\langle v_n^i | B | v_n^j \rangle = \beta_i^n \delta_{ij}. \tag{1.94}$$

This means that the new basis vectors in $\mathscr{E}_n$ are eigenvectors of $B$:

$$B|v_n^i\rangle = \beta i^{(n)} |v_n^i\rangle. \tag{1.95}$$

These vectors are automatically eigenvectors of $A$ with an eigenvalue $a_n$ since they belong to $\mathscr{E}_n$.

Eigenvectors of $A$ associated with degenerate eigenvalues are not necessarily eigenvectors of $B$. It is always possible to choose, in every eigensubspace of $A$, a basis of eigenvectors common to $A$ and $B$.

If we perform this operation in all the subsespaces $\mathscr{E}_n$, we obtain a bsis of $\mathscr{E}$, formed by eigenvectors common to $A$ and $B$.

We shall denote by $|u_{n,p}^i\rangle$ the eigenvectors common to $A$ an $B$:

$$A|u_{n,p}^i\rangle = a_n |u_{n,p}^i\rangle, \quad \text{and} \quad B|u_{n,p}^i\rangle = b_p |u_{n,p}^i\rangle. \tag{1.96}$$

The index $i$ will be used to distinguish between different basis vectors which correspond to the same eigenvalues $a_n$ and $b_p$.

### Complete sets of commting observables (C.S.C.O.)

Consider an observable $A$ and a basis $\mathscr{E}$ composed of eigenvectors $|u_n^i\rangle$ of $A$.

If none of the eigenvalues of $A$ is degenerate, the various basis vectors of $\mathscr{E}$ can be labelled by the eigenvalue $a_n$ (index $i$ is not necessary). Thefroe, specifying the eigenvalue determines in a unique way the corresponding eigenvector. In other words, there exists only one basis of $\mathscr{E}$ formed by the eigenvectors of $A$. It is said that the observable $A$ constitutes, by itself, a C.S.C.O.

On the other hand, if at least one eigenvalue of $A$ is degenerate, specifying $a_n$ is no longer always sufficient to characterize a basis vector: the basis of eigenvectors of $A$ is not unique. One can choose any basis inside each of the degenerate eigensubspaces $\mathscr{E}_n$. We can choose another observable $B$ which commute with $A$ to construct an orthonormal basis of eigenvectors common to $A$ and $B$. $A$ and $B$ form a C.S.C.O. if this basis is unique, that is, if to each of the possible pairs ofeigevalues $\{a_n, b_p\}$ there corresponds only one basis vector. For $A$ and $B$ to constitute a C.S.C.O., it is necessary and sufficient that, inside each of tese subspaces, all the $g_n$ eigenvalues of $B$ be distinct. We can add indifinitely observables until we reach the C.S.C.O.

A set of observables $A, B, C, \cdots$ is called a complete set of commuting observables if:

(i) all the observables commute by pairs.

(ii) specifying the eigenvalue of all the operators determines a unique common eigenvector. The ket then is denoted as $|a_n, b_p, c_r, \cdots\rangle$.

This means that they are C.S.C.O. if there exists a unique orthonormal basis of common eigenvectors.

Idenfitication of CSCOs is necessary in order to construct physically meaningful bases for $\mathscr{E}$. Knowing the CSCOs that are available tells the experimenter the possible sets of measurements that can be made to achieve this goal.

We list some CSCOs for specific problems. (table 31 anerson)

## 1.5 More about operators

### 1.5.1 Trace of an operator

The trace of an operator $A$, $\mathrm{Tr}\,[A]$, is the sum of its diagonal matrix elements:

$$\mathrm{Tr}\,[A] = \sum_i \langle u_i|A|u_i\rangle\,, \quad \text{and} \quad \mathrm{Tr}\,[A] = \int d\alpha\ \langle \omega_\alpha|A|\omega_\alpha\rangle\,.$$

The trace is **invariant of the basis**, meaning that a change of representation will not affect the final result.

For a discrete basis, for instance, we have

$$\sum_i \langle u_i|A|u_i\rangle = \sum_i \langle u_i| \left[\sum_k |t_k\rangle\langle t_k|\right] A|u_i\rangle = \sum_{i,j} \langle t_k|A|u_i\rangle\langle u_i|t_k\rangle = \sum_k \langle t_k|A|\mathbb{1}|t_k\rangle = \sum_k \langle t_k|A|t_k\rangle.$$

If $A$ is an observable, then $\mathrm{Tr}\,[A]$ can be calculated in a basis of eigenvectors of $A$. The diagonal matrix elements are then the eigenvalues $a_n$ of $A$ and the trace can be written

$$\mathrm{Tr}\,[A] = \sum_n g_n a_n, \quad g_n = \text{degree of degeneracy of } a_n\,. \tag{1.97}$$

We list some properties:

$$\mathrm{Tr}\,[AB] = \mathrm{Tr}\,[BA] \;\Big|\; \mathrm{Tr}\,[ABC] = \mathrm{Tr}\,[BCA] = \mathrm{Tr}\,[CAB] \ \text{(cyclic permutation)}$$

### 1.5.2 Function of an operator

To express a function of an operator $A$, $F(A)$, we use Taylor expansion:

$$F(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n = \sum_{n=0}^{\infty} f_n (x-a)^n \Longrightarrow F(A) = \sum_{n=0}^{\infty} f_n (A-a)^n\,. \tag{1.98}$$

For example, the $e^A$ operator around $a = 0$ is:

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \mathbb{1} + A + \frac{A^2}{a!} + \frac{A^3}{3!} + \cdots$$

Let $|\varphi_k\rangle$ be an eigenvector of $A$ with eigenvalue $\lambda_k$, then (assuming $a = 0$):

$$A|\varphi_k\rangle = \lambda_k|\varphi_k\rangle \implies F(A)|\varphi_k\rangle = \sum_{n=0}^{\infty} f_n A^n \lambda|\varphi_k\rangle = \sum_{n=0}^{\infty} f_n \lambda_k^n|\varphi_k\rangle = F(\lambda_k)|\varphi_k\rangle.$$

If the operator $A$ has an eigenpar $(\lambda_k, \varphi_k)$, then $(F(\lambda_k), \varphi_k)$ is the eigenpar of $F(A)$.

### Potential operator

The potential operator is a function $V(\cdot)$ with the position operator $X$ as the argument, $V(X)$.

The eigenequation associated to this function is

$$V(\boldsymbol{R})|\boldsymbol{r}\rangle = V(\boldsymbol{r})|\boldsymbol{r}\rangle\,. \tag{1.99}$$

The matrix elements in $\{|\boldsymbol{r}\rangle\}$ are:

$$\langle\boldsymbol{r}|V(\boldsymbol{R})|\boldsymbol{r}'\rangle = V(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}')\,. \tag{1.100}$$

Finally, using the eigenequation above and the fact that $V(\boldsymbol{R})$ is Hermitian (the function $V(\boldsymbol{r})$ is real), we obtain:

$$\langle\boldsymbol{r}|V(\boldsymbol{R})|\psi\rangle = V(\boldsymbol{r})\psi(\boldsymbol{r})\,. \tag{1.101}$$

This shows that the action of $V(\boldsymbol{R})$ is simply multiplication by $V(\boldsymbol{r})$.

## 1.5.3 Commutator algebra

We have seen that the commutator of two operators is

$$[A, B] = AB - BA. \tag{1.102}$$

We then present some properties:

$[A, B] = -[B, A]$
$[A, B]^\dagger = [B^\dagger, A^\dagger]$
$[F(A), A] = 0$
$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$
$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]}$ $([A, [A, B]] = [B, [A, B]] = 0)$
$[X, P] = i\hbar$

$[A + B, C + D] = [A, C] + [A, D] + [B, C] + [B, D]$
$[A, BC] = [A, B]C + B[A, C]$
$[A, B] = 0 \implies [F(A), B] = [A, F(B)] = [F(A), F(B)] = 0$
$[A, [A, B]] = [B, [A, B]] = 0 \implies [A, F(B)] = [A, B]\dfrac{dF(B)}{dB}$
$[A, [A, B]] = [B, [A, B]] = 0 \implies [F(A), B] = [A, B]\dfrac{dF(A)}{dA}$

### 1.5.4 Derivative of an operator

Let $A(t)$ be a time-dependent operator, whose derivative is $dA/dt$. In a time-independent basis $\{|u_n\rangle\}$, the matrix elements of $A$ and $dA/dt$ are:

$$A_{ij}(t) = \langle u_i|A|u_j\rangle, \quad \text{and} \quad \left(\frac{dA}{dt}\right)_{ij} = \langle u_i|\frac{dA}{dt}|u_j\rangle = \frac{d}{dt}\langle u_i|A|u_j\rangle = \frac{dA_{ij}}{dt}. \tag{1.103}$$

The last equation corresponds to the matrix elements of $dA/dt$. We see that,

> To obtain the mtrix elements of $dA/dt$, we compute the derivative of each element of $A$.

Properties of differentiation also apply here. For instance, for product rule we have

$$\langle u_i|FG|u_j\rangle = \sum_k \langle u_i|F|u_k\rangle\langle u_k|G|u_j\rangle \Longrightarrow \langle u_i|\frac{d(FG)}{dt}|u_j\rangle = \sum_k \left[\langle u_i|\frac{dF}{dt}|u_k\rangle\langle u_k|G|u_j\rangle + \langle u_i|F|u_k\rangle\langle u_k|\frac{dG}{dt}|u_j\rangle\right]$$
$$= \langle u_i|\frac{dF}{dt}G + F\frac{dG}{dt}|u_j\rangle.$$

Other two examples are

$$\frac{d(e^{At})}{dt} = Ae^{At} \overset{\text{they commute}}{=} e^{At}A, \quad \text{and} \quad \frac{d(e^{At}e^{Bt})}{dt} = Ae^{At}e^{Bt} + e^{At}Be^{Bt}.$$

### 1.5.5 Unitary operators

An operator $U$ is unitary if its inverse $U^{-1}$ is equal to its adjoint $U^\dagger$:

$$U^\dagger U = UU^\dagger = \mathbb{1}. \tag{1.104}$$

The scalar product of $|\tilde{\psi}_1\rangle = U|\psi_1\rangle$ and $|\tilde{\psi}_2\rangle = U|\psi_2\rangle$ is conserved with unitary operators:

$$\langle\tilde{\psi}_1|\tilde{\psi}_2\rangle = \langle\psi_1|U^\dagger U|\psi_2\rangle = \langle\psi_1|\psi_2\rangle (= \delta_{ij}).$$

We show some important things about $U$:

- If $A$ is a Hermitian operator, the operator $T = e^{iA}$ is unitary:

$$T^\dagger T = TT^\dagger = (e^{-iA})(e^{iA}) = \mathbb{1}.$$

- The product of two unitary operators ($U, V$ for instance) is also unitry:

$$(UV)^\dagger(UV) = V^\dagger U^\dagger UV = V^\dagger V = \mathbb{1}.$$

> When two transformations conserve the scalar product, so does the successive application of these two transformations.

- Unitary operators constitute the generalization of orthogonal operators to complex spaces.

### Change of bases

Lets consider an orthonormal basis $\{|v_i\rangle\}$ and the transformation $\{|\tilde{v}_i\rangle\}$ basis under $U$, which are also orthonormal.

These vectors constitute a basis of $\mathscr{E}$, because

$$U^\dagger|\psi\rangle = \sum_i c_i|v_i\rangle \;/U \longrightarrow UU^\dagger|\psi\rangle = \sum_i c_i U|v_i\rangle = \sum_i c_i|\tilde{v}_i\rangle.$$

Any vector $|\psi\rangle$ can be expanded on the vectors $|\tilde{v}_i\rangle$, which therefore constitues a basis.

**How can one see from the matrix representing $U$ if this operator is unitary?**

When a matrix is unitary, the sum of the product of the elements of one column and the comple conjugates of the elements of another column is:

- zero if the two columns are different.
- one if they are not.

Given that $U|\psi_u\rangle = u|\psi_u\rangle$, the square of the norm of $U|\psi_u\rangle$ is:

$$\langle\psi_u|U^\dagger U|\psi_u\rangle = u^* u\langle\psi_u|\psi_u\rangle = u^* u.$$

Since the unitary operator conserves the norm, we have $u^* u = 1$. The eigenvalues of a unitary operator must therefore be complex numbers of modulus 1.

### Unitary transformations of operators

A unitary operator $U$ permits the construction, starting from one otrhonormal basis $\{|v_i\rangle\} \in \mathscr{E}$, of another one, $\{|\tilde{v}_i\rangle\}$.

Lets define the transform $\tilde{A}$ of the operator $A$ as the operator which, in the $\{|\tilde{v}_i\rangle\}$ basis, has the same matrix elements as $A$ in $\{|v_i\rangle\}$:

$$\langle\tilde{v}_i|\tilde{A}|\tilde{v}_j\rangle = \langle v_i|A|v_j\rangle. \tag{1.105}$$

Using $|\tilde{v}\rangle = U|v\rangle$:

$$\langle v_i|U^\dagger\tilde{A}U|v_j\rangle = \langle v_i|A|v_j\rangle \Longrightarrow \boxed{\tilde{A} = UAU^\dagger} \quad \text{Definition of } \tilde{A}.$$

This can be taken to be the definition of the transform $\tilde{A}$ of the operator $A$ by the unitary transformation $U$.

How can the eigenvetors of $\tilde{A}$ be obtained from those of $A$?

$$\tilde{A}|\varphi_a\rangle = (UAU^\dagger)U|\varphi_a\rangle = UA(U^\dagger U)|\varphi_a\rangle = UA|\varphi_a\rangle = aU|\varphi_a\rangle = a|\tilde{\varphi}_a\rangle.$$

**Eigenpar of the transform $\tilde{A}$**

The eigenvectors of the transform $\tilde{A}$ of $A$ are the transforms $|\tilde{\varphi}_a\rangle$ of eigenvectors $|\varphi_a\rangle$ of $A$: the eigenvalues are **unchanged**.

- The adjoint of the transform $\tilde{A}$ of $A$ by $U$ is the transform of $A^\dagger$ by $U$:

$$(\tilde{A})^\dagger = (UAU^\dagger)^\dagger = UA^\dagger U^\dagger = \tilde{A}^\dagger.$$

- Similarly,

$$(\tilde{A})^2 = UAU^\dagger UAU^\dagger = UAAU^\dagger = \tilde{A}^2 \Longrightarrow (\tilde{A})^n = \tilde{A}^n.$$

  Also,

$$\tilde{F}(A) = F(\tilde{A}).$$

## 1.6 Two important examples of representation and observables

### 1.6.1 The $\{r\}$ and $\{p\}$ representations

Recall the following bases of $\mathscr{F}$. They are not composed of functions belonging to $\mathscr{F}$:

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_0) \quad \text{and} \quad v_{\boldsymbol{p}_0}(\boldsymbol{r}) = (2\pi\hbar)^{-3/2} e^{\frac{i}{\hbar}\boldsymbol{p}_0 \cdot \boldsymbol{r}} \tag{1.106}$$

Every sufficiently regular equare-integrable function can be expanded in one or the other of these bases. The ket associted with $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ and $v_{\boldsymbol{p}_0}(\boldsymbol{r})$ will be denoted as:

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) \Longleftrightarrow |\boldsymbol{r}_0\rangle \quad \text{and} \quad v_{\boldsymbol{p}_0}(\boldsymbol{r}) \Longleftrightarrow |\boldsymbol{p}_0\rangle. \tag{1.107}$$

Using these bases $\{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$ and $\{v_{\boldsymbol{p}_0}(\boldsymbol{r})\}$ of $\mathscr{F}$ we thus define in $\mathscr{E}_{\boldsymbol{r}}$ two representation: the $\{|\boldsymbol{r}_0\rangle\}$ and the $\{|\boldsymbol{p}_0\rangle\}$ representations.

#### Orthonormalization and closure relations

If we calculate the scalar product of two kets, we have

$$\langle \boldsymbol{r}_0 | \boldsymbol{r}'_0 \rangle = \int d^3r \; \xi^*_{\boldsymbol{r}_0}(\boldsymbol{r}) \xi_{\boldsymbol{r}'_0}(\boldsymbol{r}) = \delta(\boldsymbol{r}_0 - \boldsymbol{r}'_0) \quad \text{and} \quad \langle \boldsymbol{p}_0 | \boldsymbol{p}'_0 \rangle = \int d^3r \; v^*_{\boldsymbol{p}_0}(\boldsymbol{r}) v_{\boldsymbol{p}'_0}(\boldsymbol{r}) = \delta(\boldsymbol{p}_0 - \boldsymbol{p}'_0).$$

Thus, te baseses are therefore orthonormal in the extended sense. The fact that the set of the $|\boldsymbol{r}_0\rangle$ or that of $|\boldsymbol{p}_0\rangle$ constitutes a basis in $\mathscr{E}_{\boldsymbol{r}}$ can be expressed by a closure relation in $\mathscr{E}_{\boldsymbol{r}}$:

| Orthonormality relation | Closure relation | |
|---|---|---|
| $\langle \boldsymbol{r}_0 \| \boldsymbol{r}'_0 \rangle = \delta(\boldsymbol{r}_0 - \boldsymbol{r}'_0)$ | $\int d^3r_0 \; \|\boldsymbol{r}_0\rangle\langle\boldsymbol{r}_0\| = \mathbb{1}$ | (1.108) |
| $\langle \boldsymbol{p}_0, \boldsymbol{p}'_0 \rangle = \delta(\boldsymbol{p}_0 - \boldsymbol{p}'_0)$ | $\int d^3p_0 \; \|\boldsymbol{p}_0\rangle\langle\boldsymbol{p}_0\| = \mathbb{1}$ | (1.109) |

### Components of a ket

Consider a ket $|\psi\rangle$ corresponding to $\psi(\boldsymbol{r})$. We can expand it in each representation using the closure relation:

$$|\psi\rangle = \int d^3r_0 \; |\boldsymbol{r}_0\rangle\langle\boldsymbol{r}_0|\psi\rangle, \quad \text{where} \quad \langle\boldsymbol{r}_0|\psi\rangle = \psi(\boldsymbol{r}_0) = \int d^3r \; \xi^*_{\boldsymbol{r}_0}(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{1.110}$$

$$|\psi\rangle = \int d^3p_0 \; |\boldsymbol{p}_0\rangle\langle\boldsymbol{p}_0|\psi\rangle, \quad \text{where} \quad \langle\boldsymbol{p}_0|\psi\rangle = \tilde{\psi}(\boldsymbol{p}_0) = \int d^3r \; v^*_{\boldsymbol{p}_0}(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{1.111}$$

We see that $\tilde{\psi}(\boldsymbol{p}_0)$ is the Fourier transform of $\psi(\boldsymbol{r}_0)$. Each value corresponds to the components of $|\psi\rangle$ on the basis vector of the respective representation.

Now, we redefine the above bases to just $|\boldsymbol{r}\rangle$ and $|\boldsymbol{p}\rangle$:

$$\begin{array}{ll} \langle\boldsymbol{r}|\psi\rangle = \psi(\boldsymbol{r}) & \langle\boldsymbol{p}|\psi\rangle = \tilde{\psi}(\boldsymbol{p}) \\ \langle\boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') & \langle\boldsymbol{p},\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') \\ \displaystyle\int d^3r|\boldsymbol{r}\rangle\langle\boldsymbol{r}| = \mathbb{1} & \displaystyle\int d^3p \; |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1} \end{array} \tag{1.112}$$

### Changing from $\{|\boldsymbol{r}\rangle\}$ to $\{|\boldsymbol{p}\rangle\}$ representation

Changing from one basis to the other brinds in the numbers:

$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \langle\boldsymbol{p}|\boldsymbol{r}\rangle^* = \int d^3r' \; \langle\boldsymbol{r}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\boldsymbol{p}\rangle = \int d^3r' \; \delta(\boldsymbol{r}-\boldsymbol{r}')(2\pi\hbar)^{-3/2}e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'} = (2\pi\hbar)^{-3/2}e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}. \tag{1.113}$$

A given ket $|\psi\rangle$ is represented by $\langle\boldsymbol{r}|\psi\rangle = \psi(\boldsymbol{r})$ in the $\{|\boldsymbol{r}\rangle\}$ representation and by $\langle\boldsymbol{p}|\psi\rangle = \tilde{\psi}(\boldsymbol{p})$ in the $\{|\boldsymbol{p}\rangle\}$ representation.

Therefore,

$$\psi(\boldsymbol{r}) = \langle\boldsymbol{r}|\psi\rangle = \int d^3p \; \langle\boldsymbol{r}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\psi\rangle = (2\pi\hbar)^{-3/2}\int d^3p \; e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\tilde{\psi}(\boldsymbol{p}) \tag{1.114}$$

$$\tilde{\psi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi\rangle = \int d^3r \; \langle\boldsymbol{p}|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\psi\rangle = (2\pi\hbar)^{-3/2}\int d^3r \; e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\psi(\boldsymbol{r}) \tag{1.115}$$

$$A(\boldsymbol{p},\boldsymbol{p}') = (2\pi\hbar)^{-3}\int d^3r \; \int d^3r' \; e^{\frac{i}{\hbar}(\boldsymbol{p}\cdot\boldsymbol{r}-\boldsymbol{p}'\cdot\boldsymbol{r}')}A(\boldsymbol{r}',\boldsymbol{r}) \tag{1.116}$$

## 1.6.2 The R and P operators

We define the $X$, $Y$, $Z$ operators whsoe action, in the $\{|\boldsymbol{r}\rangle\}$ representation, is given by:

$$\begin{array}{l} \langle\boldsymbol{r}|X|\psi\rangle = x\langle\boldsymbol{r}|\psi\rangle \\ \langle\boldsymbol{r}|Y|\psi\rangle = y\langle\boldsymbol{r}|\psi\rangle \\ \langle\boldsymbol{r}|Z|\psi\rangle = z\langle\boldsymbol{r}|\psi\rangle \end{array} \tag{1.117}$$

X, Y, and Z will be considered to be the components of a vector operator $\boldsymbol{R}$. Similarly, we define the vector operator $\boldsymbol{P}$ by its components $P_x$, $P_y$, $P_z$, whose action, in the $\{|\boldsymbol{p}\rangle\}$ representation is given by:

$$\begin{array}{l} \langle\boldsymbol{p}|P_x|\psi\rangle = p_x\langle\boldsymbol{p}|\psi\rangle \\ \langle\boldsymbol{p}|P_y|\psi\rangle = p_y\langle\boldsymbol{p}|\psi\rangle \\ \langle\boldsymbol{p}|P_z|\psi\rangle = p_z\langle\boldsymbol{p}|\psi\rangle \end{array} \tag{1.118}$$

How $\boldsymbol{P}$ operator acts in the $\{|\boldsymbol{r}\rangle\}$ representation? We use the closure relation to obtain:

$$\begin{aligned}\langle \boldsymbol{r}|P_x|\psi\rangle &= \int d^3p\ \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|P_x|\psi\rangle \\ &\overset{(a)}{=} (2\pi\hbar)^{-3/2}\int d^3p\ e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}p_x\tilde{\psi}(\boldsymbol{p}) \\ \langle \boldsymbol{r}|P_x|\psi\rangle &\overset{(b)}{=} \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\boldsymbol{r}).\end{aligned}$$

In $(a)$ we have used the equation (1.113) while in $(b)$ we have used the property of the derivative of a Fourier transform. Generally, the result is:

$$\langle \boldsymbol{r}|\boldsymbol{P}|\psi\rangle = \frac{\hbar}{i}\nabla\langle \boldsymbol{r}|\psi\rangle = \frac{\hbar}{i}\nabla\psi(\boldsymbol{r})\,. \tag{1.119}$$

In the $\{|bR\rangle\}$ representation, the $\boldsymbol{P}$ operator coincides with the differential operator $(\hbar/i)\nabla$ applied to the wave functions.

If we compute the commutator say, $[X, P_x]$, we have

$$\begin{aligned}\langle \boldsymbol{r}|[X,P_x]|\psi\rangle &= \langle \boldsymbol{r}|(XP_x - P_xX)|\psi\rangle \\ &= \langle \boldsymbol{r}|XP_x|\psi\rangle - \langle \boldsymbol{r}|P_xX|\psi\rangle \\ &= \int d^3r'\ \langle \boldsymbol{r}|X|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|P_x|\psi\rangle - \int d^3r'\ \langle \boldsymbol{r}|P_x|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|X|\psi\rangle \\ &= \int d^3r'\ \left[x'\delta(\boldsymbol{r}-\boldsymbol{r}')\right]\frac{\hbar}{i}\frac{\partial}{\partial x}\langle \boldsymbol{r}'|\psi\rangle - \int d^3r'\ \left[\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(\boldsymbol{r}-\boldsymbol{r}')\right]x'\langle \boldsymbol{r}'|\psi\rangle \\ &= \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\langle \boldsymbol{r}|\psi\rangle) \\ &= \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle \\ \langle \boldsymbol{r}|[X,P_x]|\psi\rangle &= i\hbar\langle \boldsymbol{r}|\psi\rangle.\end{aligned}$$

Thus, one finds $[X, P_x] = i\hbar$. In the same way, we find all the other commutators between the components of $\boldsymbol{R}$ and $\boldsymbol{P}$:

Canonical commutation relations
$$[R_i, R_j] = 0, \quad [P_i, P_j] = 0, \quad [R_i, P_j] = i\hbar\delta_{ij}, \quad i,j = 1,2,3\,. \tag{1.120}$$

**R and P are Hermitian**

All the components of $\boldsymbol{R}$ and $\boldsymbol{P}$ are Hermitian operators.

For example,

$$\langle \varphi|X|\psi\rangle = \int d^3r\ \varphi^*(\boldsymbol{r})x\psi(\boldsymbol{r}) = \left[\int d^3r\ \varphi(\boldsymbol{r})x\psi^*(\boldsymbol{r})\right]^* = \langle \psi|X|\varphi\rangle^*.$$

### Eigenvectors of R and P

Consider the action of $X$ on the ket $|\boldsymbol{r}_0\rangle$:

$$\langle \boldsymbol{r}|X|\boldsymbol{r}_0\rangle = x\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle = x\delta(\boldsymbol{r}-\boldsymbol{r}_0) = x_0\delta(\boldsymbol{r}-\boldsymbol{r}_0) = x_0\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle.$$

The components in $\{|\boldsymbol{r}\rangle\}$ representation of the ket $X|\boldsymbol{r}_0\rangle$ are equal to those of the ket $\boldsymbol{r}_0$ multiplied by $x_0$:

$$X|\boldsymbol{r}_0\rangle = x_0|\boldsymbol{r}_0\rangle. \tag{1.121}$$

Omitting the index zero, and doing the same for the other components of $\boldsymbol{R}$ and $\boldsymbol{P}$ in their respective representations yield:

$$\begin{array}{l} X|\boldsymbol{r}\rangle = x|\boldsymbol{r}\rangle \\ Y|\boldsymbol{r}\rangle = y|\boldsymbol{r}\rangle \\ Z|\boldsymbol{r}\rangle = z|\boldsymbol{r}\rangle \end{array}, \quad \text{and} \quad \begin{array}{l} P_x|\boldsymbol{p}\rangle = p_x|\boldsymbol{p}\rangle \\ P_y|\boldsymbol{p}\rangle = p_y|\boldsymbol{p}\rangle \\ P_z|\boldsymbol{p}\rangle = p_z|\boldsymbol{p}\rangle \end{array} \tag{1.122}$$

### R and P are observables

We have already demonstrated the closure relation for each representation $\{|\boldsymbol{r}\rangle\}$ and $\{|\boldsymbol{p}\rangle\}$ in equation (1.112). Therefore, $\boldsymbol{R}$ and $\boldsymbol{P}$ are observables. In a three-dimensional space, is necessary to specify the eigenvalues $x_o, y_o, z_o$ as they uniquely determines the corresponding eigevector $|\boldsymbol{r}_0\rangle$.

The set of the three operators $X, Y, Z$ and the set of the three operators $P_x, P_y, P_z$ constitute a CSCO in $\mathscr{E}_{\boldsymbol{r}}$.

Recall that an operator must have eigenvectors that span the whole state vector, so missing one coordinate will degenerate it and therefore is no longer uniquely determined. One can also mix X with P as $\{X, P_y, P_z\}$ to create CSCOs.

## Chapter 2

# Postulates of Quantum Mechanics

## 2.1 Introduction

In classical mechanics, the motion of any physical system is determined through the position $\boldsymbol{r} = (x, y, z)$ and the velocity $\boldsymbol{v} = (\dot{x}, \dot{y}, \dot{z})$. One usually introduces generalized coordinates $q_i(t)$ whose derivatives with respect to time $\dot{q}_i(t)$. are the generalized velocities. With these coordinates, the position and velocity of any point can be calculated. Using the Lagrangian $\mathcal{L}(q_i, \dot{q}_i, t)$ one defines the conjugate momentum $p_i$ os each of the generalized cooridnates $q_i$:

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}.$$

The $q_i(t)$ and $p_i(t)$ are called **fundamental dynamical variables**. All the physical quantities associated with the system (energy, angular momentum, etc) can be expressed in terms of the fundamental dynamical variables.

The motion (evolution) of a system can be studied by Lagrange's equations or the Hamilton-Jacobi canonical equation:

$$\text{Hamilton-Jacobi equations} \qquad \frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}.$$

The classical description of a physical system can be summarized as follows:

- The state of the system at time $t_0$ is defined by specifying $N$ generalized coordinates $q_i(t_0)$ and their $N$ conjugate momenta $p_i(t_0)$.
- Knowing the state of the system at $t_0$, allows to predict with certainty the result of any measurement performed at time $t_0$.
- The time evolution of the state of the system is given by the **Hmailton-Jacobi** equations. The state of the system is known for all time if its initial state is known.

## 2.2 Statements of the postulates

### 2.2.1 State and measurable physical quantites of a system

The quantum state of a particle at a fixed time is characterized by a ket of the space $\mathscr{E}_{\boldsymbol{r}}$.

**First postulate: Sate of a system**

At time $t_0$, the state of an isolated physical system is defined by specifying a ket $|\psi(t_0)\rangle \in \mathscr{E}_{\boldsymbol{r}}$.

Recall that, sinsce $\mathscr{E}$ is a vector space, a linear combination of state vectors is a state vector.

**Second postulate: Measurable physical quantities**

Every measurable physical quantity $\mathcal{A}$ is described by an operator $A$ acting in $\mathscr{E}$: this operator is an **observable**.

In this sense, a state is represented by a vector, while a physical quantity by an operator.

**Third postulate: Outcomes of measurements**

The only possible result of the measurement of a physical quantity $\mathcal{A}$ is one of the eigenvalues of the corresponding observable $A$.

- A measurement of $\mathcal{A}$ gives **always** a real value, since $A$ is Hermitian by definition.
- If the spectrum of $A$ is discrete, the results that can be obtained by measuring $\mathcal{A}$ are **quantized**.

### 2.2.2 Principle of spectral decomposition

Consider a system whose state is characterized, at a given time, by $|\psi\rangle$, which is assumed normalized. We want to predict the result of the measurement, at thi time, of a physical quantity $\mathcal{A}$ associated with the observable $A$.

#### Discrete spectrum

If all eigenvalues $a_n$ of $A$ are non-degenerate, there is associated with each of them a **unique** eigenvector $|u_n\rangle$. As $A$ is an observable, the set of $|u_n\rangle$ which we assume normalized, conssitutes a basis in $\mathscr{E}$ and we can expand $|\psi\rangle$:

$$A|u_n\rangle = a_n|u_n\rangle \Longrightarrow |\psi\rangle = \sum_n c_n|u_n\rangle$$

The probability $P(a_n)$ of finding $a_n$ when $\mathcal{A}$ is measured is therefore:

$$P(a_n) = |c_n|^2 = |\langle u_n|\psi\rangle|^2.$$

If, however, some of the eigenvalues $a_n$ are degenerate, several orthonormalized eigenvectors $|u_n^i\rangle$ corresponds to them and we can still expand $|\psi\rangle$ on the orthonormal basis $\{|u_n^i\rangle\}$:

$$A|u_n^i\rangle = a_n|u_n^i\rangle,\ i = 1, 2, \cdots, g_n \Longrightarrow |\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i|u_n^i\rangle. \tag{2.1}$$

The probability now becomes

$$P(a_n) = \sum_{i=1}^{g_n} |c_n^i|^2 = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2. \tag{2.2}$$

**Foruth postulate (discrete case): Result of a measurement**

When $\mathcal{A}$ is measured on a system in the normalized state $|\psi\rangle$, the probability $P(a_n)$ of obtaining the eigenvalue $a_n$ of the observable $A$ is the discrete projection of $\psi$ onto the eigensubspace $\mathscr{E}_n$:

$$P(a_n) = \langle\psi|P_n|\psi\rangle = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2, \quad P_n = \sum_{i=1}^{g_n} |u_n^i\rangle\langle u_n^i|.$$

$\{|u_n^i\rangle\}$ is a set of orthonormal vectors which forms a basis in the eigensubspace $\mathscr{E}_n$.

### Continuous case

If now the spectrum of $A$ is continuous and non-degenerate, the eigenvectors of $A$ forms a continuous basis in $\mathscr{E}$, in terms of which $|\psi\rangle$ can be expanded:

$$A|v_\alpha\rangle = \alpha|v_\alpha\rangle \Longrightarrow |\psi\rangle = \int d\alpha\, c(\alpha)|v_\alpha\rangle.$$

In this case, we cannot define the probability on a single point; we must define a probability density function. The differential probability of obtaining a value included betwen $\alpha$ and $\alpha + d\alpha$ is

$$dP(\alpha) = \rho(\alpha)d\alpha, \quad \text{with} \quad \rho(\alpha) = |c(\alpha)|^2 = |\langle v_\alpha|\psi\rangle|^2.$$

**Fourth postulate (continuous case, non-degenerate): Result of a measurement**

If $\mathcal{A}$ is measured in the normalized state $|\psi\rangle$, the probability of obtaining a result within betwen $\alpha_1$ and $\alpha_2$ is the continuous projection of $\psi$ onto that interval:

$$P(\alpha_1 < \alpha < \alpha_2) = \langle\psi|P_{\alpha_1,\alpha_2}|\psi\rangle = \int_{\alpha_1}^{\alpha_2} |\langle v_\alpha|\psi\rangle|^2\, d\alpha\,, \quad P_{\alpha_1,\alpha_2} = \int_{\alpha_1}^{\alpha_2} |v_\alpha\rangle\langle v_\alpha|\, d\alpha. \tag{2.3}$$

In cases where the state $|\psi\rangle$ is **not normalized**, we then use the following expressions:

$$\begin{array}{ll} \text{Discrete case} & \text{Continuous case} \\ P(a_n) = \dfrac{1}{\langle\psi|\psi\rangle}\displaystyle\sum_{i=1}^{g_n} |c_n^i|^2 & \rho(\alpha) = \dfrac{1}{\langle\psi|\psi\rangle}|c(\alpha)|^2. \end{array} \tag{2.4}$$

On the other hand, two proportional state vectors, $|\psi'\rangle = ae^{i\theta}|\psi\rangle$, represent **the same** physical state:

$$|\langle u_n^i|\psi'\rangle|^2 = |e^{i\theta}\langle u_n^i|\psi\rangle|^2 = |\langle u_n^i|\psi\rangle|^2.$$

$a$ is simplified when dividing by $\langle\psi'|\psi'\rangle$.

**Global versus relative phase factor**

A global phase factor does not affect the physical preditions, but the relative phases of the coefficients of an expansion are significant.

### 2.2.3 Reduction of the wave packet

We want to measure at a given point the physical quantity $\mathcal{A}$. If the ket $|\psi\rangle$ before the measurement is knwon, the fourth postulate allows us to predict the probability of the various possible outcomes. Immbediately after the measurement, we cannot speak of probability, as we have alreade got the result (collapse).

If the measurement of $\mathcal{A}$ resulted in $a_n$ (assuming discrete spectrum of $A$), the state of the system immediately after this measurement is the eigenvector $|u_n\rangle$ associate with $a_n$:

$$\text{State of collapse} \qquad |\psi\rangle \xrightarrow{(a_n)} |u_n\rangle. \tag{2.5}$$

- If we perform a second measurement of $\mathcal{A}$ immediately after the first one, we shall always find the same result $a_n$.
- We use just after the measurement to assume the system had not time to evolve, because otherwise the state evolves and we need the sixth postulate to keep track of this motion.

When the eigenvalue $a_n$ is degenerate, then the state just before the measurement is written as (equation (2.1)):

$$|\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle.$$

And the state of collapse just after the measurement is

$$\text{State of collapse} \qquad |\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{1}{\sqrt{\sum_{i=1}^{g_n} |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle. \tag{2.6}$$

The square root factor is the normalization so that we get a unitary norm of the state. We rewrite the above expression in the following fifth postulate.

**Firfth postulate: State of collapse**

If the measurement of the $\mathcal{A}$ in the state $|\psi\rangle$ gives the result $a_n$, the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the eigensubspace $\mathscr{E}_n$ associated with $a_n$:

$$|\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}} \tag{2.7}$$

It is not an arbitrary ket of $\mathscr{E}_n$, but the part of $|\psi\rangle$ that belongs to $\mathscr{E}_n$.

### 2.2.4 Time evolution of Systems

**Sixth postulate: Time evolution of the system**

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrodinger equation:

$$ih\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle\,, \tag{2.8}$$

where $H(t)$ is the **Hamiltonian operator** (observable) associated with the total energy of the system.

### 2.2.5 Quantization rules

We will discuss how to construct, for a physical quantity $\mathcal{A}$ already deffined in classical mechanics, the operator $A$ which rescribes it in quantum mechanics.

## 2.3 The physical interpretation of the postulates

### 2.3.1 Quantization rules are consistent with probabilistic interpretation

Lets consider a one-dimensional problem. If the particle is in the normalized state $|\psi\rangle$, the probability that a measurement of its position will yield a result included between $x$ and $x + dx$ is equal to (equation (2.4)):

$$dP(x) = |\langle x|\psi\rangle|^2 \, dx.$$

Now, to the eigenvector $|p\rangle$ of the observable $P$ corresponds the plane wave:

$$\langle x|p\rangle = (2\pi\hbar)^{-1/2} e^{\frac{ipx}{\hbar}}. \tag{2.9}$$

and we have seen that de Broglie relations associate with this wave a well-defined momentum which is precisely $p$. In ddition, the probability of finding, for a particle in $|\psi\rangle$, a momnetum between $p$ and $p + dp$ is:

$$dP(p) = |\langle p|\psi\rangle|^2 \, dp = |\tilde{\psi}(p)|^2 \, dp. \tag{2.10}$$

### 2.3.2 The measurement process

There is the question of the "fundamental" perturbation involved in the observation of quantum system. The origin of these problems lies in hte fact that the system under study is treated independently from the measurement device, although hteir interaction s essential to the observation process. One should actually consider the system and the measurement device together as a whole. This raise delicate questions concerning the details of the measurement process.

The nondeterministic formulation of the fourth and fifth postulates is related to the problems that we have mentiones. OFr example, the abrup change from one stat evector to another de to the measurement corrsponds to the fundamental perturbation of which we have spoken. We shall consider here only ideal measurements: the perturbation they provoke is due only to the quantum mechanical aspect of th emeasurement. Of course, real devices always present imperfections that affect the measurement and the system.

### 2.3.3 Mean value of an observable in a given state

The predictions deduced from the fourth postulate are expressed in terms of probabilities. To verigy them, it would be necessary to perform a large nuvmber of measurements under identical ocnditions. This means measuring the same quantity in a large number of systems which are all in the same quantum state. If these predictions are correct, the proportion of $N$ identical experiments resulting in a given event will approach, as $N \to \infty$, the theorically predicted probability $P$ of this event. In practice, of course, $N$ is finite, and statisticla techniques must be used to interpret the results.

The **mean value of an observable** $A$ in the state $|\psi\rangle$, which we shall denote by $\langle A\rangle_\psi$, or $\langle A\rangle$, is defined as the average of the results obtained when a large number $N$ of measurements of this observable are performed on systems which are all in the state $|\psi\rangle$. When $|\psi\rangle$ is given, we can compute the probabilities of findins all the possible results, and therefore, $\langle A\rangle_\psi$ is known.

If $|\psi\rangle$ is normalized, $\langle A\rangle$ is given by

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle \tag{2.11}$$

Assuming discrete spectrum, out of $N$ measurements of $\mathcal{A}$, the eigenvalue $a_n$ will be obtained $N(a_n)$ times, with

$$\lim_{N\to\infty}\frac{N(a_n)}{N}=P(a_n),\quad \text{and}\quad \sum_n N(a_n)=N. \tag{2.12}$$

In the limit, we can approximate therefore the mean value of the results as

$$\langle A\rangle_\psi=\lim_{N\to\infty}\frac{1}{N}\sum_n a_n N(a_n)=\sum_n a_n P(a_n). \tag{2.13}$$

The last expression is then treated:

$$\begin{aligned}\langle A\rangle_\psi&=\sum_n a_n P(a_n)=\sum_n a_n\langle\psi|P_n|\psi\rangle=\sum_n a_n\sum_{i=1}^{g_n}\langle\psi|u_n^i\rangle\langle u_n^i|\psi\rangle=\sum_n\sum_{i=1}^{g_n}\langle\psi|a_n|u_n^i\rangle\langle u_n^i|\psi\rangle\\&=\sum_n\sum_{i=1}^{g_n}\langle\psi|A|u_n^i\rangle\langle u_n^i|\psi\rangle=\langle\psi|A\left[\sum_n\sum_{i=1}^{g_n}|u_n^i\rangle\langle u_n^i|\right]|\psi\rangle=\langle\psi|A\mathbb{1}|\psi\rangle=\langle\psi|A|\psi\rangle.\end{aligned}$$

In the continuous case, we have something similar:

$$\lim_{N\to\infty}\frac{dN(\alpha)}{N}=dP(\alpha). \tag{2.14}$$

In the limit, we can approximate the mean value of the results as

$$\langle A\rangle_\psi=\lim_{N\to\infty}\frac{1}{N}\int\alpha\,dN(\alpha)=\int\alpha\,dP(\alpha). \tag{2.15}$$

The last expression is then treated:

$$\begin{aligned}\langle A\rangle_\psi&=\int\alpha\,dP(\alpha)=\int\alpha\langle\psi|v_\alpha\rangle\langle v_\alpha|\psi\rangle\,d\alpha=\int\langle\psi|A|v_\alpha\rangle\langle v_\alpha|\psi\rangle\,d\alpha\\&=\langle\psi|A\left[\int d\alpha\,|v_\alpha\rangle\langle v_\alpha|\right]|\psi\rangle=\langle\psi|A\mathbb{1}|\psi\rangle=\langle\psi|A|\psi\rangle.\end{aligned}$$

- If the ket $|\psi\rangle$ is not normalized, then we use

$$\text{Mean value of } A\qquad \boxed{\langle A\rangle_\psi=\frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}}. \tag{2.16}$$

- In practice, one often places oneself in a particular representation to compute $\langle A\rangle_\psi$.

$$\begin{aligned}\langle X\rangle_\psi&=\langle\psi|X|\psi\rangle=\int d^3r\,\langle\psi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|X|\psi\rangle=\int d^3r\,\psi^*(\boldsymbol{r})x\psi(\boldsymbol{r}).\\\langle P_x\rangle_\psi&=\langle\psi|P_x|\psi\rangle=\int d^3r\,\tilde\psi^*(\boldsymbol{p})p_x\tilde\psi(\boldsymbol{p}),\quad\text{or}\\\langle P_x\rangle_\psi&=\langle\psi|P_x|\psi\rangle=\int d^3r\,\langle\psi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|P_x|\psi\rangle=\int d^3\,\psi^*(\boldsymbol{r})\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\boldsymbol{r})\right].\end{aligned}$$

### 2.3.4 The root mean square deviation

$\langle A \rangle$ indicates the order of magnitude of the values of the observables $A$ when the system is in the state $|\psi\rangle$. However, this mean values does not give any idea of the dispersion of the results we expect when measuring $A$.

We therefore define the **root mean square deviation** $\Delta A$ as

$$\text{RMS deviation} \qquad \Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}\,. \tag{2.17}$$

If this definition is applied to the observable $\boldsymbol{R}$ and $\boldsymbol{P}$, we can shown, using commutation realtions, that for any state $|\psi\rangle$, we have

$$\text{Heisenberg relations} \qquad \begin{array}{l} \Delta X \cdot \Delta P_x \geq \frac{\hbar}{2} \\ \Delta Y \cdot \Delta P_y \geq \frac{\hbar}{2} \\ \Delta Z \cdot \Delta P_z \geq \frac{\hbar}{2} \end{array}\,. \tag{2.18}$$

### 2.3.5 Compatibility of observables

#### Compatibility and commutation rules

Let be two commutate observable $A$ and $B$ $[A, B] = 0$, and assume discrete spectrum. There exists a basis of the state space composed of eigenkets commont to $A$ and $B$, which we denote $|a_n, b_p, i\rangle$:

$$\begin{aligned} A|a_n, b_p, i\rangle &= a_n |a_n, b_p, i\rangle \\ B|a_n, b_p, i\rangle &= b_p |a_n, b_p, i\rangle. \end{aligned}$$

For any $a_n$ and $b_p$, there exists at least one state $|a_n, b_p, i\rangle$ for which a measurement of $A$ will always give $a_n$ and a measurement of $B$ will always give $b_p$. These observables which can be simultaneously determined are said to be **compatible**.

The initial state of a system $|\psi\rangle$ can always be written as

$$|\psi\rangle = \sum_{n,p,i} c_{n,p,i} |a_n, b_p, i\rangle.$$

Assume we measure $A$ and then immediately we measure $B$. First, the probability of having $a_n$ is

$$P(a_n) = \sum_{p,i} |c_{n,p,i}|^2. \tag{2.19}$$

When we then measure $B$, the system is no long in the state $|\psi\rangle$ but, if we found $a_n$ in the state $|\psi'_n\rangle$ we have

$$|\psi'_n\rangle = \frac{1}{\sqrt{\sum_{p,i} |c_{n,p,i}|^2}} \sum_{p,i} c_{n,p,i} |a_n, b_p, i\rangle.$$

The probability of obtaining $b_p$ when it is known that the first measurement was $a_n$ is then

$$P_{a_n}(b_p) = \frac{1}{\sum_{p,i} |c_{n,p,i}|^2} \sum_{i} |c_{n,p,i}|^2. \tag{2.20}$$

The probability $P(a_n, b_p)$ of obtaining $a_n$ in the first measureement and $b_p$ in the second is then a composite event, we must first find $a_n$ and then find $b_p$. Therefore,

$$P(a_n, b_p) = P(a_n)P_{a_n}(b_p) = \sum_i |c_{n,p,i}|^2. \tag{2.21}$$

The state of the system becomes imediately after the second measuremet

$$|\psi''_{n,p}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{2.22}$$

$|\psi''_{n,p}\rangle$ is an eigenvector common to $A$ and $B$ with the eigenvalues $a_n$ and $b_p$, respectively.

If we do the same in opposite order, that is, measuring $B$ and then $A$ we have

$$P(b_p, a_n) = \sum_i |c_{n,p,i}|^2, \quad \text{and} \quad |\psi''_{p,n}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{2.23}$$

**Consequence of compatible observables**

When two observables are compatible, the physical predictions ae the **same**, whatever the order of performing the two measurements. The probability and the state after the last measurements are for both cases:

$$P(a_n, b_p) = P(b_p, a_n) = \sum_i |c_{n,p,i}|^2 = \sum_i |\langle a_n, b_p, i|\psi\rangle|^2, \quad \text{and} \tag{2.24}$$

$$|\psi''_{n,p}\rangle = |\psi''_{p,n}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{2.25}$$

When two observables $A$ and $B$ are compatibles, the measurement of $B$ does not cause any loss of information previously obtained from the measurement of $A$, and viceversa.

New measurement of $A$ or $B$ will yields the same values again without fail.

Preparation of a state

## 2.4 Physical implications of the Schrodinger equation

Recall the Schrodinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi\rangle. \tag{2.26}$$

### 2.4.1 General properties of the Schrodinger equation

The ir no indeterminacy in the time evolution of a quantum system. Indeterminacy appears only when a physical quantity is measured.

Between two measurements, the state vectors evolves (following Shcrodinger equation) in a perfectly deterministic way.

### Supeorposition

The equation (2.26) is linear and homogeneous, then their slutions are linearly superposable:

$$|\psi(t_0)\rangle = \lambda_1|\psi_1(t_0)\rangle + \lambda_2|\psi_2(t_0)\rangle \Longrightarrow |\psi(t)\rangle = \lambda_1|\psi_1(t)\rangle + \lambda_2|\psi_2(t)\rangle. \tag{2.27}$$

### Conservation of probability

Since the Hamiltonian operator $H(t)$ is Hermitian, the square of the norm of the state vector $\langle\psi(t)|\psi(t)\rangle$ does not depend on time:

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= \left[\frac{d}{dt}\langle\psi(t)|\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{d}{dt}|\psi(t)\rangle\right] \\
&= \left[-\frac{1}{i\hbar}\langle\psi(t)|H(t)\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{1}{i\hbar}H(t)|\psi(t)\rangle\right] \\
&= -\frac{1}{i\hbar}\langle\psi(t)|H(t)|\psi(t)\rangle + \frac{1}{i\hbar}\langle\psi(t)|H(t)|\psi(t)\rangle \\
\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= 0.
\end{aligned}$$

The property of conservation of the norm which we have derived is expressed by the equation

$$\langle\psi(t)|\psi(t)\rangle = \int d^3r\ |\psi(\boldsymbol{r},t)|^2 = \langle\psi(t_0)|\psi(t_0)\rangle = 1. \tag{2.28}$$

This implies that time evolution does not modify the global probability of finding the particle in all space, which always remains equal to 1.

### Evolution of the mean value of an observable

The mean value of the observable $A$ at the instant $t$ is

$$\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle. \tag{2.29}$$

The mean value may depends on time by the state $\psi(t)$, but also by the observator itself $A(t)$. If we differentiate the above equation with time we have

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|A(t)|\psi(t)\rangle &= \left[\frac{d}{dt}\langle\psi(t)|\right]A(t)|\psi(t)\rangle + \langle\psi(t)|A\left[\frac{d}{dt}|\psi(t)\rangle\right] + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle \\
&= \frac{1}{i\hbar}\langle\psi(t)|[A(t)H(t) - H(t)A(t)]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle.
\end{aligned}$$

Therefore,

Evolution of the mean value of $A$ $$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[A,H(t)]\rangle + \langle\frac{\partial A}{\partial t}\rangle. \tag{2.30}$$

The mean value $\langle A \rangle$ is a number whch depends only on time $t$. It is this value that must be compared to the value taken on by the classical uantity $\mathcal{A}(\boldsymbol{r}, \boldsymbol{p}, t)$.

We can apply the equation (2.30) to the observables $\boldsymbol{R}$ and $\boldsymbol{P}$, assuming a scalar stationary potential $V(\boldsymbol{r})$:

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{R}).$$

We also have

$$\frac{d}{dt}\langle \boldsymbol{R} \rangle = \frac{1}{i\hbar}\langle [\boldsymbol{R}, H] \rangle = \frac{1}{\hbar}\langle [\boldsymbol{R}, \frac{\boldsymbol{P}^2}{2m}] \rangle = \frac{i\hbar}{m}\boldsymbol{P}, \quad \text{and} \quad \frac{d}{dt}\langle \boldsymbol{P} \rangle = \frac{1}{i\hbar}\langle \boldsymbol{P}, H \rangle = \frac{1}{i\hbar}\langle [\boldsymbol{P}, V(\boldsymbol{R})] \rangle = -i\hbar \nabla V(\boldsymbol{R}).$$

Therefore, we have the **Ehrenfest's theorem**:

$$\text{Ehrenfest's theorem} \qquad \begin{aligned} \frac{d}{dt}\langle \boldsymbol{R} \rangle &= \frac{1}{m}\langle \boldsymbol{P} \rangle \\ \frac{d}{dt}\langle \boldsymbol{P} \rangle &= -\langle \nabla V(\boldsymbol{R}) \rangle \end{aligned}. \tag{2.31}$$

classical limits of the Ehrenfest's theorem

### 2.4.2 Conservative systems

When the Hamiltonian of a physical system **does not** depend explicitly on time, the system is said to be **conservative**. It can also be said that the total energy of the system is constant of the motion.

#### Solution of the Schrodinger equation

Lets consider the eigenequation of $H$ (assuming discrete spectrum):

$$H|\varphi_{n,\tau}\rangle = E_n|\varphi_{n,\tau}\rangle. \tag{2.32}$$

$\tau$ is used to denote the set of indices other than $n$ necessary to uniquely characterizes a unique vector $|\varphi_{n,\tau}\rangle$. Since $H$ does not depend on time, neither $E_n$ nor $|\varphi_{n,\tau}\rangle$. Because $|\varphi_{n,\tau}\rangle$ form a basis, it is always possible to expand the state $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \sum_{n,\tau} c_{n,\tau}(t)|\varphi_{n,\tau}\rangle, \quad \text{with} \quad c_{n,\tau}(t) = \langle \varphi_{n,\tau}|\psi(t)\rangle.$$

All the time dependence of $|\psi(t)\rangle$ is contained within $c_{n,\tau}(t)$. Let us project the Schrodinger equation onto each of the states $|\varphi_{n,\tau}\rangle$:

$$\begin{aligned} i\hbar\frac{d}{dt}\langle \varphi_{n,\tau}|\psi(t)\rangle &= \langle \varphi_{n,\tau}|H|\psi(t)\rangle \\ i\hbar\frac{d}{dt}c_{n,\tau}(t) &= E_n c_{n,\tau}(t). \end{aligned}$$

This equation can be integrated to give

$$c_{n,\tau}(t) = c_{n,\tau}(t_0)e^{-E_n(t-t_0)/\hbar}. \tag{2.33}$$

When $H$ does not depend on time, to find $|\psi(t)\rangle$ given $|\psi(t_0)\rangle$, proceed as follows:

- Expand $|\psi(t_0)\rangle$ in terms of the eigenstates of $H$:

$$|\psi(t_0)\rangle = \sum_n \sum_\tau c_{n,\tau}(t_0)|\varphi_{n,\tau}\rangle, \quad \text{with} \quad c_{n,\tau}(t_0) = \langle\varphi_{n,\tau}|\psi(t_0)\rangle.$$

- To obtain $|\psi(t)\rangle$, multiply each coefficient $c_{n,\tau}(t_0)$ of the expansion by the term $e^{-iE_n(t-t_0)/\hbar}$:

$$|\psi(t)\rangle = \sum_n \sum_\tau c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{2.34}$$

  or, in the continuous case,

$$|\psi(t)\rangle = \sum_\tau \int dE\ c_\tau(E,t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{2.35}$$

### Stationary states

An important special case is that in which $|\psi(t_0)\rangle$ is itself an eigenstate of $H$. Then, the expansion of $|\psi(t_0)\rangle$ involves only eigenvalue of $H$ with the same eigenvalue:

$$|\psi(t_0)\rangle = \sum_\tau c_{n,\tau}(t_0)|\varphi_{n,\tau}\rangle.$$

We notice there is no summation over $n$, and the passage from $|\psi(t_0)\rangle$ to $|\psi(t)\rangle$ involves only one factor of $e^{-iE_n(t-t_0)/\hbar}$, which can be taken outisde the summation over $\tau$:

$$|\psi(t)\rangle = \sum_\tau c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle = e^{-iE_n(t-t_0)/\hbar}\sum_\tau c_{n,\tau}(t_0)|\varphi_{n,\tau}\rangle = e^{-iE_n(t-t_0)/\hbar}|\psi(t_0)\rangle.$$

$|\psi(t)\rangle$ and $|\psi(t_0)\rangle$ therefore differe only by a glboal phase factor. Theese two states are physically indistinguishable.

All the physical properties of a system which is an eigenstate of $H$ do not vary over time: the eigenstates of $H$ are called **stationary states**.

The state of the system will no longer evolver after the first masurement and will always remain an eigenstate of $H$ with eigenvalue of $E_k$. A second measurement of the energy at any subsequent time will always yield the same result $E_k$ as the first one.

### Constants of the motion

A constant of the motion is an observable $A$ which does not depends explicitly on time and which commutes with $H$:

$$\text{Constant of the motion } A \qquad \frac{\partial A}{\partial t} = 0 \wedge [A,H] = 0\,. \tag{2.36}$$

For a conservative system, $H$ is therefore itself a constant of the motion.

- The mean value of $A$ does not evolve over time:

$$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle [A, H(t)]\rangle + \langle \frac{\partial A}{\partial t}\rangle = 0.$$

- Since $A$ and $H$ are observables which commute, we can always find for them a system of common eigenvectors:

$$H|\varphi_{n,p,\tau}\rangle = E_n|\varphi_{n,p,\tau}\rangle$$
$$A|\varphi_{n,p,\tau}\rangle = a_p|\varphi_{n,p,\tau}\rangle$$

  Since the states $|\varphi_{n,p,\tau}\rangle$ are eigenstates of $H$, they are stationary states. But it is also an eigenstate of $A$.

  When $A$ is a constant of motion, there exist stationary states of the physical system ($|\varphi_{n,p,\tau}\rangle$) that always remain, for all $t$, eigenstates of $A$ with the same eigenvalue $a_p$. The eigenvalues of $A$ are called **good quantum numbers**.

- The probability of finding the eigenvalue $a_p$, when the constant of motion $A$ is measured, is not time-dependent.

$$|\psi(t_0)\rangle = \sum_{n,p,\tau} c_{n,p,\tau}(t_0)|\varphi_{n,p,\tau}\rangle, \quad |\psi(t)\rangle = \sum_{n,p,\tau} c_{n,p,\tau}(t)|\varphi_{n,p,\tau}\rangle, \quad \text{with} \quad c_{n,p,\tau}(t) = c_{n,p,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}.$$

  The probability $P(a_p, t_0)$ of finding $a_p$ when $A$ is measured at $t_0$ on the system of state $|\psi(t_0)\rangle$ is

$$P(a_p, t_0) = \sum_{n,\tau} |c_{n,p,\tau}(t_0)|^2. \quad \text{Similarly,} \quad P(a_p, t) = \sum_{n,\tau} |c_{n,p,\tau}(t)|^2.$$

  We see from the coefficeint relation equation that $c_{n,p,\tau}(t)$ and $c_{n,p,\tau}(t_0)$ have the same modulus. Therefore,

$$P(a_p, t) = P(a_p, t_0). \tag{2.37}$$

If all but one of the probabilities $P(a_p, t_0)$ are zero, the physical stystem at $t_0$ is in an eigenstate of $A$ with an eigenvalue of $a_k$. Since the $P(a_p, t)$ do not depend on $t$, the state of the system at time $t$ remains an eigenstate of $A$ with en eigenvalue of $a_k$.

### Bohr frequencies of a system

Let $B$ be an arbitrary observable of the system. Its time derivative is

$$\frac{d}{dt}\langle B\rangle = \frac{1}{i\hbar}\langle [B, H]\rangle + \langle \frac{\partial B}{\partial t}\rangle.$$

For a conservative system, we know how to construct $|\psi(t)\rangle$ (2.34). Therefore, we can compute explicitly $\langle\psi(t)|B|\psi(t)\rangle$ and not only $d\langle B\rangle/dt$:

$$\begin{aligned}\langle B\rangle(t) &= \langle\psi(t)|B|\psi(t)\rangle \\ &= \left[\sum_{n',\tau'} c^*_{n',\tau'}(t_0)e^{iE_{n'}(t-t_0)/\hbar}\langle\varphi_{n',\tau'}|\right] B \left[\sum_{n,\tau} c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle\right] \\ &= \sum_{n,\tau}\sum_{n',\tau'} c^*_{n',\tau'}(t_0)c_{n,\tau}(t_0)\langle\varphi_{n',\tau'}|B|\varphi_{n,\tau}\rangle e^{i(E_{n'}-E_n)(t-t_0)/\hbar}.\end{aligned}$$

If we assume $B$ does not dependt explicity on time, the matrix elements $\langle\varphi_{n',\tau'}|B|\varphi_{n,\tau}\rangle$ are constant. The evolution of $\langle B\rangle(t)$ is described by a series of oscilatting terms, whose frequencies

$$\text{Bohr frequencies of the system} \qquad \nu_{n',n} = \frac{1}{2\pi}\frac{|E_{n'} - E_n|}{\hbar} = \left|\frac{E_{n'} - E_n}{h}\right|$$

are characteristic of the system under consideration, but independent of $B$ and the initial state of the system. The importance of each frequency $\nu_{n'n}$ depends on the matrix elements $\langle\varphi_{n',\tau'}|B|\varphi_{n,\tau}\rangle$. This is the origin of thr selection rules which indicate what frequencies can be emitted or absorbed under given conditions. One would have to study the non-diagonal matrix elements $n \neq n'$ of the various atomis operator such as the electric and magnetic dipoles, etc.

Using the $\langle B\rangle(t)$ expression, we can say that the mean value of a constant of the motiion is always time-independent. The only terms of $\langle B\rangle$ that are non-ero are thus constant.

Time-energy uncertainty relation

## 2.5 The superposition principle and physical predictions

One of the important consequences of the first postulate, when it is combined with the others, is the appearance of **interference effects**.

## 2.6 Evolution operator

The transformation of $|\psi(t_0)\rangle$ into $|\psi(t)\rangle$ is linear. Therefore, there exists a linear operator $U(t,t_0)$ such that

$$\text{Evolution operator} \qquad |\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle\,, \tag{2.38}$$

where $U(t,t_0)$ is the **evolution operator** of the system.

### 2.6.1 General properties

From (2.38) we know that

$$U(t_0,t_0) = \mathbb{1}. \tag{2.39}$$

If we substitute the linear operator into the Shcrodinger equation, we obtain:

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = H(t)U(t,t_0)|\psi(t_0)\rangle \Longrightarrow i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)U(t,t_0). \tag{2.40}$$

This a first-order differential equation completely defined $U(t,t_0)$. Equations (2.39) and (2.40) can be condenses into a single integral form:

$$U(t,t_0) = \mathbb{1} = \int_{t_0}^{t} H(t')U(t',t_0)\,dt. \tag{2.41}$$

Lets know take three instants $t'', t'', t$ so that $t'' < t' < t$, then

$$\left.\begin{array}{l}|\psi(t)\rangle = U(t,t')|\psi(t')\rangle \\ |\psi(t')\rangle = U(t',t'')|\psi(t'')\rangle\end{array}\right\} \Longrightarrow |\psi(t)\rangle = U(t,t')U(t',t'')|\psi(t'')\rangle = U(t,t'')|\psi(t'')\rangle.$$

From last expression, we have:

$$U(t,t')U(t',t'') = U(t,t'') \tag{2.42}$$

If we set $t = t''$ and interchange the roles of $t$ and $t'$ we have

$$\mathbb{1} = U(t',t)U(t,t') \Longrightarrow U(t',t) = U^{-1}(t,t'). \tag{2.43}$$

On the other hand, the evolution operator between two instants separated by $dt$ is :

$$d|\psi(t)\rangle = |\psi(t+dt)\rangle - |\psi(t)\rangle = -\frac{i}{\hbar}H(t)||\psi(t)\rangle\ dt.$$

From this we have

$$|\psi(t+dt)\rangle = \left[\mathbb{1} - \frac{i}{\hbar}H(t)\ dt\right]|\psi(t)\rangle = U(t+dt,t)|\psi(t)\rangle.$$

That is, we have the **infinitesimal evolution operator**:

$$\text{Infinitesimal evolution operator} \qquad U(t+dt,t) = \mathbb{1} - \frac{i}{\hbar}H(t)\ dt\ . \tag{2.44}$$

Since $H(t)$ is Hermitian, $U(t+dt,t)$ is unitary. It is not surprising that the evolution operator conserves the norm of vectors on which it acts. We saw preivously that the norm of the state vector does not change over time.

### 2.6.2 Case of conservative systems

When the operator $H$ does not depend on time, equation (2.40) can be integrated easily:

$$U(t,t_0) = e^{-iH(t-t_0)/\hbar}. \tag{2.45}$$

Applying this operator on a state vector $|\varphi_{n,\tau}\rangle$ yields:

$$U(t,t_0)|\varphi_{n,\tau}\rangle = e^{-iH(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle = e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{2.46}$$

## 2.7 One-dimensional Gaussian wave packet (G1)

## 2.8 Particle in an infinite potential well

### 2.8.1 Introduction (H1)

### 2.8.2 Distribution of the momentum values in a stationary state

We have seen that the stationary states of the particle correspond to the energies

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.47}$$

and to the wave functions

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, \tag{2.48}$$

where $a$ is the width of the well.

The probability of a measurement of the momentum $P$ of the particle yielding a result between $p$ and $p + dp$ is

$$\bar{P}_n(p)\, dp = |\bar{\varphi}_n(p)|^2\, dp, \quad \text{with} \tag{2.49}$$

$$\begin{aligned}
\bar{\varphi}_n(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_0^a \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} e^{-ipx/\hbar}\, dx \\
&= \frac{1}{2i\sqrt{n\hbar a}} \int_0^a \left[ e^{(\frac{n\pi}{a} - \frac{p}{\hbar})x} - e^{-i(\frac{n\pi}{a} + \frac{p}{\hbar})x} \right] dx \\
&= \frac{1}{2i}\sqrt{\frac{a}{\pi\hbar}} e^{i(\frac{n\pi}{a} - \frac{pa}{2\hbar})} \left[ F(p - \frac{n\pi\hbar}{a}) + (-1)^{n+1} F(p + \frac{n\pi\hbar}{a}) \right], \quad \text{with} \quad F(p) = \frac{\sin(pa/2\hbar)}{pa/2\hbar}.
\end{aligned} \tag{2.50}$$

The function inside the brakets in equation (2.50) is even if $n$ is odd, and odd if $n$ is even. The probability density $\bar{P}_n(p)$ is therefore an even function of $p$ in all cases, so that

$$\text{Mean value of the momentum in the energy state } E_n \qquad \langle P \rangle_n = \int_{-\infty}^{\infty} \bar{P}_n(p) p\, dp = 0. \tag{2.51}$$

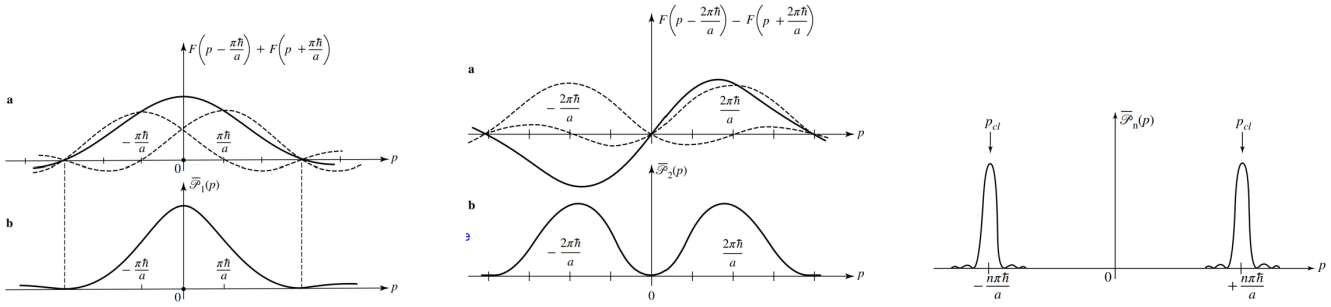
In the same way, we can compute $\langle P^2 \rangle_n$. Using the fact that in the $\{|x\rangle\}$ representation $P$ acts like $-i\hbar\partial_x$ and performing an integration by parts, we obtain:

$$\langle P^2 \rangle_n = \hbar^2 \int_0^a \left| \frac{d\varphi_n}{dx} \right|^2 dx = \hbar^2 \int_0^a \frac{2}{a} \left( \frac{n\pi}{a} \right)^2 \cos^2 \frac{n\pi x}{a}\, dx = \left( \frac{n\pi x}{a} \right)^2. \tag{2.52}$$

Using both $\langle P \rangle_n$ and $\langle P^2 \rangle_n$ we get:

$$\Delta P_n = \sqrt{\langle P^2 \rangle_n - \langle P \rangle_n^2} = \frac{n\pi\hbar}{a}.$$

We can plot the probability density $\bar{P}_n(p)$ for different values of $n \in \{1, 2, \text{large}\}$. The resutls are illustrated in the followign plot. We can see that as $n$ increase, the interference term between $F(p - n\pi\hbar/a)$




**(a)** Ground state ($n = 1$) **(b)** First excited state ($n = 2$) **(c)** State for large $n$

and $F(p + n\pi\hbar/a)$ is negligible:

$$\bar{P}_n(p) = \frac{a}{4\pi\hbar} \left[ F\left( p - \frac{n\pi\hbar}{a} \right) + (-1)^{n+1} F\left( p + \frac{n\pi\hbar}{2} \right) \right]^2 \approx \frac{a}{4\pi\hbar} \left[ F^2\left( p - \frac{n\pi\hbar}{a} \right) + F^2\left( p + \frac{n\pi\hbar}{a} \right) \right].$$

In this limit, is then possible to predict with almost complete certainty the results of a meqasurement of the momentum of the particle in the state $|\varphi_n\rangle$: the value will be nearly equalt to $\pm\frac{n\pi\hbar}{a}$, with accuraccy increasing as $n$ grows.

- The momentum of a classical particle of energy $E_n$ is:

$$\frac{p_{cl}^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \longrightarrow p_{cl} = \pm\frac{n\pi\hbar}{a}.$$

  When $n$ is large, the two peaks of $\bar{P}_n(p)$ therefore correspond to the classical values of the momentum.

- For large $n$, although the absolute value of the momentum is well-defined, its sign is not. This is why $\Delta P_n$ is large: the rms deviation reflects the distance between the two peaks, it is no longer related to their widths.

### 2.8.3 Evolution of the particle's wave function

Time evolution appears only when the state vector is a inear combination of several kets $|\varphi_n\rangle$.

#### Wave function at $t$

Assuming that at $t = 0$ we have

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|\varphi_1\rangle + |\varphi_2\rangle],$$

we apply formula of this chapter to get

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-i\frac{\pi^2\hbar}{2ma^2}}|\varphi_1\rangle + e^{-2i\frac{\pi^2\hbar}{ma^2}}|\varphi_2\rangle\right] \propto \frac{1}{\sqrt{2}}[|\varphi_1\rangle + e^{-i\omega_{21}t}|\varphi_2\rangle], \quad \text{with} \quad \omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\pi^2\hbar}{2ma^2}.$$

#### Evolution of the shape of the wave packet

The shape of the wave packet is given by the probability density:

$$|\psi(x,t)|^2 = \frac{1}{2}\varphi_1^2(x) + \frac{1}{2}\varphi_2^2(x) + \varphi_1(x)\varphi_2(x)\cos\omega_{21}t.$$

We see that the time variation is due to the interference term in $\varphi_1\varphi_2$. Only one Bohr frequency appears, $\nu_{21} = (E_2 - E_1)/\hbar$.

#### Motion of the center of the wave packet

The mean value $\langle X\rangle$ of the position of the particle at $t$ is done by first doing $X' = X - a/2$. By Symmetry, the diagonal matrix elements of $X'$ are zero:

$$\langle\varphi_1|X'|\varphi_2\rangle \propto \int_0^a \left(x - \frac{a}{2}\right)\sin^2\frac{\pi x}{a}\,dx = 0, \quad \text{and} \quad \langle\varphi_2|X'|\varphi_2\rangle \propto \int_0^a \left(x - \frac{a}{2}\right)\sin^2\frac{2\pi x}{a}\,dx = 0.$$

We then have

$$\langle X'\rangle(t) = \text{Re}\left(e^{-i\omega_{21}t}\langle\varphi_1|X'|\varphi_2\rangle\right),$$

with

$$\langle\varphi_1|X'|\varphi_2\rangle = \langle\varphi_1|X|\varphi_2\rangle - \frac{a}{2}\langle\varphi_1|\varphi_2\rangle = \frac{2}{a}\int_0^a x\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx = -\frac{16a}{9\pi^2}.$$

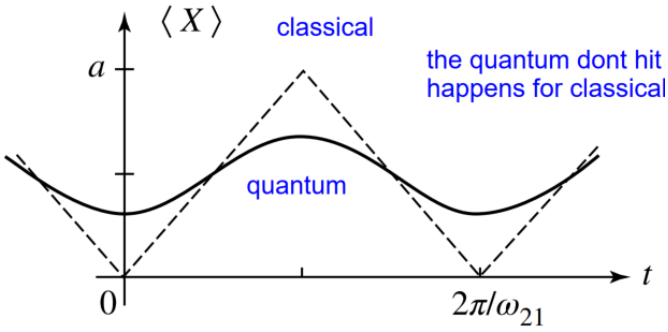



**Figure 2.2** Time variation of $\langle X \rangle$ corresponding to the wave packet's motion. QM predicts that the center of the wave packet will turn back before hitting the wall

Therefore,

$$\langle X \rangle(t) = \frac{a}{2} - \frac{16a}{9\pi^2} \cos \omega_{21} t.$$

We immediately notice a very clear difference between these two typoe of motion. Before the center of the wave packet has touched the wall, the action of the potential on the edges of this packet is sufficient to make it turn back.

- The mean value of the energy of the particle in $|\psi(t)\rangle$ is

$$\langle H \rangle = \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{5}{2}E_1$$
$$\langle H^2 \rangle = \frac{1}{2}E_1^2 + \frac{1}{2}E_2^2 = \frac{17}{2}E_1^2,$$

  which gives

$$\Delta H = \frac{3}{2}H_1.$$

  We have seen that the wave packet evolves appreciably over a time of the order of $\Delta t \approx 1/\omega_{21}$. Therefore,

$$\Delta H \Delta t = \frac{3}{2}E_1 \frac{\hbar}{3E_1} = \frac{\hbar}{2}. \tag{2.53}$$

### 2.8.4 Perturbation created by a position measurement

## 2.9 Shcrodinger and Heisenberg pictures

### 2.9.1 Time-dependent reference frames

The state of a system can be evaluated in various **reference frames** that evolve in time.

The state $|\psi(t)\rangle$ in one reference frame evolves in time according to the Schrodinger equation

$$i\hbar\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle.$$

A second reference frame that may evolve in time relative to the first one if we assume the existence of a time-dependent unitary operator that operates over the first frame provifing an effective state in the second frame:

$$\text{Effective state of the second frame} \qquad |\psi_E(t)\rangle = F(t)|\psi(t)\rangle, \quad F(t_0) = \mathbb{1}\,. \tag{2.54}$$

The effective state obeys the **effective Schrodinger equation** obtained by inserting $|\psi(t)\rangle = F^\dagger(t)|\psi_E(t)\rangle$ in the Schrodinger equation of the first frame:

$$\text{Effective Schrodinger equation and Hamiltonian} \qquad \begin{aligned} &i\hbar\partial_t|\psi_E(t)\rangle = H_E(t)|\psi_E(t)\rangle \\ &H_E(t) = F(t)H(t)F^\dagger(t) - i\hbar F(t)\left(\partial_t F^\dagger(t)\right) \end{aligned} \tag{2.55}$$

Frame transformations are generally used to simplify calculations and time dependence of the Schrodinger equation.

### 2.9.2 Schrodinger, Heisenberg, and interaction pictures

They are different frames of reference, and are distinguished by the specfic time-dependent unitary transformations.

- **Schrodinger picture** State vectors $|\psi_S(t)\rangle$ evolve in time under the action of the Hamiltonian $|\psi_S(t)\rangle = U(t,t_0)|\psi_S(t)\rangle$. Position and momentum operators have no time dependence.
- **Heisenberg picture** Defined by the adjoint of the evolution operator of the S picture, so that its application on the Schrodinger-picture state vector $|\psi_H\rangle = U^\dagger(t,t_0)|\psi_S(t)\rangle = |\psi_S(t_0)\rangle$ vanishes the time dependence. On the other hand, operators that have no time dependence in the S picture may now depend on time.
- **Interaction picture** Used when the S picture Hamiltonian is time dependent. In this picture, operators and state vectors generally evolve in time.

### 2.9.3 Schrodinger picture

Position and momentum operators have no explicit tiem dependence in this picture. However, other operators with time dependence may be constructed.

The expectation value of an operator $A_S(t)$ wo;; generally have time dependence that results from both the time dependence of $|\psi_S(t)\rangle$ and from the operator itself:

$$\langle A_S(t)\rangle(t) = \langle\psi_S(t)|A_S(t)|\psi_S(t)\rangle \longrightarrow \frac{d}{dt}\langle A_S\rangle = \frac{1}{i\hbar}\langle[A_S, H_S]\rangle + \langle\frac{\partial A_S}{\partial t}\rangle\,. \tag{2.56}$$

Ehrenfest's equations are obtained by replacing $A_S(t)$ with the position and momentum operator $\boldsymbol{R} = (X,Y,Z)$ and $\boldsymbol{P} = (P_x, P_y, P_z)$, and noting that $\partial_t\boldsymbol{R} = \partial_t\boldsymbol{P} = 0$:

$$\text{Ehrenfest's equations} \qquad \begin{aligned} &\frac{d}{dt}\langle\boldsymbol{R}\rangle = \frac{1}{m}\langle\boldsymbol{P}\rangle \\ &\frac{d}{dt}\langle\boldsymbol{P}\rangle = -\langle\nabla V(\boldsymbol{R})\rangle \end{aligned} \quad , \quad \langle V(\boldsymbol{R})\rangle = \left[\langle\partial_X V(\boldsymbol{R})\rangle, \langle\partial_Y V(\boldsymbol{R})\rangle, \langle\partial_Z V(\boldsymbol{R})\rangle\right]. \tag{2.57}$$

### 2.9.4 Heisenberg picture

This picture vanishes the time dependence of S picture state vector by applying the adjoint of the time evolution oeprator $U^\dagger(t,t_0)$, which defines a unitary transformation.

An arbitrary operator $A_S(t)$ in the S picture is transformed to the H picture as

$$\text{Heisenberg operator} \qquad A_H(t) = U^\dagger(t,t_0)A_S(t)U(t,t_0)\,.$$

The time-dependent expectation value of $A_H(t)$ in the H picture is equivalent to that of $A_S(t)$, which must be the same in any picture. The evolution of the operator $A_H(t)$ is then given by:

$$\begin{aligned}
\frac{d}{dt}A_H(t) &= -\frac{1}{i\hbar}U^\dagger(t,t_0)H_S(t)A_S(t)U(t,t_0) + U^\dagger(t,t_0)\frac{dA_S(t)}{dt}U(t,t_0) + \frac{1}{i\hbar}U^\dagger(t,t_0)A_S(t)H_S(t)U(t,t_0)\\
&= -\frac{1}{i\hbar}U^\dagger(t,t_0)H_S(t)U(t,t_0)U^\dagger(t,t_0)A_S(t)U(t,t_0) + U^\dagger(t,t_0)\frac{dA_S(t)}{dt}U(t,t_0)\\
&\quad + \frac{1}{i\hbar}U^\dagger(t,t_0)A_S(t)U(t,t_0)U^\dagger(t,t_0)H_S(t)U(t,t_0)\\
i\hbar\partial_t A_H(t) &= [A_H(t),H_H(t)] + i\hbar U^\dagger(t,t_0)(\partial_t A_S(t))U(t,t_0).
\end{aligned}$$

In the table, $H_S$ and $|\psi_S(t)\rangle$ are the S picture Hamiltonian and state vector.

Heisenberg picture quantities and dynamics

| | |
|---|---|
| $\lvert\psi_H\rangle$ | $\equiv U^\dagger(t,t_0)\lvert\psi_S(t)\rangle = \lvert\psi_S(t_0)\rangle$ |
| $A_H(t)$ | $\equiv U^\dagger(t,t_0)A_S(t)U(t,t_0)$ |
| $H_H$ | $= H_S,$ for time-independent $H_S$ |
| $H_H(t)$ | $= H_S(t),$ for $[H_S(t),H_S(t')]=0$ |
| $\langle A_H(t)\rangle(t)$ | $= \langle\psi_H\lvert A_H(t)\rvert\psi_H\rangle$ |
| | $= \langle\psi_S(t_0)\lvert U^\dagger(t,t_0)A_S(t)U(t,t_0)\rvert\psi_S(t_0)\rangle$ |
| | $= \langle\psi_S\lvert A_S(t)\rvert\psi_S(t)\rangle = \langle A_S(t)\rangle(t)$ |
| $i\hbar\partial_t A_H(t)$ | $= [A_H(t),H_H(t)] + i\hbar U^\dagger(t,t_0)\,(\partial_t A_S(t))\,U(t,t_0)$ |

The effective Hamiltonian of the H picture is $H_E = 0$. Therefore, the effect Schrodinger equation $i\hbar\partial_t|\psi_H\rangle = 0$ is solved by $|\psi_H\rangle = |\psi_S(t_0)\rangle$. In the H picture, only operators evolve in time following the ODE in the last line of the table.

An advantage of Heisenberg picture is that it leads to equations formally similar to those of classical mechanics.

### 2.9.5 Interaction picture

Obtained with a unitary transformation of state vectors and operators of the S picture. This picture removes some of the time dependence of the S picture state vectors, while also altering the time dependence of operators. The interaction picture is typically used with a time-dependent S picture Hamiltonian

$$\text{Time-dependent S picture Hamiltonian} \qquad H_S(t) = H_0 + W(t)\,, \tag{2.58}$$

where the eigenstates of $H_0$ are knwon, and $W(t)$ is a time-dependent **perturbation** which induces time-dependent dynamics and **transitions** between the eigenstates of $H_0$. To transform into the interaction picture, an evolutino operator $U_0(t,t_0) = e^{-iH_0(t-t_0)/\hbar}$ is associated with $H_0$. The transformed state vector and arbitrary operator expressed in the interaction picture are

$$\text{Transformed state vector and operator} \qquad \begin{aligned} |\psi_I(t)\rangle &= U_0^\dagger(t,t_0)|\psi_S(t)\rangle \\ A_I(t) &= U_0^\dagger(t,t_0)A_S(t)U_0(t,t_0) \end{aligned} \tag{2.59}$$

The effective Schrodinger equation in the interaction picture is

$$i\hbar\partial_t|\psi_I(t)\rangle = H_E(t)|\psi_I(t)\rangle, \quad \text{where} \quad H_E(t) = U_0^\dagger(t,t_0)W(t)U(t,t_0) \tag{2.60}$$

is the effective Hamiltonian. If $W(t) = 0$, then the interaction picture reduces to the H picture: $H_E(t) = 0$ and $|\psi_I(t)\rangle = |\psi_S(t_0)\rangle$.

## 2.10 The density operator

To determine the state of a system at a given time, it suffices to perform on the system a set of measurements corresponding to a CSCO. However, in practice, the state of the system is often not perfectly determined. How can we incorporate into the formalism the incomplete information we possess about the state of the system, so that our predictions make maximum use of this partial information? We will then introduce the **density operator**.

### 2.10.1 Concept of a statistical mixture of states

When one has incomplete information about a system, one typically appeals to the concept of probability. This incomplete information is presented in the following way:

> The state of this system may be either the state $|\psi_1\rangle$ with probability $p_1$ or $|\psi_2\rangle$ with probability $p_2$. Obviously,
>
> $$\sum_k p_k = 1.$$

We say then we are dealing with a **statistica mixture** of states $|\psi_1\rangle, |\psi_2\rangle, \cdots$ with probabilities $p_1, p_2, \cdots$.

- The various states are not necessarily orthogonal. However, they can always be chosen normalized.
- Probabilities intervene at two different levels: a) initial information about the system, b) postulates concerning the meassurement nature.
- It is impossible, in general, to describe a statistical mixture by an average state vector which would be a superposition of the states $|\psi_k\rangle$.

### 2.10.2 The pure case

The density operator is an **average operator** which permits a simple description of the statistical mixture of states. We will first consider the case where the state of the system is perfectly known, that is, a **pure state**. Characterizing the system by its state vector if completely equivalent to characterizing it by acertain operator acting in the state space.

### Description by a state vector

Let be a system whise state vector is

$$|\psi(t)\rangle = \sum_n c_n(t)|u_n\rangle, \quad \text{with} \quad \sum_n |c_n(t)|^2 = 1.$$

If $A$ is an observable with $A_{np} = \langle u_n|A|u_p\rangle$, then the mean value of $A$ is

$$\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle = \sum_{n,p} c_n^*(t)c_p(t)A_{np}.$$

Finally, the evolution of $|\psi(t)\rangle$ is

$$i\hbar\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle.$$

### Description by a density operator

We introduce the density operator $\rho(t)$ as

$$\text{Density operator} \qquad \rho(t) = |\psi(t)\rangle\langle\psi(t)|\,. \tag{2.61}$$

The density operator is represented in $\{|u_n\rangle\}$ basys by a matrix called te **density matrix** whose elements are:

$$\rho_{pn}(t) = \langle u_p|\rho(t)|u_n\rangle = c_n^*(t)c_p(t).$$

The specification of $\rho(t)$ suffices to characterize the quantum state of the system.

First, we have the following normalization condition

$$\text{Normalization condition} \qquad \sum_n |c_n(t)|^2 = \sum_n \rho_{nn}(t) = \text{Tr}\left[\rho(t)\right] = 1.$$

Secondly, the mean value of $A$ is

$$\text{Mean value of } A \qquad \langle A\rangle(t) = \sum_{n,p}\langle u_p|\rho(t)|u_n\rangle\langle u_n|A|u_p\rangle = \sum_p \langle u_p|\rho(t)|u_p\rangle = \text{Tr}\left[\rho(t)A\right].$$

Finally, the time evolution of the operator can be deduced from the Schrodinger equation above:

$$\begin{aligned}\text{Time evolution of } \rho(t) \qquad \partial_t\rho(t) &= (\partial_t|\psi(t)\rangle)\langle\psi(t)| + |\psi(t)\rangle(\partial_t\langle\psi(t)|) \\ &= \frac{1}{i\hbar}H(t)|\psi(t)\rangle\langle\psi(t)| - \frac{1}{i\hbar}|\psi(t)\rangle\langle\psi(t)| \\ \partial_t\rho(t) &= \frac{1}{i\hbar}[H(t),\rho(t)].\end{aligned} \tag{2.62}$$

The probabilities $P(a_n)$ are then given by

$$P(a_n) = \text{Tr}\left[P_n\rho(t)\right], \quad P_n = \text{Eigensubspace of } a_n.$$

### Properties of the density operator in a pure case

In a pure case, a system can be described just as well by a density operator as by a state vector. However, the density operator presents a certain number of advantages. Using this operator eliminates the drawbacks related to the existence of an arbitrary global phase factor for the state vector. Also, by looking the above formulas we see that the expression are linear with respect to $\rho(t)$. Furtheremore, we have

$$\rho^\dagger(t) = \rho(t), \quad \underbrace{\rho^2(t) = \rho(t), \quad \text{Tr}\left[\rho^2(t)\right] = 1}_{\text{Only for pure case}}. \tag{2.63}$$

## 2.10.3 A statistical mixture of states (non-pure case)

### Definition of the density operator

Lets consider a system for which the various probabilities are arbitrary, on the condition that they satisfy the relations:

$$\begin{cases} 0 \leq p_1, p_2, \cdots, p_k, \cdots \leq 1 \\ \sum_k p_k = 1 \end{cases}$$

How does one calculate hte probability $P(a_n)$ that a measurement of the observable $A$ will yield the result $a_n$? Let $P_k(a_n) = \langle\psi_k|P_n|\psi_k\rangle$ be the probability of finding $a_n$ if the state vector were $|\psi_k\rangle$. To obtain the desired probability $P(a_n)$, one must weight $P_k(a_n)$ by $p_k$ and then sum over $k$:

$$P(a_n) = \sum_k p_k P_k(a_n) = \sum_k p_k \text{Tr}\left[\rho_k P_n\right] = \text{Tr}\left[\sum_k p_k \rho_k P_n\right] = \text{Tr}\left[\rho P_n\right]. \tag{2.64}$$

We see that the linearity of the formulas whih use the density operator enables us to express all physical predictions in terms of $\rho$.

The same density operator can be interpreted as several different statistical mixtures of pure states. This situation is sometimes described as the **multiple preparations** of the same density operator.

### General properties of the density operator

Since the coefficients $p_k$ are real, $\rho$ is obviously a Hermitian operator. The trace of $\rho$ is

$$\text{Tr}\left[\rho\right] = \sum_k p_k \text{Tr}\left[\rho_k\right] \overset{(a)}{=} \sum_k p_k 1 = 1.$$

In $(a)$ we saw that the trace of $\rho_k$ (trace of pure states) is always 1. We can also generalize the formula of the mean value to statistical mixture:

$$\langle A\rangle = \sum_n a_n P(a_n) = \text{Tr}\left[\rho \sum_n a_n P_n\right] = \text{Tr}\left[\rho A\right]. \tag{2.65}$$

Now let us calculate the time evolution of the density operator. We will assume that, unlike the state of the system, its Hamiltoninan $H(t)$ is well known. If the system at the initial time $t_0$ has the probability $p_k$ og being the state $|\psi_k\rangle$, then, at a subsequent time $t$, it has the same probability $p_k$ of being in the state $|\psi_k(t)\rangle$ given by

$$\begin{cases} i\hbar\partial_t|\psi_k(t)\rangle = H(t)|\psi_k(t)\rangle \\ |\psi_k(t_0)\rangle = |\psi_k\rangle \end{cases}$$

The density operator at the instant $t$ will then be

$$\rho(t) = \sum_k p_k \rho_k(t), \quad \text{with} \quad \rho_k(t) = |\psi_k(t)\rangle\langle\psi_k(t)|. \tag{2.66}$$

According to the pure case, $\rho_k(t)$ obeys the evolution equation (2.62). Thus,

$$\text{Time evolution of } \rho(t) \qquad i\hbar\partial_t\rho(t) = [H(t), \rho(t)]\,. \tag{2.67}$$

So, we could generalize most of theequations except to the one pointed out previously. Since $\rho$ is no longer a projector (as in the pure case), we have, in general:

$$\rho^2(t) \neq \rho(t).$$

and, consequently,

$$\text{Tr}\left[\rho^2\right] \leq 1.$$

Finally, we see from a previous equation that, for any ket $|u\rangle$, we have

$$\langle u|\rho|u\rangle = \sum_k p_k \langle u|\rho_k|u\rangle = \sum_k p_k |\langle u|\psi_k\rangle|^2 \Longrightarrow \langle u|\rho|u\rangle \geq 0.$$

Consequently, $\rho$ is a positive operator.

### Populations; coherences

What is the physical meaning of the matrix element $\rho_{np}$ in the $\{|u_n\rangle\}$ basis? We analyze first the diagional elements $\rho_{nn}$:

$$\rho_{nn} = \sum_k p_k [\rho_k]_{nn} = \sum_k p_k |c_n^{(k)}|^2, \quad \text{with} \quad |c_n^{(k)}|^2 \geq 0.$$

$\rho_{nn}$ represents the average probability of finding the system in the state $|u_n\rangle$. Thats why $\rho_{nn}$ is called the population of the state $|u_n\rangle$.

A similar calculation can be carried out for non-diagonal elements $\rho_{np}$:

$$\rho_{np} = \sum_k p_k c_n^{(k)} c_p^{(k)*}.$$

We see that $c_n^{(k)} c_p^{(k)*}$ is a cros term. It reflects the **interference effects** between the states $|u_n\rangle$ and $|u_p\rangle$ which can appear when the state $|\psi_k\rangle$ is a coherent linear superposition of these states. $\rho_{np}$ is the average of these cross terms, taken over all possible states of the statistical mixture. We can see that $\rho_{nn}$ is the sym of real positive numbers, while $\rho_{np}$ is the sum of complex numbers.

If $\rho_{np} \neq 0$, means that a certain coherence subsists between these states (interference effects). This is why non-diagonal elements of $\rho$ are often called **coherences**.

- The distinction between populations and coherences obviously depends on the basis $\{|u_n\rangle\}$ chosen in the state space. Since $\rho$ is Hermitian, it is always possible to find an orthonormal basis $\{|\chi_l\rangle\}$ where $\rho$ is diagonal and can be written as

$$\rho = \sum_l \pi_l |\chi_l\rangle\langle\chi_l|.$$

Since $\rho$ is positive and $\mathrm{Tr}\,[\rho] = 1$, we have

$$\begin{cases} 0 \leq \pi_l \leq 1 \\ \sum_l \pi_l = 1 \end{cases}$$

$\rho$ can thus be considered to describe a statistical mixture of the states $|\chi_l\rangle$ with the probabilities $\pi_l$ (no coherence between the states $|\chi_l\rangle$).

- If the kets $|u_n\rangle$ are eigenvectors of the Hamiltoninan $H$ (assumed time-independent), the populations are constant, and the coherences oscillates at the Bohr frequencies of the system.
- $\rho$ can have coherences only between states whose populations are not zero ($\rho_{nn}\rho_{pp} \geq |\rho_{np}|^2$).

### 2.10.4 Separate description of part of a physical system. Concept of a partial trace

## Chapter 3

# The quantum harmonic oscillator

# 3.1 Introduction

## 3.1.1 Importance of the harmonic oscillator in physics

The simplest example is a particle of mass $m$ moving in a potential which depends only on $x$ and has the form

$$V(x) = \frac{1}{2}kx^2, \quad k > 0.$$

The particle is attracted towards the $x = 0$ by a restoring force:

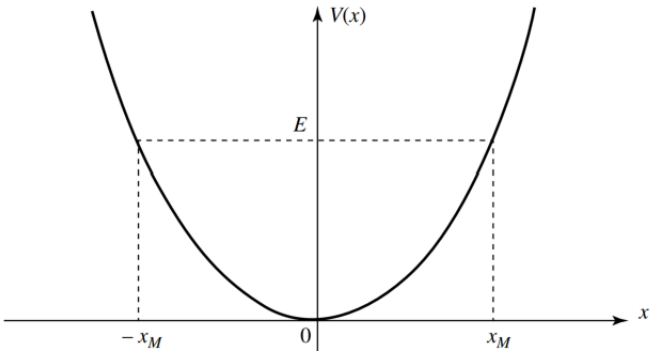



**Figure 3.1** Potential energy $V(x)$ of a 1D harmonic oscillator.

$$F_x = \frac{dV}{dx} = -kx.$$

In classical mechanics, the motion of the particle is a sinusoidal oscillation about $x = 0$ with angular frequency $\omega = \sqrt{k/m}$.

**Various systems are governed by the harmonic oscillator equations**

Whenever one studies the behavior of a system in the neighborhood of a stable equilibrium position, one arrives at equations which, in the limit of small oscillations, are those of a harmonic oscillator.

## 3.1.2 The harmonic oscillator in classical mechanics

The motion of the particle is governed by the dynamics equation

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx} = -kx \longrightarrow x = x_M \cos(\omega t - \varphi). \tag{3.1}$$

The kinetic energy of the particle is

$$T = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{p^2}{2m}, \tag{3.2}$$

where $p = mv$ is the momentum of the paticle. The total energy after substitution of $x_M$ is

$$E = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2}m\omega^2x_M^2.$$

- The potential can be expanded in Taylor's series around $x_0$:

$$V(x) = \underbrace{V(x_0)}_{a} + V'(x_0)(x - x_0) + \underbrace{\frac{1}{2!}V^{(2)}(x_0)}_{b}(x - x_0)^2 + \underbrace{\frac{1}{3!}V^{(3)}(x_0)}_{c}(x - x_0)^3 + \cdots$$

The force derived from the potential in the neighborhood of $x_0$ is

$$F_x = -\frac{dV}{dx} = -2b(x - x_0) - 3c(x - x_0)^2 + \cdots \tag{3.3}$$

The point $x = x_0$ is a stable equilibrium for the particle: $F_x(x_0) = 0$. In adittion, if the amplitude of the motion of the particle about $x_0$ is sufficiently small, we can keep with the linear term only and we have a harmonic oscillator since the dynamics equation can be approximated by

$$m\frac{d^2x}{dt^2} \approx -2b(x - x_0).$$

For higher energies $E$, the particle will be in period but not sinusoidal motion (as signal in Fourier series) between the limits $x_1$ and $x_2$. We then say that we are dealing with an **anharmonic oscillator**.

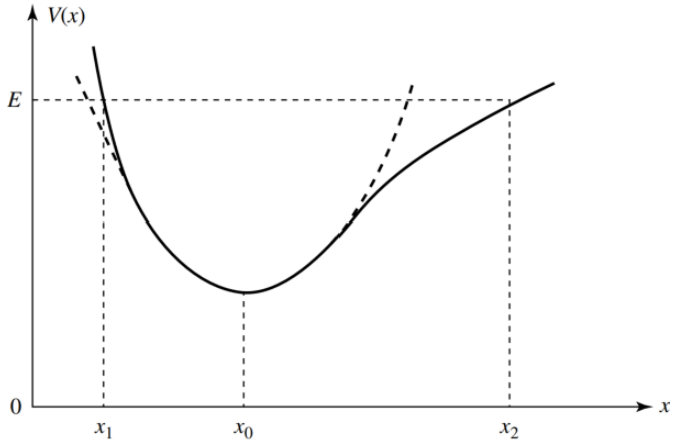



**Figure 3.2** Any potential can be approximated by a parabolic potential. In $V(x)$, a classical particle of energy $E$ oscillates between $x_1$ and $x_2$.

### 3.1.3 General properties of the quantum mechanical Hamiltonian

In QM, the classical quantities $x$ and $p$ are replaced respectively by the observables $X$ and $P$, which satisfy

$$[X, P] = i\hbar.$$

It is then easy to obtain the Hamiltonian operator of the system from the total energy

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2.$$

Since $H$ is time-independent (conservative system), the quantum mechanical study of the harmonic oscillator reduces to the solution of the eigenequation:

$$H|\varphi\rangle = E|\varphi\rangle$$

which is written, in the $\{|x\rangle\}$ representation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right]\varphi(x)=E\varphi(x).$$

Let us indicate some properties of the potential function:

- **The eigenvalues of the Hamiltonian are positive**. If $V(x)$ has a lower bound, the eigenvalues $E$ of $H$ are greater than the minimum of $V(x)$:

$$V(x)\leq V_m \quad \text{requires} \quad E>V_m.$$

  We have chosen for the harmonic oscillator that $V_m=0$.
- **The eigenfunctions of $H$ have a definite parity** due to that $V(-x)=V(x)$ is an even function. We shall see that the eigenvalues of $H$ are not degenerate; the wave functions associated with the stationary tates are necessarily either even or odd.
- **The energy spectrum is discrete**.

## 3.2 Eigenvalues of the Hamiltonian

### 3.2.1 Notation

It is easy to see that the observables $\hat{X}$ and $\hat{P}$

Dimensionless observables $$\hat{X}=\frac{X}{\sigma}, \quad \hat{P}=\frac{\sigma P}{\hbar}, \quad \text{where} \quad \sigma=\sqrt{\frac{\hbar}{m\omega}}=\text{Oscillator length } (m).$$

are dimensionless. With these new operators, the canonical commutation is

$$\text{Canonical commutation} \qquad [\hat{X},\hat{P}]=i \tag{3.4}$$

and the Hamiltonian can be put in the form

$$H=\hbar\omega\hat{H}, \quad \text{with} \quad \hat{H}=\frac{1}{2}(\hat{X}^2+\hat{P}^2). \tag{3.5}$$

In consequence, we seek the solutions of the following eigenequation

$$\hat{H}|\varphi_\nu^i\rangle=\epsilon_\nu|\varphi_\nu^i\rangle,$$

where the operator $\hat{H}$ and the eigenvalues $\epsilon_\nu$ are **dimensionless**.

If $\hat{X}$ and $\hat{P}$ were numbers and not operators, we could write the sum $\hat{X}^2+\hat{P}^2$ appearing in the definition of $\hat{H}$ in the form of a product $(\hat{X}-i\hat{P})(\hat{X}+i\hat{P})$. However, the introuction of operators proportional to $\hat{H}\pm i\hat{P}$ enables us to simplify considerably out search for eigenvalues and eigenvectors of $\hat{H}$. We therefore set

$$\begin{aligned} a&=\frac{1}{\sqrt{2}}(\hat{X}+i\hat{P}) \\ a^\dagger&=\frac{1}{\sqrt{2}}(\hat{X}-i\hat{P}) \end{aligned} \quad\Longleftrightarrow\quad \begin{aligned} \hat{X}&=\frac{1}{\sqrt{2}}(a^\dagger+a) \\ \hat{P}&=\frac{i}{\sqrt{2}}(a^\dagger-a) \end{aligned}. \tag{3.6}$$

The commutator of $a$ and $a^\dagger$ is

$$[a, a^\dagger] = \frac{1}{2}[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}] = \frac{i}{2}[\hat{P}, \hat{X}] - \frac{i}{2}[\hat{X}, \hat{P}] = 1 \longrightarrow \boxed{[a, a^\dagger] = 1}\,. \tag{3.7}$$

If we do $aa^\dagger$ we obtain

$$a^\dagger a = \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P}) = \frac{1}{2}(\hat{X}^2 + \hat{P}^2 + i\hat{X}\hat{P} - i\hat{P}\hat{X}) = \frac{1}{2}(\hat{X}^2 + \hat{P}^2 - 1).$$

Comparing with $\hat{H}$ we see that

$$\boxed{\hat{H} = a^\dagger a + \frac{1}{2} = aa^\dagger - \frac{1}{2}}\,.$$

We see that we canot put $\hat{H}$ in a product of linear terms, due to the non-commutatitivty of $\hat{X}$ and $\hat{P}$ ($1/2$ term).

We introduce another operator:

$$\text{Operator } N \qquad \boxed{N = a^\dagger a}\,. \tag{3.8}$$

This operator is Hermitian

$$N^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = N. \tag{3.9}$$

And its relation with $\hat{H}$ is

$$\hat{H} = N + \frac{1}{2} \tag{3.10}$$

so that the eigenvectors of $\hat{H}$ are eigenvectors of $N$, and viceversa. The commutators with $a$ and $a^\dagger$ are:

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a \longrightarrow \boxed{[N, a] = -a} \tag{3.11}$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger [a, a^\dagger] + [a^\dagger, a^\dagger]a = a^\dagger \longrightarrow \boxed{[N, a^\dagger] = a^\dagger}\,. \tag{3.12}$$

The study of the harmonic oscilator is based on these operatores $a$, $a^\dagger$, and $N$. The eigenequation for $N$ is

$$\text{Eigenequation of } N \qquad \boxed{N|\varphi_\nu^i\rangle = \nu|\varphi_\nu^i\rangle}\,. \tag{3.13}$$

When this is solved, we know that the eigenvector $|\varphi_\nu^i\rangle$ of $N$ is also an eigenvector of $H$ with the eigenvalue $E_\nu = (\nu + 1/2)\hbar\omega$:

$$H|\varphi_\nu^i\rangle = (\nu + 1/2)\hbar\omega|\varphi_\nu^i\rangle. \tag{3.14}$$

The solution of the eigenequation of $N$ will be based on the commutation relation $[a, a^\dagger] = 1$.

### 3.2.2 Determination of the spectrum

#### Lemmas

- **Properties of the eigenvalues of** $N$ The eigenvalues $\nu$ of the operator $N$ are positive or zero. We can see this by looking the qaure of the norm of the vector $a|\varphi_n u^i\rangle$

$$\|a|\varphi^i_\nu\rangle\|^2 = \langle\varphi^i_\nu|a^\dagger a|\varphi^i_\nu\rangle = \langle\varphi^i_\nu|N|\varphi^i_\nu\rangle = \nu\langle\varphi^i_\nu|\varphi^i_\nu\rangle \geq 0 \Longrightarrow \boxed{\nu \geq 0}\,.$$

- **Properties of the vector** $a|\varphi^i_\nu\rangle$
  - i) $\nu = 0 \Longrightarrow a|\varphi^i_{\nu=0}\rangle = 0$. If $\nu = 0$ is an eigenvalue of $N$, all eigenvectors $|\varphi^i_0\rangle$ associated with this eigenvalue satisfy the relation

$$a|\varphi^i_0\rangle = 0. \tag{3.15}$$

    Anyn vector which satisfy this relation is therefore an eigenvector of $N$ with the eigenvalue $\nu = 0$.
  - ii) $\nu > 0 \Longrightarrow a|\varphi^i_\nu\rangle$ is a non-zero eigenvector of $N$ with eigenvalue $\nu - 1$.

$$\begin{array}{rl} [N,a]|\varphi^i_\nu\rangle & = -a|\varphi^i_\nu\rangle \\ Na|\varphi^i_\nu\rangle & = aN|\varphi^i_\nu\rangle - a|\varphi^i_\nu\rangle \\ N[a|\varphi^i_\nu\rangle] & = a\nu|\varphi^i_\nu\rangle - a|\varphi^i_\nu\rangle \end{array} \Longrightarrow \boxed{N[a|\varphi^i_\nu\rangle] = (\nu-1)[a|\varphi^i_\nu\rangle]}\,.$$

- **Properties of the vector** $a^\dagger|\varphi^i_\nu\rangle$
  - i) $a^\dagger|\varphi^i_\nu\rangle$ is always non-zero. We study it with the square of the norm:

$$\|a^\dagger|\varphi^i_\nu\rangle\|^2 = \langle\varphi^i_\nu|aa^\dagger|\varphi^i_\nu\rangle = \langle\varphi^i_\nu|(N+1)|\varphi^i_\nu\rangle = (\nu+1)\langle\varphi^i_\nu|\varphi^i_\nu\rangle.$$

    As $\nu \geq 0$ by lemma 1, the ket $a^\dagger|\varphi^i_\nu\rangle$ always has non-zero norm and, consequently, is never zero.
  - ii) $a^\dagger|\varphi^i_\nu\rangle$ is an eigenvector of $N$ with eigenvalue $N+1$. We do it analoguisly to lemma IIb):

$$\begin{array}{rl} [N,a^\dagger]|\varphi^i_\nu\rangle & = a^\dagger|\varphi^i_\nu\rangle \\ Na^\dagger|\varphi^i_\nu\rangle & = a^\dagger N|\varphi^i_\nu\rangle + a^\dagger|\varphi^i_\nu\rangle \\ N[a^\dagger|\varphi^i_\nu\rangle] & = \nu a^\dagger|\varphi^i_\nu\rangle + a^\dagger|\varphi^i_\nu\rangle \end{array} \Longrightarrow \boxed{N[a^\dagger|\varphi^i_\nu\rangle] = (\nu+1)[a^\dagger|\varphi^i_\nu\rangle]}\,.$$

#### The spectrum of $N$ is composed of non-negative integers

If $\nu$ is non-integral, we can therefore construct a non-zero eigenvector of $N$ with a strictly negative eigenvalue. Since this is impossible by lemma 1, the hypothesis of non-integral $\nu$ must be rejected.

> $\nu$ can only be a non-negative integer.

We conclude that the eigenvalues of $H$ are of the form

$$\text{Eigenvalue of } H \qquad \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n \in \mathbb{N}_0^+}\,. \tag{3.16}$$

In QM, the energy of the harmonic oscillator is **quantized**. The smallest value (ground state) is $\hbar\omega/2$.

#### Interpretation of the $a$ and $a^\dagger$ operators

We have seen that, given $|\varphi_n^i\rangle$ with eigenvalue $E_n$, application of $a$ gives an eigenvector associated with $E_{n-1}$ while application of $a^\dagger$ yields the energy $E_{n+1}$.

Thats why $a^\dagger$ is said to be a **creation operator** and $a$ an **annihilation operator**; their action on an eigenvector of $N$ makes an energy quantum $\hbar\omega$ appear or dissapear.

### 3.2.3 Degeneracy of the eigenvalues

#### The grounds state is non-degenerate

The eigenstates of $H$ associated with $E_0 = \hbar\omega/2$ (or eigenvector of $N$ associated with $n = 0$), according to lemma II, must all satisfy the equation

$$a|\varphi_0^i\rangle = 0.$$

To find the degeneracy of the $E_0$ level, all we must do is see how many li kets satisfy the above. We can write the above equation using the definition of $\hat{X}, \hat{P}$ and $a$ in terms of them, in the form

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}X + \frac{i}{\sqrt{m\hbar\omega}}P\right]|\varphi_0^i\rangle = 0.$$

In the $\{|x\rangle\}$ representation, this relation becomes

$$\left(\frac{m\omega}{\hbar}x + \frac{d}{dx}\right)\varphi_0^i(x) = 0, \quad \text{where} \quad \varphi_0^i(x) = \langle x|\varphi_0^i\rangle.$$

Therefore we msut solve a first-order differential equation, which solution is

$$\varphi_0^i(x) = ce^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{3.17}$$

The various solutions of the ODE are all proportional to each other. Consequently, there exists only one ket $|\varphi_0\rangle$ that satisfies the initial equation: the ground sate $E_0 = \hbar\omega/2$ is not degenerate.

#### All the states are non-degenerate

We use recurrence to show that all other states are also non-degenerate. We need to prove that if $E_n$ is non degenerate, the level $E_{n+1}$ is not either.

Lets assume there exists only one vector $|\varphi_n\rangle$ such that

$$N|\varphi_n\rangle = n|\varphi_n\rangle.$$

Then consider an eigenvector $|\varphi_{n+1}^i\rangle$ corresponding to the eigenvalue $n+1$

$$N|\varphi_{n+1}^i\rangle = (n+1)|\varphi_{n+1}^i\rangle.$$

We know that the ket $a|\varphi_{n+1}^i\rangle$ is not zero and that it is an eigenvector of $N$ with eigenvalue $n$. Since this ket is not degenerae by hypothesis, there exists a number $c^i$ such that

$$a|\varphi_{n+1}^i\rangle = c^i|\varphi_n\rangle/a^\dagger \longrightarrow a^\dagger a|\varphi_{n+1}^i\rangle = N|\varphi_{n+1}^i\rangle = (n+1)|\varphi_{n+1}^i\rangle = c^i a^\dagger|\varphi_n\rangle.$$

We have,

$$|\varphi_{n+1}^i\rangle = \frac{c^i}{n+1}a^\dagger|\varphi_n\rangle.$$

We see that all kets $|\varphi_{n+1}^i\rangle$ associated with the eigenvalue $n+1$ are proportional to $a^\dagger|\varphi_n\rangle$. They are proportional to each other: the eigenvalue $n+1$ is not degenerate.

Since the eigenvalue $n=0$ is not degenerate, the eigenvalue $n=1$ is not either, nor is $n=2$, etc.: all the eigenvalues of $N$ and, consequently, all those of $H$, are non-degenerate. Now, we can just write $|\varphi_n\rangle$ for the eigenvector of $H$ associated with $E_n$.

## 3.3 Eigenstates of the Hamiltonian

### 3.3.1 The $\{\varphi_n\}$ representation

Since none of the eigenvalues of $N$ ($H$) is degenerate, $N$ ($H$) alon constitutes a CSCO in $\mathscr{E}_c$.

#### The basis vectors in terms of $|\psi_0\rangle$

We assume that the vector $|\varphi_0\rangle$ which satsfies $a|\varphi_0\rangle = 0$, is normalized. According to lemma III, the vector $|\varphi_1\rangle$ is proportional to $a^\dagger|\varphi_0\rangle$ in the form

$$|\varphi_1\rangle = c_1 a^\dagger|\varphi_0\rangle.$$

We shall determine $c_1$ by requiring $|\varphi_1\rangle$ to e normalized and choosing the phase of $|\varphi_1\rangle$ such that $c_1$ is real and positive. The square of the norm of $|\varphi_1\rangle$ is

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2\langle\varphi_0|aa^\dagger|\varphi_0\rangle = |c_1|^2\langle\varphi_0|(a^\dagger a+1)|\varphi_0\rangle = |c_1|^2[\underbrace{\langle\varphi_0|N|\varphi_0\rangle}_{0\langle\varphi_0|\varphi_0\rangle}+\langle\varphi_0|\varphi_0\rangle] = |C_1|^2.$$

We find that $c_1 = 1$:

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2 = 1 \Longrightarrow |\varphi_1\rangle = a^\dagger|\varphi_0\rangle. \tag{3.18}$$

We can do the same to constrcut $|\varphi_2\rangle$ from $|\varphi_1\rangle$ and get $c_2$ and so on. In general, if we know $|\varphi_{n-1}\rangle$ (normalized), then the normalized vector $|\varphi_n\rangle$ is written

$$|\varphi_n\rangle = c_n a^\dagger|\varphi_{n-1}\rangle, \quad \text{so that} \quad c_n = \frac{1}{\sqrt{n}}.$$

In fact, we can express all $|\varphi_n\rangle$ in terms of $|\varphi_0\rangle$ by recursion:

Excited states in terms of the ground state $$|\varphi_n\rangle = \frac{1}{\sqrt{n}}(a^\dagger)^n|\varphi_0\rangle\,. \tag{3.19}$$

#### Orthonormalization and closure relations

Since $H$ is Hermitian, the kets $|\varphi_n\rangle$ corresponding to different values of $n$ are orthogonal so that they satisfy the orthonormalization relation:

$$\langle\varphi_n'|\varphi_n\rangle = \delta_{nn'}.$$

In addition, $H$ is an obsrvable; the set of the $|\varphi_n\rangle$ therefore constitutes a basis in $\mathscr{E}_x$, which is expressed by the closure relation

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = \mathbb{1}.$$

### Action of the various operators

The observables $X$ and $P$ are linear combinations of the operators $a$ and $a^\dagger$. Therefore, all physical quantities can be expressed in terms of the latters. The action of $a$ and $a^\dagger$ on the vectors of the $\{|\varphi_n\rangle\}$ basis is

$$\text{Action of } a \text{ and } a^\dagger \qquad \begin{array}{l} a^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle \\ a|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle \end{array} \overset{\text{Adjoint}}{\longrightarrow} \begin{array}{l} \langle\varphi_n|a = \sqrt{n+1}\langle\varphi_{n+1}| \\ \langle\varphi_n|a^\dagger = \sqrt{n}\langle\varphi_{n-1}| \end{array} \tag{3.20}$$

Note that $a$ decreases or increases $n$ by one unit depending on wheter it acts on the $|\varphi_n\rangle$ or on the bra $\langle\varphi_n|$, similarly for $a^\dagger$. The expressions for $X$ and $P$ are then:

$$X|\varphi_n\rangle = \sqrt{\frac{\hbar}{m\omega}}\frac{1}{\sqrt{2}}(a^\dagger + a)|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n+1}|\varphi_{n+1}\rangle + \sqrt{n}|\varphi_{n-1}\rangle] \tag{3.21}$$

$$P|\varphi_n\rangle = \sqrt{m\hbar\omega}\frac{i}{\sqrt{2}}(a^\dagger - a)|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}[\sqrt{n+1}|\varphi_{n+1}\rangle - \sqrt{n}|\varphi_{n-1}\rangle] \tag{3.22}$$

The matrix elements of $a, a^\dagger, X, P$ in the $\{|\varphi_n\rangle\}$ representation are therefore

$$\langle\varphi_{n'}|a|\varphi_n\rangle = \sqrt{n}\delta_{n',n-1} \tag{3.23}$$

$$\langle\varphi_{n'}|a^\dagger|\varphi_n\rangle = \sqrt{n+1}\delta_{n',n+1} \tag{3.24}$$

$$\langle\varphi_{n'}|X|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \tag{3.25}$$

$$\langle\varphi_{n'}|P|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}[\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}] \tag{3.26}$$

The matrices representing $a$ and $a^\dagger$ are Hermitian conjugates of each other, while matrices representing $X$ and $P$ are both Hermitian.

### Eigenstates of $a$

Does $a$ have eigenstates? that is, can we express any vector as

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle?$$

We begin with $a|\alpha\rangle = \alpha|\alpha\rangle$ in the left side:

$$a|\alpha\rangle = a\mathbb{1}|\alpha\rangle = a\sum_{n=0}^{\infty}|n\rangle\langle n|\alpha\rangle = \cancelto{0}{a|0\rangle}c_0 + \sum_{n=1}^{\infty}c_n a|\alpha\rangle = \sum_{n=1}^{\infty}\sqrt{n}|n-1\rangle c_n = \sum_{n=0}^{\infty}c_{n+1}\sqrt{n+1}|n\rangle.$$

On the right side, we have

$$\alpha|\alpha\rangle = \alpha\mathbb{1}|\alpha\rangle = \alpha\sum_{n=0}^{\infty}|n\rangle\langle n|\alpha\rangle = \alpha\sum_{n=0}^{\infty}c_n|n\rangle.$$

Equating both side results:

$$\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = \alpha \sum_{n=0}^{\infty} c_n|n\rangle / \langle m|$$
$$\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}\langle m|n\rangle = \alpha \sum_{n=0}^{\infty} c_n\langle m|n\rangle$$
$$c_{m+1}\sqrt{m+1} = \alpha c_m$$

from which we get

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle.$$

We normalize it:

$$\begin{aligned}\langle\alpha|\alpha\rangle = 1 &= \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m\alpha^n}{\sqrt{m!}\sqrt{n!}} c_0^* c_0 \langle m|n\rangle \\ &= \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n}!|c_0|^2 \\ &= |c_0|^2 e^{|\alpha|^2} = 1 \longrightarrow c_0 = e^{-\frac{|\alpha|^2}{2}}.\end{aligned}$$

Therefore, we finally get:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{3.27}$$

### 3.3.2 Wave functions associated with the stationary states

We know that $\varphi_0(x)$ is the ground sate:

$$\varphi_0(x) = \langle x|\varphi_0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.$$

To obtain the functions $\varphi_n(x)$, all we need to do is use expression (3.19) and the fact that in $\{|x\rangle\}$ $a^\dagger$ is represented by

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]. \tag{3.28}$$

since $X$ is represented by multiplication by $x$, and $P$ by $-i\hbar\partial_x$. We thus obtain

$$\varphi_n(x) = \langle x|\varphi_n(x)\rangle = \frac{1}{\sqrt{n!}}\langle x|(a^\dagger)^n|\varphi_0\rangle = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]^n \varphi_0(x). \tag{3.29}$$

That is,

Excited state
$$\varphi_n(x) = \underbrace{\left[\frac{1}{2^n n!}\left(\frac{\hbar}{m\omega}\right)^n\right]^{1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\frac{m\omega}{\hbar}x - \frac{d}{dx}\right]^n}_{\text{Hermite polynomial}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}. \tag{3.30}$$

When $n$ increases, the region of the Ox axis in which $\varphi_n(x)$ takes on non-negligible values becomes larger. It follows that the mean value of the potential energy grows with $n$. In addition, the number of zeros of $\varphi_n(x)$ is $n$, this mplies that the mean kinetic energy of the particle increases with $n$.

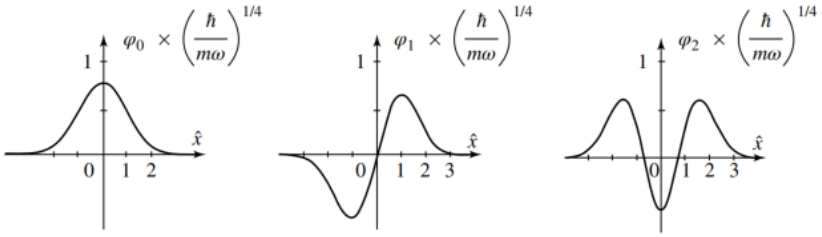



*Figure 4: Wave functions associated with the first three levels of a harmonic oscillator.*

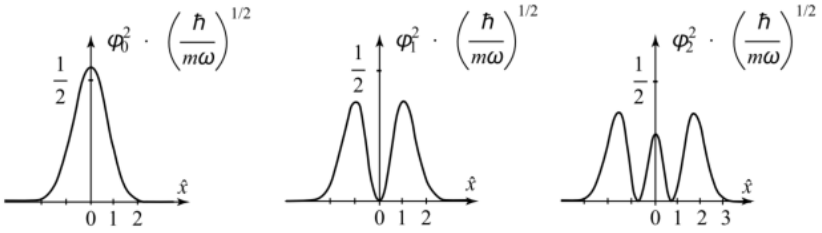



*Figure 5: Probability densities associated with the first three levels of a harmonic oscillator.*

## 3.4 Discussion

### 3.4.1 Mean values and rms eviations of $X$ and $P$ in a state $|\varphi_n\rangle$

Neither $X$ nor $P$ comutes with $H$, and the eigenstates $|\varphi_n\rangle$ of $H$ are not eigenstates of $X$ or $P$. Consequently, if the harmonics oscillator is in stationary state $|\varphi_n\rangle$, a measurement of the observable $X$ or $P$ can, a priori, yield any result.

We will compute the mean values of $X, P$ in such stationary state and also theirs rms deviation in order to set the uncertainty relation. We will use equations (3.22), which show that neither $X$ nor $P$ has diagonal matrix elements:

$$\langle\varphi_n|X|\varphi_n\rangle = \langle\varphi_n|P|\varphi_n\rangle = 0. \tag{3.31}$$

To obtain the rms deviations, we must calculate the mean value of $X^2$ and $P^2$. First, we note that

$$X^2 = \frac{\hbar}{2m\omega}(a^\dagger + a)(a^\dagger + a) = \frac{\hbar}{2m\omega}(a^{\dagger 2} + aa^\dagger + a^\dagger a + a^2)$$
$$P^2 = -\frac{m\hbar\omega}{2}(a^\dagger - a)(a^\dagger - a) = -\frac{m\hbar\omega}{2}(a^{\dagger 2} - aa^\dagger - a^\dagger a + a^2)$$

The terms $a^2$ and $a^{\dagger 2}$ do not contribute to the diagonal matrix elements, since $a^2|\varphi_n\rangle$ is proportional to $|\varphi_{n-2}\rangle$ and $a^{\dagger 2}|\varphi_n\rangle$ to $|\varphi_{n+2}\rangle$; both are orthogonal to $|\varphi_n\rangle$. The rest of the terms yields:

$$\langle\psi_n|(a^\dagger a + aa^\dagger)|\varphi_n\rangle = \langle\varphi_n|(2a^\dagger a + 1)|\varphi_n\rangle = 2n + 1.$$

Therefore, we have:

$$(\Delta X)^2 = \langle\varphi_n|X|\varphi_n\rangle - \langle\varphi_n|X^2|\varphi_n\rangle = \langle\varphi_n|X^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega} = \sigma^2\left(x + \frac{1}{2}\right). \tag{3.32}$$

$$(\Delta P)^2 = \langle\varphi_n|P|\varphi_n\rangle - \langle\varphi_n|P^2|\varphi_n\rangle = \langle\varphi_n|P^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega = \frac{\hbar^2}{\sigma^2}\left(x + \frac{1}{2}\right). \tag{3.33}$$

The product is therefore

$$\text{Uncertainty relation} \qquad \Delta X \Delta P = \left(n + \frac{1}{2}\right)\hbar\,. \tag{3.34}$$

We see that the lower bound is attained for $n = 0$, that is, for the ground state.

### 3.4.2 Properties of the ground state

In classical mechanics, the lowest energy of the harmonic oscilaltor is obtained when the particle is at rest. In QM, the moninum energy sate is $|\varphi_0\rangle$, whose energy is not zero, and the associates wave function has a certain spatial extension, characterized by the rms deviation $\Delta X = \sqrt{\hbar/2m\omega}$. The ground state correesponds to a compromie in which the sum of the kinetic and potential energy is as small as possible (uncertainty limitation).

The QHO possesses the peculiarity that due to the form of $V(x)$, the $\Delta X \Delta P$ attains its lower value at the ground state $|\varphi_0\rangle$. This is related to the fact that the wave function of the ground state is Gaussian.

### 3.4.3 Time evolution of the mean values

Consider thw state at $t = 0$

$$|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n(0)|\varphi_n\rangle.$$

Its state $|\psi(t)\rangle$ at $t$ can be obtained by using the evolution operator for conservative systems:

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-iE_n t/\hbar}|\varphi_n\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-i(n+1/2)\omega t}|\varphi_n\rangle. \tag{3.35}$$

The mean value of any physical quantity $A$ is

$$\langle\varphi(t)|A|\varphi(t)\rangle = \sum_{m,n=0}^{\infty} c_m^*(0)c_n(0)A_{mn}e^{i(m-n)\omega t}, \quad \text{with} \quad A_{mn} = \langle\varphi_m|A|\varphi_n\rangle.$$

The time evolution of the mean values involves only the frequency $\omega/2\pi$ and its various harmonics, which constitutes the Bohr frequencies of the harmonics oscillator.

If we consider $X$ and $P$, we know that the only non-zero elements $X_{mn}$ and $P_{mn}$ are those for which $m = n \pm 1$. Consequently, the mean values of $X$ and $P$ include only terms in $e^{\pm\omega t}$. Moreover, the form of the harmonics oscillator potential implies that for all $|ket\varphi_n$ the mean values of $X$ and $P$ rigorously satisfy the classical equations of motion. Using Ehrenfest theorem:

$$\begin{aligned} \frac{d}{dt}\langle X\rangle &= \frac{1}{i\hbar}\langle[X,H]\rangle = \frac{\langle P\rangle}{m} \\ \frac{d}{dt}\langle P\rangle &= \frac{1}{i\hbar}\langle[P,H]\rangle = -m\omega^2\langle X\rangle \end{aligned} \quad \xrightarrow{\int dt} \quad \begin{aligned} \langle X\rangle(t) &= \langle X\rangle(0)\cos\omega t + \frac{1}{m\omega}\langle P\rangle(0)\sin\omega t \\ \langle P\rangle(t) &= \langle P\rangle(0)\cos\omega t + m\omega\langle X\rangle(0)\sin\omega t \end{aligned} \tag{3.36}$$

- In a stationary state $|\varphi_n\rangle$, the behavior of the harmonic oscillator is totally different from that predicted by classical mechanics. The mean values of all the observables are constant over time.

# 3.5 Stationary states in the $\{|x\rangle\}$ representation

## 3.5.1 Hermite polynomials

### Definition

Let be the Gaussian function

$$F(z) = e^{-z^2} \tag{3.37}$$

The successive derivatives are

$$F'(z) = -2ze^{-z^2}, \quad F''(z) = (4z^2 - 2)e^{-z^2}, \quad \cdots, \quad F^{(n)}(z) = (-1)^n H_n(z)e^{-z^2}.$$

If we have $F^{(n-1)}$, its differentiation will yields $F^{(n)}$ and we can obtain the above general equation:

$$H_n(z) = \left(2z - \frac{d}{dz}\right) H_{n-1}(z), \tag{3.38}$$

where $H_n(z)$ is the nth-degree **Hermite polynomial**:

$$\text{Hermite polynomial} \qquad H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}. \tag{3.39}$$

The parity of $H_n(x)$ is $(-1)^n$, and it has $n$ real zeros between which one finds those of $H_{n-1}$.

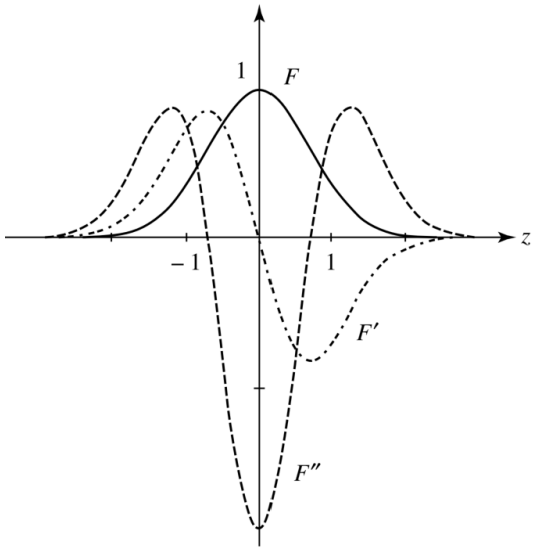



**Figure 3.1** Shape of the Gaussian function $F(z)$ and its first and second derivatices.

### Generating function

Consider the function

$$F(z+\lambda) = e^{-(z+\lambda)^2} \overset{\text{Taylor}}{=} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} F^{(n)}(z) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (-1)^n H_n(z) e^{-z^2}.$$

Multiplying this relation by $e^{z^2}$ and replacing $\lambda$ by $-\lambda$ we obtain:

Generating function of Hermite polynomials
$$e^{z^2}F(z-\lambda) = e^{-\lambda^2+2\lambda z} = \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}H_n(z)\,. \tag{3.40}$$

The Hermite polynomials can therefore be obtained from the series expansion in $\lambda$ for the function $e^{-\lambda^2+2\lambda z}$.

### Recurrence relations; differential equation

We can obtain other recurrence relation by using the equation (3.40). For instance, differentiating equation (3.40) with respect to $z$ and using its expansion:

$$\frac{d}{dz}H_n(z) = 2nH_{n-1}(z). \tag{3.41}$$

If we differentiate with respect to $\lambda$, we get

$$H_n(z) = 2zH_{n-1}(z) - 2(n-1)H_{n-2}(z). \tag{3.42}$$

Finally, we can obtain an ODE differentiating equation (3.41) and using (3.38):

$$\frac{d^2}{dz^2}H_n(z) = 2n\frac{d}{dz}H_{n-1}(z) = 2n[2zH_{n-1}(z) - H_n(z)] = 2z\frac{d}{dz}H_{n-1}(z) - 2nH_n(z),$$

Thus,

ODE satisfied by Hermite polynomials
$$\left[\frac{d^2}{dz^2} - 2z\frac{d}{dz} + 2n\right]H_n(z) = 0\,. \tag{3.43}$$

## 3.5.2 The eigenfunctions of the harmonic oscillator Hamiltonian

### Generating function

### $\varphi_n(x)$ in terms of the Hermite polynomials

What is $\varphi(x) = \langle x|\varphi\rangle$?

We know that $a|\varphi_0\rangle = 0|\varphi_0\rangle$, so we replace the $\{|x\rangle\}$ representation

$$\langle x|a|\varphi_0\rangle = \langle x|\frac{1}{\sqrt{2}}\left(\frac{x}{\sigma} + \frac{ip\sigma}{\hbar}\right)|\varphi_0\rangle = 0$$
$$\frac{1}{\sqrt{2}}\left(\frac{x}{\sigma} + \sigma\frac{\partial}{\partial x}\right)\varphi_0(x) =$$
$$\frac{\partial\varphi_0(x)}{\partial x} = -\frac{x}{\sigma^2}\varphi_0(x).$$

Its solution is

$$\varphi_0(x) = ce^{-\frac{x^2}{2\sigma^2}} \xrightarrow{\text{normalization}} \varphi_0(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4}e^{-\frac{x^2}{2\sigma^2}}.$$

The general form is the following:

$$\text{Excited state in } \{|x\rangle\} \qquad \varphi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\beta^2 x^2/2} H_n(\beta x)\,. \tag{3.44}$$

The shape of $\varphi_n(x)$ is therefore analogous to that of the nth-order derivative of the Gaussian function $F(x)$. Moreover, $\varphi_n(x)$ is of parity $(-1)^n$ and posseses $n$ zeros interposed between those of $\varphi_{n+1}(x)$. Recall this is related to the increase in the average kinetic energy of the states $|\varphi_n\rangle$ when $n$ increases.

### Recurrence relations

Lets write the action of $a$ and $a^\dagger$ (3.20) in the $\{|x\rangle\}$ representation. The action of them in this representation is

$$a \longrightarrow \frac{\beta}{\sqrt{2}}\left[x + \frac{1}{\beta^2}\frac{d}{dx}\right] \qquad a^\dagger \longrightarrow \frac{\beta}{\sqrt{2}}\left[x - \frac{1}{\beta^2}\frac{d}{dx}\right]. \tag{3.45}$$

Then equation (3.20) becomes:

$$\text{Action of } a, a^\dagger \text{ in } \{|x\rangle\} \qquad \begin{aligned} \frac{\beta}{\sqrt{2}}\left[x + \frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) &= \sqrt{n}\varphi_{n-1}(x) \\ \frac{\beta}{\sqrt{2}}\left[x - \frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) &= \sqrt{n+1}\varphi_{n+1}(x) \end{aligned} \tag{3.46}$$

Taking the sum and difference:

$$\begin{aligned} x\beta\sqrt{2}\varphi_n(x) &= \sqrt{n}\varphi_{n-1}(x) + \sqrt{n+1}\varphi_{n+1}(x) \\ \frac{\sqrt{2}}{\beta}\frac{d}{dx}\varphi_n(x) &= \sqrt{n}\varphi_{n-1}(x) - \sqrt{n+1}\varphi_{n+1}(x) \end{aligned}$$

Replacing in them the function $\varphi_n(x)$ of equation x yields two recursive equations for $H(x)$ (setting $\hat{x} = \beta x$):

$$\begin{aligned} 2\hat{x}H_n(\hat{x}) &= 2nH_{n-1}(\hat{x}) + H_{n+1}(\hat{x}) \\ 2\left[-\hat{x}H_n(\hat{x}) + \frac{d}{d\hat{x}}H_n(\hat{x})\right] &= 2nH_{n-1}(\hat{x}) - H_{n+1}(\hat{x}) \end{aligned}$$

## 3.6 The isotropic three-dimensional harmonic oscillator

The main idea is the same, but here there is an extension of the problem.

The spinless particle of mass $m$ is subjected to a central force

$$\boldsymbol{F} = -k\boldsymbol{r}. \tag{3.47}$$

This force is derived from the potential energy:

$$V(\boldsymbol{r}) = \frac{1}{2}k\boldsymbol{r}^2 = \frac{1}{2}m\omega^2\boldsymbol{r}^2, \quad \omega = \sqrt{\frac{k}{m}}. \tag{3.48}$$

The classical Hamiltonian is therefore:

$$\text{Classical Hamiltonian} \qquad \mathcal{H}(\boldsymbol{r},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}m\omega^2\boldsymbol{r}^2 \,. \tag{3.49}$$

Using the quantization rules, we get the Hamiltonian operator:

$$\text{Hamiltonian operator} \qquad H = \frac{\boldsymbol{P}^2}{2m} + \frac{1}{2}m\omega^2\boldsymbol{R}^2 \,. \tag{3.50}$$

Since the Hamiltonian is time-independent, we shall solve its eigenequation $H|\psi\rangle = E|\psi\rangle$, where $|\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}$ the state space of the particle in three-dimensional space.

**Isotropic QHO**

Due to $V(\boldsymbol{r})$ only depends on the distance $r = |\boldsymbol{r}|$ of the particle from the origin (invariant to rotations), this harmonic oscillator is said to be **isotropic**.

$$V(\boldsymbol{r}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2). \tag{3.51}$$

It is defined by a single frequency $\omega = \omega_x = \omega_y = \omega_z$.

### 3.6.1 Separation of variables in cartesian coordinates

We assume the state space is a separable function so that:

$$\mathscr{E}_{\boldsymbol{r}} = \mathscr{E}_x \otimes \mathscr{E}_y \otimes \mathscr{E}_z. \tag{3.52}$$

The expression for the Hamiltonian is therefore

$$H = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega(Z^2 + Y^2 + Z^2) = H_z + H_y + H_z, \quad \text{with} \quad H_k = \frac{P_k^2}{2m} + \frac{1}{2}m\omega^2R_k^2. \tag{3.53}$$

Each operator acts in its own state space $\mathscr{E}_k$. $H_x, H_y, H_z$ commute, and also with the sum $H$. Consequently, the eigenequation can be solved by seeking the eigenvectors of $H$ that are also eigenvectors of $H_x, H_y, H_z$:

$$\begin{array}{ll} H_x|\varphi_{n_x}\rangle = \left(n_x + \frac{1}{2}\right)\hbar\omega|\varphi_{n_x}\rangle & |\varphi_{n_x}\rangle \in \mathscr{E}_x \\ H_y|\varphi_{n_y}\rangle = \left(n_y + \frac{1}{2}\right)\hbar\omega|\varphi_{n_y}\rangle & |\varphi_{n_y}\rangle \in \mathscr{E}_y \\ H_z|\varphi_{n_z}\rangle = \left(n_z + \frac{1}{2}\right)\hbar\omega|\varphi_{n_z}\rangle & |\varphi_{n_z}\rangle \in \mathscr{E}_z \end{array} \quad , \quad n_x, n_y, n_z \in \mathbb{N}_0^+.$$

The eigenstates common to $H, H_x, H_y, H_z$ are of the form:

$$|\psi_{n_x,n_y,n_z}\rangle = |\varphi_{n_z}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle. \tag{3.54}$$

According to the above Hamiltonian and the eigenequations, we have

$$H|\psi_{n_x,n_y,n_z}\rangle = E_{n_x,n_y,n_z}|\psi_{n_x,n_y,n_z}\rangle = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega|\psi_{n_x,n_y,n_z}\rangle. \tag{3.55}$$

The eigenvectors of $H$ are seen to be the **tensor product** os the eigenvectors of $H_x, H_y, H_z$ while the eigenvalues of $H$ to be the **sum** of eigenvalues of these operators. The energy levels $E_n$ of the isotropic 3D QHO are of the form:

$$\text{Energy levels} \qquad E_n = \left(n + \frac{3}{2}\right)\hbar\omega, \quad n = n_x + n_y + n_z \in \mathbb{N}_0^+ . \tag{3.56}$$

The $a$ operators are defined analogolously:

$$\text{Operator } a \text{ and } a^\dagger \qquad \begin{aligned} a_j &= \frac{1}{\sqrt{2}}\left(\frac{R_j}{\sigma_j} + \frac{iP_j\sigma_j}{\hbar}\right) \\ a_j^\dagger &= \frac{1}{\sqrt{2}}\left(\frac{R_j}{\sigma_j} - \frac{iP_j\sigma_j}{\hbar}\right) \end{aligned}, \quad \text{with} \quad [a_i, a_j^\dagger] = \delta_{ij} . \tag{3.57}$$

The action of $a_x$ and $a_x^\dagger$ on the state $|\psi_{n_x,n_y,n_z}\rangle$ is:

$$a_x|\psi_{n_x,n_y,n_z}\rangle = (a_x|\varphi_{n_x}\rangle)|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x}|\varphi_{n_x-1}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x}|\varphi_{n_x-1,n_y,n_z}\rangle \tag{3.58}$$

$$a_x^\dagger|\psi_{n_x,n_y,n_z}\rangle = (a_x^\dagger|\varphi_{n_x}\rangle)|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x+1}|\varphi_{n_x+1}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x+1}|\varphi_{n_x+1,n_y,n_z}\rangle. \tag{3.59}$$

And for the other dimensions is analogous. We also know that

$$|\varphi_{n_x}\rangle = \frac{1}{\sqrt{n_x!}}(a_x^\dagger)^{n_x}|\varphi_0\rangle, \quad a_x \in \mathscr{E}_x : \quad a_x|\varphi_0\rangle = 0.$$

In $\mathscr{E}_y$ and $\mathscr{E}_z$ we have something similar. Consequently, we can write

$$\text{Excited state} \qquad |\psi_{n_x,n_y,n_z}\rangle = \frac{1}{\sqrt{n_x!n_y!n_z!}}(a_x^\dagger)^{n_x}(a_y^\dagger)^{n_y}(a_z^\dagger)^{n_z}|\psi_{0,0,0}\rangle , \tag{3.60}$$

where $|\psi_{0,0,0}\rangle$ is the tensor product of the ground states of each dimension:

$$a_x|\psi_{0,0,0}\rangle = a_y|\psi_{0,0,0}\rangle = a_z|\psi_{0,0,0}\rangle = 0.$$

Finally, the associated wave functions is of the form

$$\langle \boldsymbol{r}|\psi_{n_x,n_y,n_z}\rangle = \langle z|\langle y|\langle x|\varphi_{n_z}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z), \tag{3.61}$$

where $\varphi_{n_x}, \varphi_{n_y}, \varphi_{n_z}$ are stationary wave functions of the one-dimensional harmonics oscillator. For instance,

$$\langle \boldsymbol{r}|\psi_{0,0,0}\rangle = \left(\frac{1}{\pi\sigma^2}\right)^{3/4} e^{-\frac{1}{2\sigma^2}(x^2+y^2+z^2)}, \quad \omega = \omega_x = \omega_y = \omega_z. \tag{3.62}$$

### 3.6.2 Degeneracy of the energy levels

We have that $\{H_x, H_y, H_z\}$ constitutes a CSCO in $\mathscr{E}_{\boldsymbol{r}}$ (Others CSCOs are $\{H_x, H_y, H\}, \{X, P_y, H_z\}$) so that there exists a unique ket $|\psi_{n_x,n_y,n_z}\rangle$ corresponding to a given set of eigenvalues for $H_x, H_y, H_z$. However, $H$ alone does not form a CSCO since the energy levels $E_n$ are **degenerate**. Choosing an eigenvalue of $H$, $E_n = (n + 3/2)\hbar\omega$, all the kets $\{|\psi_{n_x,n_y,n_z}\rangle\}$ basis that satisfy

$$n_x + n_y + n_z = n$$

are eigenvectors of $H$ with eigenvalue $E_n$. The degree of degeneracy $g_n$ of $E_n$ is equal to the number of different sets $\{n_x, n_y, n_z\}$ satisfying the above equation. It is equal then to

$$\text{Degree of degeneracy of } E_n \qquad g_n = \frac{(n+1)(n+2)}{2}. \tag{3.63}$$

Therefore, only the ground state $E_n = 3\hbar\omega/2$ is non-degenerate.

**Ejemplo 3.1** **Measurements of energies**

a) Measurement with $H$ and result if $\hbar\omega(1+3/2)$, then $n_x + n_y + n_z = 1$.
b) Measurement with $H_x$ and result is $n_x = 0$, then $n_y + n_z = 1$.
c) Measurement with $H_z$ and result is $n_z = 1$, then $n_y = 0$.

Therefore, the state is

$$|0,0,1\rangle = |n_x = 0, n_y = 0, n_z = 1\rangle.$$

## 3.7 Coherent states of the harmonic oscillator

We know that quantum mechanics must yield the same results as classical mechanics in the limiting casr where the harmonic oscillator has an energy much greater than the quantum $\hbar\omega$.

It is possible to construct quantum mechanics states leading to physical predictions which are almost identical to the classical ones, at least for a macroscopic oscillator? Such quantum sistems do exist: they are coherent linear superpositions of all the states $|\varphi_n\rangle$. We shall call them **quasi-classical states** or coherent states of the harmonic oscillator.

It is important to understand, in the framework of quantum mechanics, how to move gradually from the case in which thee results given by the classical approximation are sufficient to the case in which quantum effects are preponderant.

The position, momentum, and energy of a harmonic oscillator are described in QM by operators which do not commute. It is not possible to construct a state in which they are all perfectly well-defined.

Theregore, we shall only look for a state vector such that for all $t$, the mean values $\langle X\rangle$, $\langle P\rangle$, and $\langle H\rangle$ are as close as possible to the corresponding classical values: the compromise if then that none of these three observables is perfectly known. Nevertheless, the rms deviation $\Delta X$, $\Delta Y$, and $\Delta H$ are, in the macroscopic limit, completely negligible.

### 3.7.1 Quasi-classical states

#### Introducing $\alpha_0$ to characterize a classical motion

The classical quantitites of motion of a 1D harmonics oscillator of mass $m$ and angular frrequency $\omega$ are

$$\text{Equations of motion for CHO} \qquad \begin{aligned} \frac{d}{dt}x(t) &= \frac{1}{m}p(t) \\ \frac{d}{dt}p(t) &= -m\omega^2 x(t) \end{aligned}. \tag{3.64}$$

The classical state of the HO is determined at time $t$ when we know its position $x(t)$ and its momentum $p(t)$. We shall therefore combine them into a single complex number $\alpha(t)$ given by:

$$\text{Displacement coordinate} \qquad \alpha(t) = \frac{1}{\sqrt{2}}\left(\frac{x(t)}{\sigma} + i\frac{\sigma p(t)}{\hbar}\right) \quad (-). \tag{3.65}$$

Then, the equations of motions turn to

$$\frac{d}{dt}\alpha(t) = -i\omega\alpha(t) \longrightarrow \alpha(t) = \alpha_0 e^{-i\omega t}, \quad \alpha_0 = \alpha(0) \tag{3.66}$$

We can plot this evolution in a geometrical representation of the evolution of the state of the system through the **phase-space diagram** as shown in the following figure. According to the solution of the

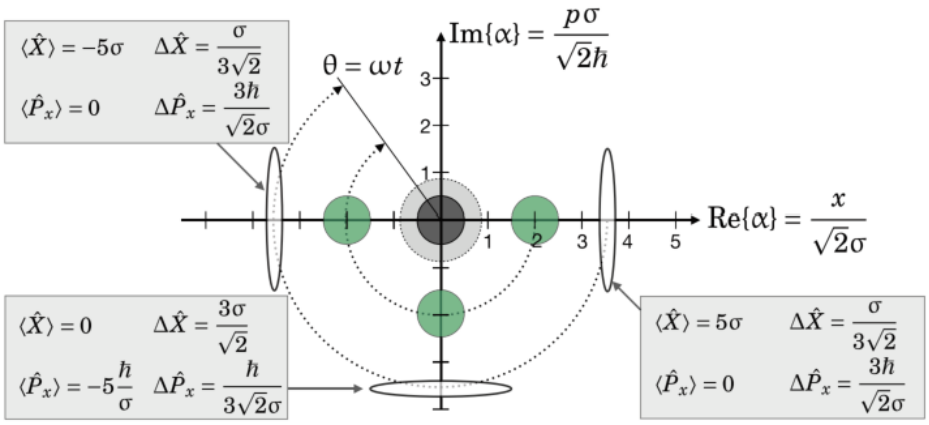



**Figure 3.1** Illustration of four HO states in the phase-space diagram: black=ground state, gray=first excited state, ovals=squeezed state, green=coherent state.

ODE, we have

$$x(t) = \frac{1}{\sqrt{2}}(\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t}), \quad p(t) = -\frac{i}{\sqrt{2}}(\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t}). \tag{3.67}$$

As for the classcal energy $\mathcal{H}$ of the system, it is constant in time and equal to:

$$\mathcal{H} = \frac{1}{2m}p(0)^2 + \frac{1}{2}m\omega^2 x^2(0) = \frac{\hbar\omega}{2}\left[\left(\frac{x(0)}{\sigma}\right)^2 + \left(\frac{\sigma p(0)}{\hbar}\right)^2\right] = \hbar\omega|\alpha_0|^2.$$

For a macroscopic oscillator, the energy $\mathcal{H}$ is much greater than the quantum $\hbar\omega$, so

$$\text{Macroscopic regime} \qquad |\alpha_0| \gg 1\,. \tag{3.68}$$

## Conditions defining quasi-classical states

We are looking for a quantum mechanical state for which at every instant the mean values $\langle X\rangle$, $\langle P\rangle$, and $\langle H\rangle$ are practically equal to the values of $x$, $p$, and $\mathcal{H}$ which correspond to a given classical motion.

The time evolution of the matrix element $\langle a\rangle(t) = \langle\psi(t)|a|\psi(t)\rangle$ is given by

$$i\hbar\partial_t\langle a\rangle(t) = \langle[a, H]\rangle(t)$$

The commutator is $[a, H] = [a, a^\dagger a] = \hbar\omega a$, which implies that the solution of the above ODE is

$$\langle a\rangle(t) = \langle a\rangle(0)e^{-i\omega t}. \tag{3.69}$$

The evolution of $\langle a^\dagger\rangle(t)$ satisfies the adjoint equation:

$$\langle a^\dagger\rangle(t) = \langle a^\dagger\rangle(0)e^{i\omega t} = \langle a\rangle^*(0)e^{i\omega t}.$$

The equation (3.69) is anaologous to equation (3.66). We can substitute $\langle a\rangle(t)$ and $\langle a^\dagger\rangle(t)$ in the mean value of $X$ and $P$ to get:

$$\langle X\rangle(t) = \frac{1}{\sqrt{2}}(a + a^\dagger) = \frac{1}{\sqrt{2}}[\langle a\rangle(0)e^{-i\omega t} + \langle a\rangle^* e^{i\omega t}] \tag{3.70}$$

$$\langle P\rangle(t) = \frac{i}{\sqrt{2}}(a^\dagger - a) = \frac{i}{\sqrt{2}}[\langle a\rangle^* e^{i\omega t} - \langle a\rangle(0)e^{-i\omega t}] \tag{3.71}$$

It is necessary and sufficient to set at $t = 0$ the condition $\langle a\rangle(0) = \alpha_0$, which resembles to the classical motion. The normalized state vector $|\psi(t)\rangle$ of the oscillator must therefore satisfy the condition

$$\text{First condition} \qquad \langle\psi(0)|a|\psi(0)\rangle = \alpha_0.$$

We must now require the mean value

$$\langle H\rangle = \hbar\omega\langle a^\dagger a\rangle(0) + \frac{\hbar\omega}{2} \tag{3.72}$$

to be equal to the classical energy $\mathcal{H}$. Given that for a classical oscillator $|\alpha_0|$ is much greater than $1$, we shall neglect the term $\hbar\omega/2$ with respect to $\hbar\omega|\alpha_0|^2$. The second condition on the state vector can now be written:

$$\text{Second condition} \qquad \langle\psi(0)|a^\dagger a|\psi(0)\rangle = |\alpha_0|^2. \tag{3.73}$$

The two conditions are sufficient to determine the normalized state vector $|\psi(0)\rangle$.

#### Quasi-classical states are eigenvectors of the operator $a$

If a normalized vector $|\psi(0)\rangle$ satisfy the relation

$$a|\psi(0)\rangle = \alpha_0|\psi(0)\rangle, \tag{3.74}$$

then the two conditions above are satisfied. The quasi-classical state, associated with a classical motion characterized by the parameter $\alpha_0$ is such that $|\psi(0)\rangle$ is an eigenvector of the operator $a$ with the eigenvalue $\alpha_0$. We will denote the eigenvector of $a$ with eigenvalue $\alpha$ by $|\alpha\rangle$:

$$\text{Eigenvector of } a \text{ with eigenvalue } \alpha \qquad a|\alpha\rangle = \alpha|\alpha\rangle. \tag{3.75}$$

### 3.7.2 Properties of the $|\alpha\rangle$ states

#### Expansion of $|\alpha\rangle$ on the basis of the stationary states $|\varphi_n\rangle$

Let us determine the ket $|\alpha\rangle$ wich is a solution of (3.74) by using an expansion on $|\varphi_n\rangle$:

$$|\alpha\rangle = \sum_n c_n(\alpha)|\varphi_n\rangle.$$

We then have

$$a|\alpha\rangle = \sum_n c_n(\alpha)\sqrt{n}|\varphi_{n-1}\rangle$$

and, substituting this into (3.75) yields

$$c_{n+1}(\alpha) = \frac{\alpha}{\sqrt{n+1}}c_n(\alpha).$$

This relation enable us to determine by recurrence all the coefficient $c_n(\alpha)$ in terms of $c_0(\alpha)$:

$$c_n(\alpha) = \frac{\alpha^n}{\sqrt{n!}}c_0(\alpha). \tag{3.76}$$

When $c_0(\alpha)$ is fixed, all the $c_n(\alpha)$ are also fixed. The vectoer $|\alpha\rangle$ is therefore unique. We shall choose $c_0(\alpha)$ real, positive and normalized with $|\alpha\rangle$, which determines it completely:

$$\sum_n |c_n(\alpha)|^2 = |c_0(\alpha)|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = |c_0(\alpha)|^2 e^{|\alpha|^2} = 1. \tag{3.77}$$

We the convenction we have chosen we have $c_0(\alpha) = e^{-|\alpha|^2/2}$ and finally,

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle. \tag{3.78}$$

This result was also obtained by Cris displacing the $|\varphi_0\rangle$ from the origin by $x_0$ (lecture 14). It began with $|\psi\rangle = S(x_0)|\varphi_0\rangle$ and got some expression. Then, we replaced $|\psi\rangle$ by $|\alpha\rangle$ with the corresponding transformation: $\alpha = x_0/(\sqrt{2}\sigma)$.

### Possible values of the energy in an $|\alpha\rangle$ state

Assuming an oscillator in the state $|\alpha\rangle$, we see from (3.78) that a measurement of the energy can yield the result $E_n = (n + 1/2)\hbar\omega$ with the probability:

$$\text{Probability of having } E_n \qquad P_n(\alpha) = |\langle\alpha|\varphi_n\rangle|^2 = \frac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2}. \tag{3.79}$$

The probability obtained corresponds to a **Poisson distribution**. We have from its a recurrence relation:

$$P_n(\alpha) = \frac{|\alpha|^2}{n}P_{n-1}(\alpha).$$

$P_n(\alpha)$ reaches its maximum when $n$ is the integral part of $|\alpha|^2$.

### Calculation of mean values and uncertainties

The mean value can be obtaines expressing them in terms of the $a$ operators, and using (3.78):

$$\begin{array}{l}
\langle X\rangle_\alpha = \langle\alpha|X|\alpha\rangle = \sqrt{2}\sigma\text{Re}\,(\alpha)\,, \quad \langle X^2\rangle_\alpha = \frac{\sigma^2}{2}[(\alpha+\alpha^*)^2+1] \\
\langle P\rangle_\alpha = \langle\alpha|P|\alpha\rangle = \frac{\sqrt{2}\hbar}{\sigma}\text{Im}\,(\alpha)\,, \quad \langle P^2\rangle_\alpha = \frac{m\hbar\omega}{2}[1-(\alpha-\alpha^*)^2] \\
\langle N\rangle_\alpha = \langle\alpha|N|\alpha\rangle = |\alpha|^2, \quad \langle N^2\rangle_\alpha = - \\
\langle H\rangle_\alpha = \langle\alpha|H|\alpha\rangle = \hbar\omega\left[|\alpha|^2+\frac{1}{2}\right], \quad \langle H^2\rangle_\alpha = \hbar^2\omega^2\left[|\alpha|^4+2|\alpha|^2+\frac{1}{4}\right]
\end{array} \tag{3.80}$$

Therefore, we have:

$$\Delta X_\alpha = \frac{\sigma}{\sqrt{2}}, \quad \Delta P_\alpha = \frac{\hbar}{\sqrt{2}\sigma}, \quad \Delta N_\alpha = |\alpha|, \quad \Delta H_\alpha = \hbar\omega|\alpha|. \tag{3.81}$$

The $XP$ uncertainty relation is therefore:

$$\Delta X_\alpha \Delta P_\alpha = \frac{\hbar}{2}. \tag{3.82}$$

### The displacement operator $D(\alpha)$

Let be the operator define by

Displacement operator
$$D(\alpha) = T(\langle X\rangle)S(\langle P\rangle)e^{i\langle X\rangle\langle P\rangle/\hbar} = e^{\alpha a^\dagger - \alpha^* a}. \tag{3.83}$$

This operator is unitary since

$$D^\dagger(\alpha) = e^{\alpha^* a - \alpha a^\dagger} \implies D(\alpha)D^\dagger(\alpha) = D^\dagger(\alpha)D(\alpha) = 1.$$

The argument of the exponential can be defined with the commutator $[\alpha a^\dagger, -\alpha^* a] = \alpha^*\alpha$ so that using the Glauber formula for exponential yields:

$$D(\alpha) = e^{-|\alpha|^2/2}e^{\alpha a^\dagger}e^{-\alpha^* a}$$

Now, the action of $D(alpha)$ into a ket $|\varphi_0\rangle$ can be considerd by parts. First,

$$e^{-\alpha^* a}|\varphi_0\rangle = \left[1 - \alpha^* a + \frac{\alpha^{*2}}{2!}a^2 + \cdots\right]|\varphi_0\rangle = |\varphi_0\rangle.$$

Because it returns the same ket, we are left with the second exponential:

$$D(\alpha)|\varphi_0\rangle = e^{-|\alpha|^2/2}e^{\alpha a^\dagger}|\varphi_0\rangle = e^{-|\alpha|^2/2}\sum_n \frac{(\alpha a^\dagger)^n}{n!}|\varphi_0\rangle = e^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle.$$

Comparing with (3.78) we have

$$|\alpha\rangle = D(\alpha)|\varphi_0\rangle. \tag{3.84}$$

$D(\alpha)$ is therefore the unitary transformation which transforms the ground state $|\varphi_0\rangle$ into the quasi-classical state $|\alpha\rangle$.

---

**Ejemplo 3.2** **Translation with D**

Let be

$$D(\alpha) = e^{\frac{1}{\sqrt{2}}(5+10i)a^\dagger - \frac{1}{\sqrt{2}}(5-10i)a}.$$

We identify $\alpha = 5 + 10i$ and $\alpha^* = 5 - 10i$. Using the result of mean values (3.80) we have

$$\langle X\rangle = 5\sigma, \quad \text{and} \quad \langle P\rangle = \frac{10\hbar}{\sigma}.$$

Then,

$$\varphi_0(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-x^2/2\sigma^2} \implies \langle x|D|\varphi_0\rangle = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{i\frac{x}{\hbar}\left(10\frac{\hbar}{\sigma}\right)} e^{-\frac{(x-5\sigma)^2}{2\sigma^2}}.$$

---

### Scalar product of two $|\alpha\rangle$ states. Closure relation

The $|\alpha\rangle$ states are eigenvectors of the non-Hermitian operator $a$. There is therefore no obvious reason for these states to satisfy orthogonality and closure relation.

The scalar product between $|\alpha\rangle$ and $|\alpha'\rangle$ is:

$$\langle\alpha|\alpha'\rangle = \sum_n c_n^*(\alpha)c_n(\alpha') = e^{-|\alpha|^2/2}e^{-|\alpha'|^2/2}\sum_n \frac{(\alpha^*\alpha')^n}{n!} = e^{-|\alpha|^2/2}e^{-|\alpha'|^2/2}e^{\alpha^*\alpha'}.$$

That is,

$$\text{Orthonormalization relation} \qquad |\langle\alpha|\alpha'\rangle|^2 = e^{-|\alpha-\alpha'|^2}. \tag{3.85}$$

We see that **they are not orthogonal**, unless $\alpha = \alpha'$.

However, **they do satisfy the closure relation**:

$$\frac{1}{\pi}\iint |\alpha\rangle\langle\alpha|\, d\{\mathrm{Re}\,(\alpha)\}d\{\mathrm{Im}\,(\alpha)\} = \cdots = \sum_n |\varphi_n\rangle\langle|_\rangle n| = 1.$$

## 3.7.3 Time evolution of a quasi-classical state

Given the initial state $|\psi(0)\rangle = |\alpha_0\rangle$, How do its physical properties evolve over time?

### A quasi-classical state always remains an eigenvector of $a$

We use the time eovlution assuming conservative system (Hamiltonian time-independent)

$$\begin{aligned}
|\psi(t)\rangle &= e^{-iE_nt/\hbar}|\alpha_0\rangle = e^{-i\omega t(a^\dagger a+1/2)}|\alpha_0\rangle = e^{-i\omega t/2}e^{-i\omega t\overbrace{a^\dagger a}^{N}}|\alpha_0\rangle = e^{-i\omega t/2}e^{-i\omega tN}|\alpha_0\rangle \\
&= e^{-i\omega t/2}e^{-i\omega tN}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle = e^{-i\omega t/2}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}e^{-i\omega tN}|n\rangle \\
&= e^{-i\omega t/2}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n}}(\alpha_0e^{-i\omega t})^n|n\rangle = e^{-i\omega t/2}|\alpha_0e^{-i\omega t}\rangle = e^{-i\omega t/2}|\alpha(t)\rangle.
\end{aligned}$$

Thus, we have found that

$$\text{Evolution of the quasi-classical state} \qquad \boxed{|\psi(t)\rangle = e^{-\frac{i\omega t}{2}}|\alpha(t) = \alpha_0e^{-i\omega t}\rangle}. \tag{3.86}$$

We see that a quasi-classical state remains an eigenvector of $a$ for all time, with an eigenvalue $\alpha_0e^{-i\omega t}$ which is nothing more than $\alpha(t)$ obtained at the begining.

### Evolution of physical properties

We use equation (3.80) and change $\alpha$ by $\alpha_0e^{-i\omega t}$ to obtain:

$$\text{Mean values for } \alpha(t) \qquad \boxed{\begin{aligned}\langle X\rangle(t) &= \sqrt{2}\sigma\mathrm{Re}\,(\alpha(t)) \\ \langle P\rangle(t) &= \tfrac{\sqrt{2}\hbar}{\sigma}\mathrm{Im}\,(\alpha(t)) \\ \langle N\rangle &= |\alpha|^2 \\ \langle H\rangle &= \hbar\omega[|\alpha_0|^2 + \tfrac{1}{2}]\end{aligned}} \tag{3.87}$$

And the corresponding uncertainties are:

$$\text{Uncertainties} \qquad \begin{aligned} \Delta X &= \frac{\sigma}{\sqrt{2}} \\ \Delta P &= \frac{\hbar}{\sqrt{2}\sigma} \\ \Delta H &= \hbar\omega|\alpha_0| \end{aligned} \tag{3.88}$$

The uncertainty relation holds:

$$\Delta X \Delta P = \frac{\hbar}{2}.$$

Using the above mean values, we express $\alpha(t)$ as:

$$\alpha(t) = \frac{1}{\sqrt{2}}\left[\frac{\langle X\rangle(t)}{\sigma} + i\frac{\sigma\langle P\rangle(t)}{\hbar}\right]. \tag{3.89}$$

### Motion of the wave packet

Let us calculate the wave function $\psi(x,t)$. Using (3.86) and (76), we have:

$$\psi(x,t) = e^{i\theta_\alpha}\left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-i\omega t/2} e^{-\frac{x\langle P\rangle(t)}{\hbar}} e^{-\left[\frac{x-\langle x\rangle(t)}{2\Delta X}\right]^2}.$$

At $t$, the wave packet is still Gaussian. Thus, it remains minimum for all time. THe following figure shows the motion of the wave packe, performing periodc oscillation withouth becoming distorted. In free particle, this type of wave packer would become distorted as it propagates, but here the potential compensates that spreading so that the shape is always the same.

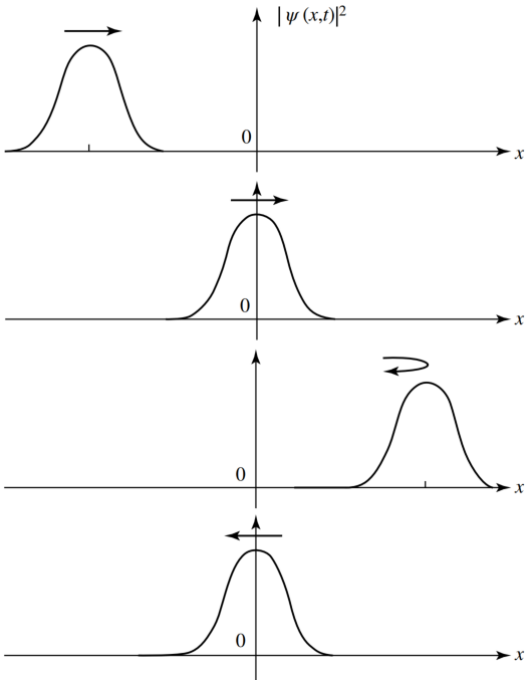



**Figure 3.2** Motion of the Gaussian wave packet associated with $|\alpha\rangle$ state. Thanks to the form of $V(x)$, the wave packet oscillates without distortion.

# Formula sheet

## 3.7.4 Useful formulas

| | | | |
|---|---|---|---|
| Closure relation (discrete) | $\sum_k \sum_{i=1}^{g_k} \lvert v_k^i\rangle\langle v_k^i\rvert = \mathbb{1}$ | Closure relation (continuous) | $\int_\beta d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert = \mathbb{1}$ |
| Glauber Formula | $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$ | Generalized uncertainty relation | $\Delta A \Delta B \geq \frac{1}{2}\lvert\langle[A,B]\rangle\rvert$ |
| Function of an operator | $F(A) = \sum_{n=0}^{\infty} f_n (A-a)^n$ | | $\Delta Q = \sqrt{\langle Q^2\rangle - \langle Q\rangle^2}$ |
| Eigenequation of $F(A)$ | $F(A)\lvert\psi\rangle = F(\lambda)\lvert\psi\rangle$ | | |
| Transformation $\{u\} \to \{v\}$ | $\mathbb{M}_{jk} = \langle u_j \rvert v_k\rangle$ | $\lvert\psi\rangle_{\{u\}} = \mathbb{M}\lvert\psi\rangle_{\{v\}}$<br>$A_{\{u\}} = \mathbb{M} A_{\{v\}} \mathbb{M}^\dagger$ | $\lvert\psi\rangle_{\{v\}} = \mathbb{M}^\dagger\lvert\psi\rangle_{\{u\}}$<br>$A_{\{v\}} = \mathbb{M}^\dagger A_{\{u\}} \mathbb{M}$ |

## 3.7.5 Basis

| Quantity | Discrete basis (sum over $j,k$) | Continuous basis (integrate over $\beta,\beta'$) |
|---|---|---|
| $\mathbb{1}$ | $= \sum \lvert v_k\rangle\langle v_k\rvert$ | $= \int d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert$ |
| $\lvert\psi\rangle = \mathbb{1}\lvert\psi\rangle$ | $= \sum \lvert v_k\rangle\langle v_k\rvert\psi\rangle$ | $= \int d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert\psi\rangle$ |
| $\langle\varphi\rvert = \langle\varphi\rvert\mathbb{1}$ | $= \sum \langle\varphi\rvert v_k\rangle\langle v_k\rvert$ | $= \int d\beta\ \langle\varphi\rvert\omega_\beta\rangle\langle\omega_\beta\rvert$ |
| $A = \mathbb{1}A\mathbb{1}$ | $= \sum\sum \lvert v_j\rangle\langle v_j\rvert A\rvert v_k\rangle\langle v_k\rvert$ | $= \iint d\beta\, d\beta'\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert A\rvert\omega_{\beta'}\rangle\langle\omega_{\beta'}\rvert$ |

| Quantity | $X$ representation | $P_x$ representation |
|---|---|---|
| $X$ | $x$ | $i\hbar\,\partial/\partial p$ |
| $P_x$ | $-i\hbar\,\partial/\partial x$ | $p$ |
| $\lvert x'\rangle$ | $\langle x\rvert x'\rangle = \delta(x-x')$ | $\langle p\rvert x'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(-ix'p/\hbar)$ |
| $\lvert p'\rangle$ | $\langle x\rvert p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ixp'/\hbar)$ | $\langle p\rvert p'\rangle = \delta(p-p')$ |
| $\lvert\psi\rangle$ | $\langle x\rvert\psi\rangle = \psi(x)$ | $\langle p\rvert\psi\rangle = \tilde{\psi}(p)$ |

Fourier transforms for 3D wavefunctions

| | |
|---|---|
| $\tilde{\psi}(\boldsymbol{p}) = \mathscr{F}[\psi(\boldsymbol{r})] = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int_{-\infty}^{\infty} d^3\boldsymbol{r}\ e^{-i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\psi(\boldsymbol{r})$ | $\psi(\boldsymbol{r}) = \mathscr{F}^{-1}\left[\tilde{\psi}(\boldsymbol{p})\right] = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int_{-\infty}^{\infty} d^3\boldsymbol{p}\ e^{i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\tilde{\psi}(\boldsymbol{p})$ |
| $\mathscr{F}\left[\psi^{(n)}(x)\right] = \left(\frac{ip}{\hbar}\right)^n \tilde{\psi}(p)$ | $\tilde{\psi}^{(n)}(p) = \mathscr{F}\left[\left(-\frac{ix}{\hbar}\right)^n \psi(x)\right]$ |
| $\tilde{\psi}(p-p_0) = \mathscr{F}\left[e^{ip_0x/\hbar}\psi(x)\right]$ | $e^{-ipx_0/\hbar}\tilde{\psi}(p) = \mathscr{F}[\psi(x-x_0)]$ |
| $\mathscr{F}[\psi(cx)] = \tilde{\psi}(p/c)/\lvert c\rvert$ | $\int_{-\infty}^{\infty} dx\ \varphi^*(x)\psi(x) = \int_{-\infty}^{\infty} dp\ \tilde{\varphi}^*(p)\tilde{\psi}(p)$ |
| $\psi(x)$ real: $[\tilde{\psi}(p)]^* = \tilde{\psi}(-p)$ | $\psi(x)$ imaginary: $[\tilde{\psi}(p)]^* = -\tilde{\psi}(-p)$ |
| $\Delta x \Delta p \geq \hbar$ | |

## Commutators

## Key points

- When a matrix has a block form, we can compute the eigenvalues in each block submatrix.
- The eigenpairs allows you to diagonalize $A = V\Lambda V^{-1}$ in the eigenbasis, where $V = [\boldsymbol{u}_1\rvert\boldsymbol{u}_2\rvert\cdots]$, $\Lambda = \text{diag}(\lambda_1, \lambda_2, \cdots)$, and $A\rvert\boldsymbol{u}_i\rangle = \lambda_i\rvert\boldsymbol{u}_i\rangle$. In the eigenbasis we can do $F(A) = VF(\Lambda)V^{-1}$.
- When $A$ is Hermitian, $V$ is unitary: $V^{-1} = V^\dagger$.

$[A,B] = -[B,A]$
$[A,B]^\dagger = [B^\dagger, A^\dagger]$
$[AB,CD] = A[B,C]D + AC[B,D] + [A,C]DB + C[A,D]B$
$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$
$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]}$ ($[A,[A,B]] = [B,[A,B]] = 0$)
$[X,P] = i\hbar$
$[H,P] = i\hbar \frac{dV(X)}{dX}$

$[A+B,C+D] = [A,C] + [A,D] + [B,C] + [B,D]$
$[F(A),A] = 0$
$[A,B] = 0 \Longrightarrow [F(A),B] = [A,F(B)] = [F(A),F(B)] = 0$
$[A,[A,B]] = [B,[A,B]] = 0 \Longrightarrow [A,F(B)] = [A,B]\frac{dF(B)}{dB}$
$[A,[A,B]] = [B,[A,B]] = 0 \Longrightarrow [F(A),B] = [A,B]\frac{dF(A)}{dA}$
$[H,X] = -\frac{i\hbar}{m}P$
$\langle \varphi_n | [A,H] | \varphi_n \rangle = 0, \ \forall A$

- If the matrix is diagonal, the exponential acts directly onto the elements.
- The evolution operator is $U = e^{-iHt/\hbar}$ and it evolves the state by matrix multiplication $U|\psi\rangle$.
- The eigenequation show you the relation of the eigenvectors that must be considered to construct the eigenvectors of the eigenbasis: $A|u_i\rangle = \lambda |u_j\rangle$. Its matrix representation is $\lambda$ in the $ji$ position.
- You can reduce the dimension of an operator to its eigensubspace when only acting inside it.
- To know the action of an operator you can stimulate it by applying $|\psi\rangle$ or $\langle\psi|$.
- In the operation $|u_i\rangle\langle u_j|$, the element will be located at $ij$ in the matrix.
- Conservative=$H$ time-independent, Stationary state=$|\psi\rangle$ projects in a single eigenstate of $H$.
- Constant of motion=$A$ time-independent and $[A,H] = 0$.

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# Index