Notes of Quantum Mechanics

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Preface

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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^∞. 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 δ_{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 α, 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 α (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 ψ as an object that is used to extract information.

Dual space and bra vectors

A **linear function** χ 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:

Adjoint	Linear to the second vector	Antilinear to the first vector
$\langle\varphi\|\psi\rangle = \langle\psi\|\varphi\rangle^*$	$\langle\varphi\|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\langle\varphi\|\psi_1\rangle + \lambda_2\langle\varphi\|\psi_2\rangle$	$\langle\lambda_1\varphi_1 + \lambda_2\varphi_2\|\psi\rangle = \lambda_1^*\langle\varphi_1\|\psi\rangle + \lambda_2^*\langle\varphi_2\|\psi\rangle$

(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 ϵ 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

$$(A^\dagger)^\dagger = A$$
$$(\lambda A)^\dagger = \lambda^* A^\dagger$$
$$(A+B)^\dagger = A^\dagger + B^\dagger$$
$$(AB)^\dagger = B^\dagger A^\dagger$$

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_ψ 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 $|w_\alpha\rangle$:

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

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:

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

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

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 α. 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

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

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

The eigenvalue λ 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 λ.

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

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 λ of its Nth 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 λ_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 λ_0. The eigenvectors associated with λ_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 λ_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 λ_0, the system will have rank$(M) = N - p$ independent equations $(1 < p < q)$. To the eigenvalue λ_0 there corresponds an eigensubspace of dimension null$(M) = p$, and λ_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 λ_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 λ 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_ψ 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_ψ 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:

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

Then the degeneracy of the eigenvalue is 1, then the block reduces to a 1×1 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 λ_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 (λ_k, φ_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	
$\langle \boldsymbol{r}_0 \| \boldsymbol{r}'_0 \rangle = \delta(\boldsymbol{r}_0 - \boldsymbol{r}'_0)$ $\langle \boldsymbol{p}_0, \boldsymbol{p}'_0 \rangle = \delta(\boldsymbol{p}_0 - \boldsymbol{p}'_0)$	$\int d^3r_0 \; \|\boldsymbol{r}_0\rangle\langle \boldsymbol{r}_0\| = \mathbb{1}$ $\int d^3p_0 \; \|\boldsymbol{p}_0\rangle\langle \boldsymbol{p}_0\| = \mathbb{1}$	(1.108) (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 ψ 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 α 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 α_1 and α_2 is the continuous projection of ψ 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** ΔA 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**:

Ehrenfest's theorem

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

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):

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

τ 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 τ:

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

$|\psi(t)\rangle$ 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

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

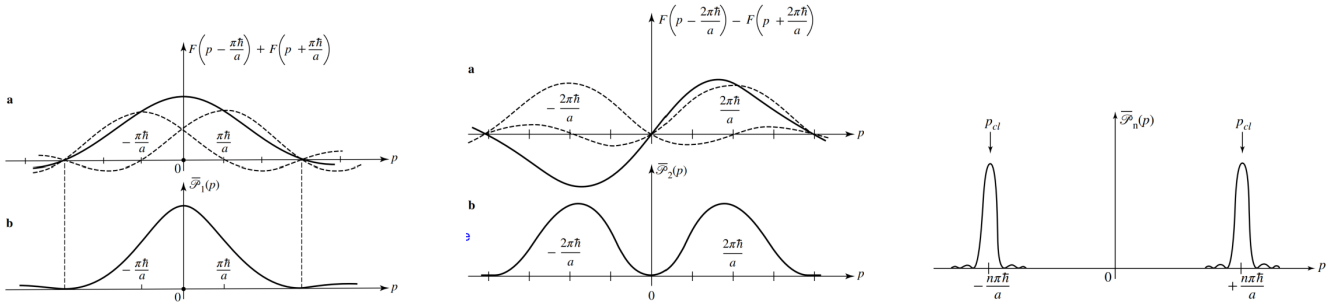
In the same way, we can compute $\langle P^2 \rangle_n$. Using the fact that in the $\{|x\rangle\}$ representation P acts like $-i\hbar\partial_x$ and performing an integration by parts, we obtain:

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

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 ΔP_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

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

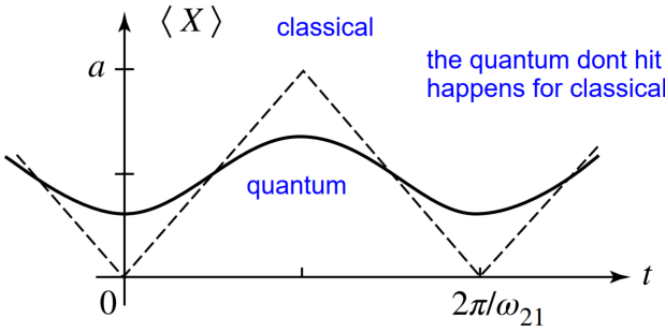


Figure 2.2 Time variation of $\langle X \rangle$ corresponding to the wave packet's motion. QM predicts that the center of the wave packet will turn back before hitting the wall

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 $A_S(t)$ who 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. In addition, because expectation values of oeprators must be **conserved** regardless the interaction used, nn arbitrary operator $A_S(t)$ in the S picture is transformed to the H picture as

Transformed state vector and operator

$$\begin{aligned} |\psi_H\rangle &= U^\dagger(t,t_0)|\psi_S(t)\rangle = |\psi_S(t_0)\rangle \\ A_H(t) &= U^\dagger(t,t_0)A_S(t)U(t,t_0) \end{aligned}.$$

As,

$$\langle A\rangle = \langle\psi_S(t)|U(t,t_0)|U^\dagger(t,0)AU(t,0)U^\dagger(t,0)|\psi_S(t)\rangle.$$

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

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

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 $|\psi_I(t)\rangle = |\psi_S(t_0)\rangle$.

Meaning of the interaction picture

In the I picture (E-picture), we are isolating the evolutino of H_0 while only allow evolve H_1.

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:

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

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:

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

We see that the linearity of the formulas which use the density operator enables us to express all physical predictions in terms of ρ.

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, ρ is obviously a Hermitian operator. The trace of ρ 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 ρ_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 ρ 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, ρ is a positive operator.

Populations; coherences

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

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

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

A similar calculation can be carried out for non-diagonal elements ρ_{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. ρ_{np} is the average of these cross terms, taken over all possible states of the statistical mixture. We can see that ρ_{nn} is the sym of real positive numbers, while ρ_{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 ρ are often called **coherences**.

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

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

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

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

  ρ can thus be considered to describe a statistical mixture of the states $|\chi_l\rangle$ with the probabilities π_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.
- ρ 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

Consider two different systems (1) and (2) and the global system (1)+(2), whose state space is the tensor product:

$$\mathscr{E} = \mathscr{E}(1) \otimes \mathscr{E}(2). \tag{2.68}$$

If $\{u_n(1)\}$ is a basis in $\mathscr{E}(1)$ and $\{v_p(2)\}$ is a basis in $\mathscr{E}(2)$, the ket $|u_n(1)\rangle|v_p(2)\rangle$ form a basis in $\mathscr{E}$.

We shall construct from ρ an operator $\rho(1)$ ($\rho(2)$) acting only in $\mathscr{E}(1)$ ($\mathscr{E}(2)$). This operation will be called **partial trace** with respect to (1) ((2)).

We introduce the operator $\rho(1)$, whose matrix elements are

$$\langle u_n(1)|\rho(1)|u'_n(1)\rangle = \sum_p (\langle u_n(1)|\langle u_n(2)|)\rho(|u'_n(1)\rangle|v_p(2)\rangle).$$

$\rho(1)$ is obtained from ρ by perfoming a partial trace on (2): $\rho(1) = \mathrm{Tr}_2\rho$. Similarly, the operator $\rho(2) = \mathrm{Tr}_1\rho$ has matrix elements:

$$\langle v_p(2)|\rho(2)|v'_p(2)\rangle = \sum_n (\langle u_n(1)|\langle v_p(2)|)\rho(|u_n(1)\rangle|v'_p(2)\rangle).$$

We now that the total trace of ρ is:

$$\mathrm{Tr}\,[\rho] = \sum_n \sum_p \left(\langle u_n(1)|\langle v_p(2)|\right) \rho \left(|u_n(1)\rangle|v_p(2)\rangle\right).$$

For the partial traces, the indices n and n' (or p and p') are not required to be equal and the summation is performed only over p (or n). We have, moreover:

$$\mathrm{Tr}\,[\rho] = \mathrm{Tr}_1[\mathrm{Tr}_2(\rho)] = \mathrm{Tr}_2[\mathrm{Tr}_1(\rho)].$$

$\rho(1)$ and $\rho(2)$ are, like ρ, operators whose trace is unitary, Hermitian, and satisfy all the general properties of a density operator.

Now, let $A(1)$ be an observable acting on $\mathscr{E}(1)$, and $\tilde{A}(1) = A(1) \otimes \mathbb{1}(2)$ its extension in $\mathscr{E}$. We have that,

$$\begin{aligned}
\langle \tilde{A}(1) \rangle =& \mathrm{Tr}\left[\rho \tilde{A}(1)\right] \\
=& \sum_{n,p} \sum_{n',p'} \left(\langle u_n(1)|\langle v_p(2)|\right) \rho \left(|u'_n(1)\rangle |v'_p(2)\rangle\right) \cdot \left(\langle u'_n(1)|\langle v'_p(2)|\right) A(1) \otimes \mathbb{1}(2) \left(|u_n(1)\rangle |v_p(2)\rangle\right) \\
=& \sum_{n,p,n',p'} \left(\langle u_n(1)|\langle v_p(2)|\right) \rho \left(|u'_n(1)\rangle |v'_p(2)\rangle\right) \cdot \langle u'_n(1)|A(1)|u_n(1)\rangle \underbrace{\langle v'_p(2)|v_p(2)\rangle}_{\delta_{pp'}} \\
=& \sum_{n,n'} \underbrace{\left[\sum_p \langle u_n(1) v_p(2)|\rho|u'_n(1) v_p(2)\rangle\right]}_{\rho(1)} \langle u'_n(1)|A(1)|u_n(1)\rangle \\
=& \sum_n \langle u_n(1)|\rho(1) A(1)|u_n(1)\rangle \\
\langle \tilde{A}(1) \rangle =& \mathrm{Tr}\left[\rho(1) A(1)\right].
\end{aligned}$$

The partial trace $\rho(1)$ enables us to calculate all the mean values $\langle \tilde{A}(1) \rangle$ as if the system (1) were and had $\rho(1)$ for a density operator. We see that $\rho(1)$ also enables us to obtain the probabilities of all the results of measurements bearing on system (1) alone.

- Sometimes, it is impossible to assign a state vector to system (1) or (2) when the state of the global system (1)+(2) is not a product state. However, one can always, thanks to the partial trace operation, assign a density operator to subssystem (1) and (2).
- The traces $\mathrm{Tr}\left[\rho^2(1)\right]$ and $\mathrm{Tr}\left[\rho^2(2)\right]$ are not generally equal to 1.
- If the global system is in product state $|\psi\rangle = |\varphi(1)\rangle|\chi(2)\rangle$, we can verify that the corresponding density operator is

$$\rho = \sigma(1) \otimes \tau(2), \quad \text{where} \quad \begin{matrix} \sigma(1) = |\varphi(1)\rangle\langle\varphi(1)| \\ \tau(2) = |\chi(2)\rangle\langle\chi(2)| \end{matrix}. \tag{2.69}$$

  The partial trace operation then yields:

$$\mathrm{Tr}_2[\sigma(1) \otimes \tau(2)] = \sigma(1), \quad \text{and} \quad \mathrm{Tr}_1[\sigma(1) \otimes \tau(2)] = \tau(2). \tag{2.70}$$

- If ρ cannot be factored out as in the previous case, there is therefore a certain correlation between systems (1) and (2), which is no longer contained in the operator $\rho = \rho(1) \otimes \rho(2)$.
- If the evolution of the global system is governed by (2.62), it is in general impossible to find a Hamiltonian operator relating to system (1) alone that would enable us to write an analogous equation for $\rho(1)$. The evolution of $\rho(1)$ is much more difficult to describe.

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:

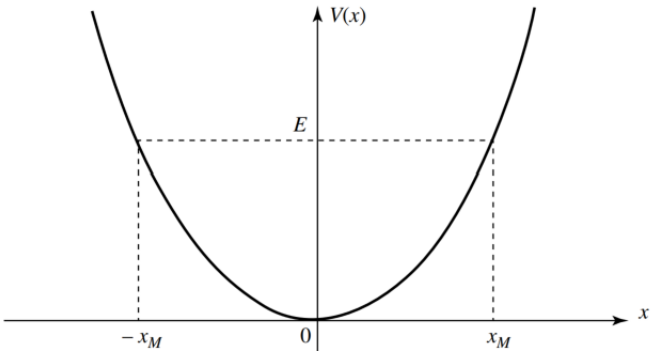


Figure 3.1 Potential energy $V(x)$ of a 1D harmonic oscillator.

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

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**.

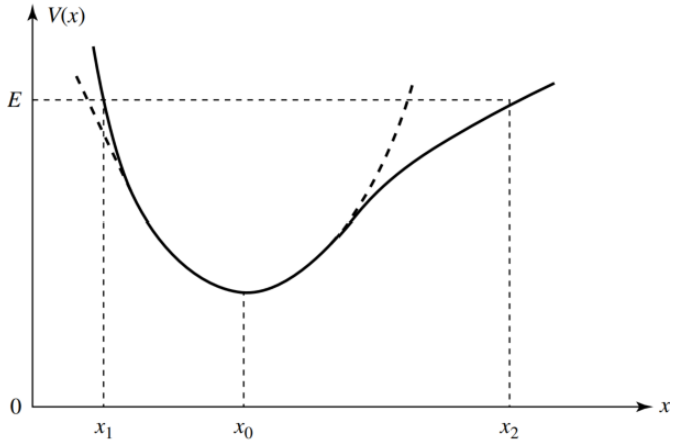


Figure 3.2 Any potential can be approximated by a parabolic potential. In $V(x)$, a classical particle of energy E oscillates between x_1 and x_2.

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 ϵ_ν 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:

$$\text{Number operator} \qquad \boxed{N = a^\dagger a}\,. \tag{3.8}$$

This operator is Hermitian

$$N^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = N.$$

And its relation with $\hat{H}$ is

$$\hat{H} = N + \frac{1}{2}, \tag{3.9}$$

so that the eigenvectors of $\hat{H}$ are eigenvectors of N, and viceversa. The commutators with a and $a^\dagger$ are:

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a \longrightarrow \boxed{[N, a] = -a} \tag{3.10}$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger [a, a^\dagger] + [a^\dagger, a^\dagger]a = a^\dagger \longrightarrow \boxed{[N, a^\dagger] = a^\dagger}\,. \tag{3.11}$$

The study of the harmonic oscilator is based on these operatores a, $a^\dagger$, and N. The eigenequation for N is

$$\text{Eigenequation of } N \qquad \boxed{N|\varphi_\nu^i\rangle = \nu|\varphi_\nu^i\rangle}\,. \tag{3.12}$$

When this is solved, we know that the eigenvector $|\varphi_\nu^i\rangle$ of N is also an eigenvector of H with the eigenvalue $E_\nu = (\nu + 1/2)\hbar\omega$:

$$H|\varphi_\nu^i\rangle = (\nu + 1/2)\hbar\omega|\varphi_\nu^i\rangle. \tag{3.13}$$

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 ν 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

$$a|\varphi^i_0\rangle = 0. \tag{3.14}$$

    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 ν 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 ν must be rejected.

> ν can only be a non-negative integer.

We conclude that the eigenvalues of H are of the form

$$\text{Eigenvalue of } H \qquad \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n \in \mathbb{N}_0^+}\,. \tag{3.15}$$

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

$$\frac{1}{\sqrt{2}}\left[\frac{X}{\sigma} + \frac{i\sigma}{\hbar}P\right]|\varphi_0^i\rangle = 0.$$

In the $\{|x\rangle\}$ representation, this relation becomes

$$\left(\frac{1}{\sigma^2}x + \frac{d}{dx}\right)\varphi_0^i(x) = 0, \quad \text{where} \quad \varphi_0^i(x) = \langle x|\varphi_0^i\rangle.$$

Therefore we msut solve a first-order differential equation, which solution is

$$\text{Ground state} \qquad \varphi_0^i(x) = ce^{-\frac{x^2}{2\sigma^2}} \overset{\text{normalization}}{\longrightarrow} \varphi_0^i(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{x^2}{2\sigma^2}}. \tag{3.16}$$

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 $c_1 = 1$:

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2 = 1 \Longrightarrow |\varphi_1\rangle = a^\dagger|\varphi_0\rangle. \tag{3.17}$$

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

$$|\varphi_n\rangle = \frac{1}{\sqrt{n}}(a^\dagger)^n|\varphi_0\rangle. \tag{3.18}$$

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

Action of a and $a^\dagger$

$$\begin{array}{ll} a^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle & \xrightarrow{\text{Adjoint}} \quad \langle\varphi_n|a = \sqrt{n+1}\langle\varphi_{n+1}| \\ a|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle & \qquad\qquad\quad \langle\varphi_n|a^\dagger = \sqrt{n}\langle\varphi_{n-1}| \end{array} \tag{3.19}$$

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:

$$X|\varphi_n\rangle = \frac{\sigma}{\sqrt{2}}(a^\dagger + a)|\varphi_n\rangle = \frac{\sigma}{\sqrt{2}}[\sqrt{n+1}|\varphi_{n+1}\rangle + \sqrt{n}|\varphi_{n-1}\rangle] \tag{3.20}$$

$$P|\varphi_n\rangle = \frac{i\hbar}{\sqrt{2}\sigma}(a^\dagger - a)|\varphi_n\rangle = \frac{i\hbar}{\sqrt{2}\sigma}[\sqrt{n+1}|\varphi_{n+1}\rangle - \sqrt{n}|\varphi_{n-1}\rangle] \tag{3.21}$$

The matrix elements of $a, a^\dagger, X, P$ in the $\{|\varphi_n\rangle\}$ representation are therefore

$$\langle\varphi_{n'}|a|\varphi_n\rangle = \sqrt{n}\delta_{n',n-1} \tag{3.22}$$

$$\langle\varphi_{n'}|a^\dagger|\varphi_n\rangle = \sqrt{n+1}\delta_{n',n+1} \tag{3.23}$$

$$\langle\varphi_{n'}|X|\varphi_n\rangle = \frac{\sigma}{\sqrt{2}}[\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \tag{3.24}$$

$$\langle\varphi_{n'}|P|\varphi_n\rangle = \frac{i\hbar}{\sqrt{2}\sigma}[\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}] \tag{3.25}$$

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 (cris, coherent states)

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 a relation of the coherent state $|\alpha\rangle$ with the energy eigenstates (eigenstates of the Hamiltonian):

Coherent state in terms of energy eigenstates
$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \,. \tag{3.26}$$

3.3.2 Wave functions associated with the stationary states

We know that $\varphi_0(x)$ is the ground sate:

$$\varphi_0(x) = \langle x|\varphi_0\rangle = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.$$

To obtain the functions $\varphi_n(x)$, all we need to do is use expression (3.18) and the fact that in $\{|x\rangle\}$ $a^\dagger$ is represented by

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]. \tag{3.27}$$

since X is represented by multiplication by x, and P by $-i\hbar\partial_x$. We thus obtain

$$\varphi_n(x) = \langle x|\varphi_n\rangle = \frac{1}{\sqrt{n!}}\langle x|(a^\dagger)^n|\varphi_0\rangle = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]^n \varphi_0(x). \tag{3.28}$$

That is,

$$\text{Excited state} \qquad \varphi_n(x) = \underbrace{\left[\frac{1}{2^n n!}\left(\frac{\hbar}{m\omega}\right)^n\right]^{1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\frac{m\omega}{\hbar}x - \frac{d}{dx}\right]^n}_{\text{Hermite polynomial}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}. \tag{3.29}$$

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.

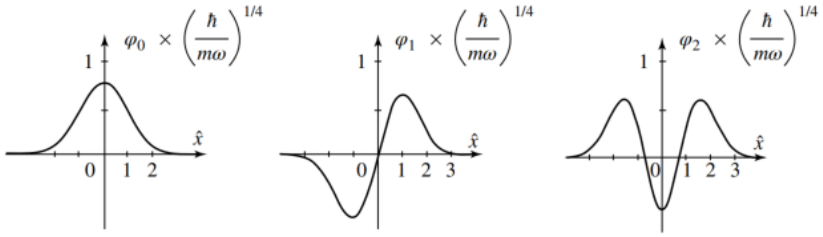


Figure 4: Wave functions associated with the first three levels of a harmonic oscillator.

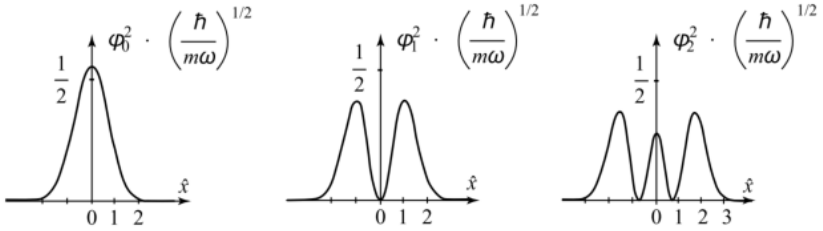


Figure 5: Probability densities associated with the first three levels of a harmonic oscillator.

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 (3.21), which show that neither X nor P has diagonal matrix elements:

$$\langle\varphi_n|X|\varphi_n\rangle = \langle\varphi_n|P|\varphi_n\rangle = 0. \tag{3.30}$$

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:

$$(\Delta X)^2 = \langle\varphi_n|X|\varphi_n\rangle - \langle\varphi_n|X^2|\varphi_n\rangle = \langle\varphi_n|X^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega} = \sigma^2\left(n + \frac{1}{2}\right). \tag{3.31}$$

$$(\Delta P)^2 = \langle\varphi_n|P|\varphi_n\rangle - \langle\varphi_n|P^2|\varphi_n\rangle = \langle\varphi_n|P^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega = \frac{\hbar^2}{\sigma^2}\left(n + \frac{1}{2}\right). \tag{3.32}$$

The product is therefore

Uncertainty relation
$$\Delta X\Delta P = \left(n + \frac{1}{2}\right)\hbar. \tag{3.33}$$

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 (57 anderson), verify - in solutions p

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:

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-iE_nt/\hbar}|\varphi_n\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-i(n+1/2)\omega t}|\varphi_n\rangle. \tag{3.34}$$

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:

$$\begin{array}{l} \frac{d}{dt}\langle X\rangle = \frac{1}{i\hbar}\langle [X,H]\rangle = \frac{\langle P\rangle}{m} \\ \frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\langle [P,H]\rangle = -m\omega^2\langle X\rangle \end{array} \xrightarrow{\int dt} \begin{array}{l} \langle X\rangle(t) = \langle X\rangle(0)\cos\omega t + \frac{1}{m\omega}\langle P\rangle(0)\sin\omega t \\ \langle P\rangle(t) = \langle P\rangle(0)\cos\omega t + m\omega\langle X\rangle(0)\sin\omega t \end{array} \tag{3.35}$$

- 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

$$F(z) = e^{-z^2} \tag{3.36}$$

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:

$$H_n(z) = \left(2z - \frac{d}{dz}\right) H_{n-1}(z), \tag{3.37}$$

where $H_n(z)$ is the nth-degree **Hermite polynomial**:

$$\text{Hermite polynomial} \qquad H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}e^{-z^2}. \tag{3.38}$$

The parity of $H_n(x)$ is $(-1)^n$, and it has n real zeros between which one finds those of H_{n-1}.

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 λ by $-\lambda$ we obtain:

$$\text{Generating function of Hermite polynomials} \qquad e^{z^2}F(z-\lambda) = e^{-\lambda^2+2\lambda z} = \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}H_n(z). \tag{3.39}$$

The Hermite polynomials can therefore be obtained from the series expansion in λ for the function $e^{-\lambda^2+2\lambda z}$.

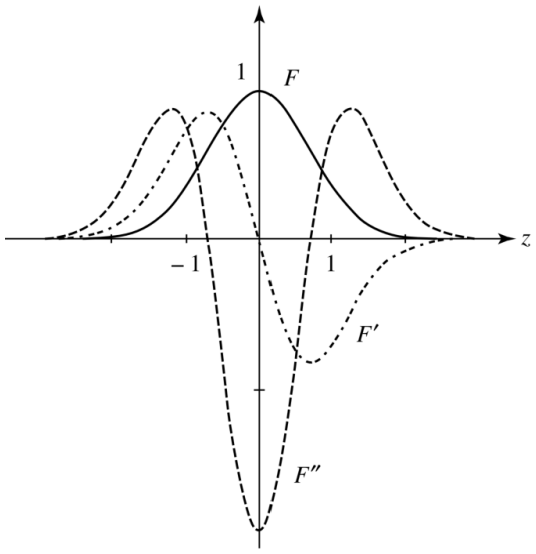


Figure 3.1 Shape of the Gaussian function $F(z)$ and its first and second derivatices.

Recurrence relations; differential equation

We can obtain other recurrence relation by using the equation (3.39). For instance, differentiating equation (3.39) with respect to z and using its expansion:

$$\frac{d}{dz}H_n(z) = 2nH_{n-1}(z). \tag{3.40}$$

If we differentiate with respect to λ, we get

$$H_n(z) = 2zH_{n-1}(z) - 2(n-1)H_{n-2}(z). \tag{3.41}$$

Finally, we can obtain an ODE differentiating equation (3.40) and using (3.37):

$$\frac{d^2}{dz^2}H_n(z) = 2n\frac{d}{dz}H_{n-1}(z) = 2n[2zH_{n-1}(z) - H_n(z)] = 2z\frac{d}{dz}H_{n-1}(z) - 2nH_n(z),$$

Thus,

ODE satisfied by Hermite polynomials $$\left[\frac{d^2}{dz^2} - 2z\frac{d}{dz} + 2n\right]H_n(z) = 0\,. \tag{3.42}$$

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:

$$\text{Excited state in } \{|x\rangle\} \qquad \varphi_n(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\frac{x^2}{2\sigma^2}} H_n\left(\frac{x}{\sigma}\right). \tag{3.43}$$

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 $a^\dagger$ (3.19) in the $\{|x\rangle\}$ representation. The action of them in this representation is

$$a \longrightarrow \frac{\beta}{\sqrt{2}}\left[x + \frac{1}{\beta^2}\frac{d}{dx}\right] \qquad a^\dagger \longrightarrow \frac{\beta}{\sqrt{2}}\left[x - \frac{1}{\beta^2}\frac{d}{dx}\right]. \tag{3.44}$$

Then equation (3.19) becomes:

$$\text{Action of } a, a^\dagger \text{ in } \{|x\rangle\} \qquad \begin{aligned} &\frac{\beta}{\sqrt{2}}\left[x + \frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) = \sqrt{n}\varphi_{n-1}(x) \\ &\frac{\beta}{\sqrt{2}}\left[x - \frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) = \sqrt{n+1}\varphi_{n+1}(x) \end{aligned} \tag{3.45}$$

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

$$\boldsymbol{F} = -k\boldsymbol{r}. \tag{3.46}$$

This force is derived from the potential energy:

$$V(\boldsymbol{r}) = \frac{1}{2}k\boldsymbol{r}^2 = \frac{1}{2}m\omega^2\boldsymbol{r}^2, \quad \omega = \sqrt{\frac{k}{m}}. \tag{3.47}$$

The classical Hamiltonian is therefore:

$$\text{Classical Hamiltonian} \qquad \mathcal{H}(\boldsymbol{r},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}m\omega^2\boldsymbol{r}^2\,. \tag{3.48}$$

Using the quantization rules, we get the Hamiltonian operator:

$$\text{Hamiltonian operator} \qquad H = \frac{\boldsymbol{P}^2}{2m} + \frac{1}{2}m\omega^2\boldsymbol{R}^2\,. \tag{3.49}$$

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**.

$$V(\boldsymbol{r}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2). \tag{3.50}$$

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:

$$\mathscr{E}_{\boldsymbol{r}} = \mathscr{E}_x \otimes \mathscr{E}_y \otimes \mathscr{E}_z. \tag{3.51}$$

The expression for the Hamiltonian is therefore

$$H = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega(Z^2 + Y^2 + Z^2) = H_z + H_y + H_z, \quad \text{with} \quad H_k = \frac{P_k^2}{2m} + \frac{1}{2}m\omega^2R_k^2. \tag{3.52}$$

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:

$$\begin{array}{ll} H_x|\varphi_{n_x}\rangle = \left(n_x + \frac{1}{2}\right)\hbar\omega|\varphi_{n_x}\rangle & |\varphi_{n_x}\rangle \in \mathscr{E}_x \\ H_y|\varphi_{n_y}\rangle = \left(n_y + \frac{1}{2}\right)\hbar\omega|\varphi_{n_y}\rangle & |\varphi_{n_y}\rangle \in \mathscr{E}_y \\ H_z|\varphi_{n_z}\rangle = \left(n_z + \frac{1}{2}\right)\hbar\omega|\varphi_{n_z}\rangle & |\varphi_{n_z}\rangle \in \mathscr{E}_z \end{array}, \quad n_x, n_y, n_z \in \mathbb{N}_0^+.$$

The eigenstates common to H, H_x, H_y, H_z are of the form:

$$|\psi_{n_x,n_y,n_z}\rangle = |\varphi_{n_z}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle. \tag{3.53}$$

According to the above Hamiltonian and the eigenequations, we have

$$H|\psi_{n_x,n_y,n_z}\rangle = E_{n_x,n_y,n_z}|\psi_{n_x,n_y,n_z}\rangle = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega|\psi_{n_x,n_y,n_z}\rangle. \tag{3.54}$$

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:

$$\text{Energy levels} \qquad E_n = \left(n + \frac{3}{2}\right)\hbar\omega, \quad n = n_x + n_y + n_z \in \mathbb{N}_0^+ . \tag{3.55}$$

The a operators are defined analogolously:

$$\text{Operator } a \text{ and } a^\dagger \qquad \begin{aligned} a_j &= \frac{1}{\sqrt{2}}\left(\frac{R_j}{\sigma_j} + \frac{iP_j\sigma_j}{\hbar}\right) \\ a_j^\dagger &= \frac{1}{\sqrt{2}}\left(\frac{R_j}{\sigma_j} - \frac{iP_j\sigma_j}{\hbar}\right) \end{aligned}, \quad \text{with} \quad [a_i, a_j^\dagger] = \delta_{ij} . \tag{3.56}$$

The action of a_x and $a_x^\dagger$ on the state $|\psi_{n_x,n_y,n_z}\rangle$ is:

$$a_x|\psi_{n_x,n_y,n_z}\rangle = (a_x|\varphi_{n_x}\rangle)|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x}|\varphi_{n_x-1}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x}|\varphi_{n_x-1,n_y,n_z}\rangle \tag{3.57}$$

$$a_x^\dagger|\psi_{n_x,n_y,n_z}\rangle = (a_x^\dagger|\varphi_{n_x}\rangle)|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x+1}|\varphi_{n_x+1}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \sqrt{n_x+1}|\varphi_{n_x+1,n_y,n_z}\rangle. \tag{3.58}$$

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

$$\text{Excited state} \qquad |\psi_{n_x,n_y,n_z}\rangle = \frac{1}{\sqrt{n_x!n_y!n_z!}}(a_x^\dagger)^{n_x}(a_y^\dagger)^{n_y}(a_z^\dagger)^{n_z}|\psi_{0,0,0}\rangle , \tag{3.59}$$

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

$$\langle \boldsymbol{r}|\psi_{n_x,n_y,n_z}\rangle = \langle z|\langle y|\langle x|\varphi_{n_z}\rangle|\varphi_{n_y}\rangle|\varphi_{n_z}\rangle = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z), \tag{3.60}$$

where $\varphi_{n_x}, \varphi_{n_y}, \varphi_{n_z}$ are stationary wave functions of the one-dimensional harmonics oscillator. For instance,

$$\langle \boldsymbol{r}|\psi_{0,0,0}\rangle = \left(\frac{1}{\pi\sigma^2}\right)^{3/4} e^{-\frac{1}{2\sigma^2}(x^2+y^2+z^2)}, \quad \omega = \omega_x = \omega_y = \omega_z. \tag{3.61}$$

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

$$\text{Degree of degeneracy of } E_n \qquad g_n = \frac{(n+1)(n+2)}{2}. \tag{3.62}$$

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 ΔX, ΔY, and ΔH are, in the macroscopic limit, completely negligible.

3.7.1 Quasi-classical states

Introducing α_0 to characterize a classical motion

The classical quantitites of motion of a 1D harmonics oscillator of mass m and angular frrequency ω are

$$\text{Equations of motion for CHO} \qquad \begin{aligned} \frac{d}{dt}x(t) &= \frac{1}{m}p(t) \\ \frac{d}{dt}p(t) &= -m\omega^2 x(t) \end{aligned} . \tag{3.63}$$

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:

$$\text{Displacement coordinate} \qquad \alpha(t) = \frac{1}{\sqrt{2}}\left(\frac{x(t)}{\sigma} + i\frac{\sigma p(t)}{\hbar}\right) \quad (-) . \tag{3.64}$$

Then, the equations of motions turn to

$$\frac{d}{dt}\alpha(t) = -i\omega\alpha(t) \longrightarrow \alpha(t) = \alpha_0 e^{-i\omega t}, \quad \alpha_0 = \alpha(0) \tag{3.65}$$

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

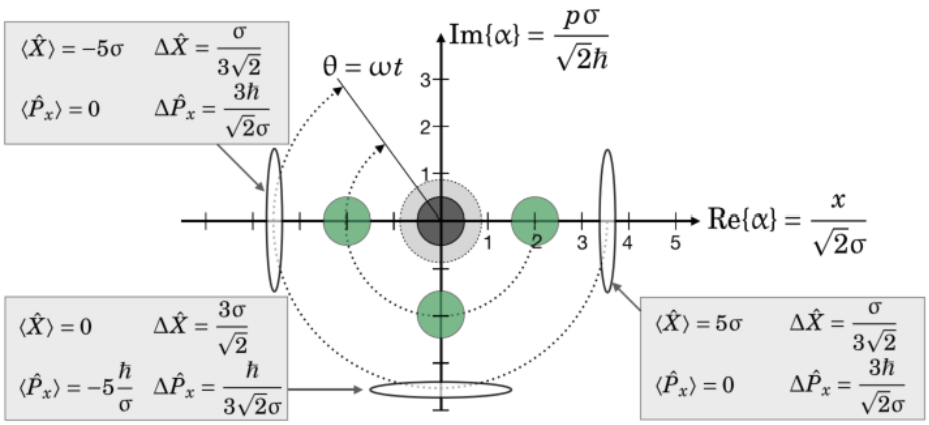


Figure 3.1 Illustration of four HO states in the phase-space diagram: black=ground state, gray=first excited state, ovals=squeezed state, green=coherent state.

ODE, we have

$$x(t) = \frac{1}{\sqrt{2}}(\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t}), \quad p(t) = -\frac{i}{\sqrt{2}}(\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t}). \tag{3.66}$$

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

$$\text{Macroscopic regime} \qquad |\alpha_0| \gg 1 . \tag{3.67}$$

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

$$\langle a\rangle(t) = \langle a\rangle(0)e^{-i\omega t}. \tag{3.68}$$

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 (3.68) is anaologous to equation (3.65). We can substitute $\langle a\rangle(t)$ and $\langle a^\dagger\rangle(t)$ in the mean value of X and P to get:

$$\langle X\rangle(t) = \frac{1}{\sqrt{2}}(a + a^\dagger) = \frac{1}{\sqrt{2}}[\langle a\rangle(0)e^{-i\omega t} + \langle a\rangle^* e^{i\omega t}] \tag{3.69}$$

$$\langle P\rangle(t) = \frac{i}{\sqrt{2}}(a^\dagger - a) = \frac{i}{\sqrt{2}}[\langle a\rangle^* e^{i\omega t} - \langle a\rangle(0)e^{-i\omega t}] \tag{3.70}$$

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

$$\langle H\rangle = \hbar\omega\langle a^\dagger a\rangle(0) + \frac{\hbar\omega}{2} \tag{3.71}$$

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:

$$\text{Second condition} \qquad \langle\psi(0)|a^\dagger a|\psi(0)\rangle = |\alpha_0|^2. \tag{3.72}$$

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

$$a|\psi(0)\rangle = \alpha_0|\psi(0)\rangle, \tag{3.73}$$

then the two conditions above are satisfied. The quasi-classical state, associated with a classical motion characterized by the parameter α_0 is such that $|\psi(0)\rangle$ is an eigenvector of the operator a with the eigenvalue α_0. We will denote the eigenvector of a with eigenvalue α by $|\alpha\rangle$:

$$\text{Eigenvector of } a \text{ with eigenvalue } \alpha \qquad a|\alpha\rangle = \alpha|\alpha\rangle. \tag{3.74}$$

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 (3.73) 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 (3.74) 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 $c_0(\alpha)$:

$$c_n(\alpha) = \frac{\alpha^n}{\sqrt{n!}}c_0(\alpha). \tag{3.75}$$

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:

$$\sum_n |c_n(\alpha)|^2 = |c_0(\alpha)|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = |c_0(\alpha)|^2 e^{|\alpha|^2} = 1. \tag{3.76}$$

We the convenction we have chosen we have $c_0(\alpha) = e^{-|\alpha|^2/2}$ and finally,

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle. \tag{3.77}$$

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 (3.77) that a measurement of the energy can yield the result $E_n = (n + 1/2)\hbar\omega$ with the probability:

$$\text{Probability of having } E_n \qquad P_n(\alpha) = |\langle\alpha|\varphi_n\rangle|^2 = \frac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2}. \tag{3.78}$$

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 (3.77):

$$\begin{array}{ll} \langle X\rangle_\alpha = \langle\alpha|X|\alpha\rangle = \sqrt{2}\sigma \mathrm{Re}\,(\alpha)\,, & \langle X^2\rangle_\alpha = \frac{\sigma^2}{2}[(\alpha+\alpha^*)^2+1] \\ \langle P\rangle_\alpha = \langle\alpha|P|\alpha\rangle = \frac{\sqrt{2}\hbar}{\sigma}\mathrm{Im}\,(\alpha)\,, & \langle P^2\rangle_\alpha = \frac{m\hbar\omega}{2}[1-(\alpha-\alpha^*)^2] \\ \langle N\rangle_\alpha = \langle\alpha|N|\alpha\rangle = |\alpha|^2, & \langle N^2\rangle_\alpha = - \\ \langle H\rangle_\alpha = \langle\alpha|H|\alpha\rangle = \hbar\omega\left[|\alpha|^2+\frac{1}{2}\right], & \langle H^2\rangle_\alpha = \hbar^2\omega^2\left[|\alpha|^4+2|\alpha|^2+\frac{1}{4}\right] \end{array} \tag{3.79}$$

Therefore, we have:

$$\Delta X_\alpha = \frac{\sigma}{\sqrt{2}}, \quad \Delta P_\alpha = \frac{\hbar}{\sqrt{2}\sigma}, \quad \Delta N_\alpha = |\alpha|, \quad \Delta H_\alpha = \hbar\omega|\alpha|. \tag{3.80}$$

The XP uncertainty relation is therefore:

$$\Delta X_\alpha \Delta P_\alpha = \frac{\hbar}{2}. \tag{3.81}$$

The displacement operator $D(\alpha)$

Let be the operator define by

$$\text{Displacement operator} \qquad D(\alpha) = T(\langle X\rangle)S(\langle P\rangle)e^{i\langle X\rangle\langle P\rangle/\hbar} = e^{\alpha a^\dagger - \alpha^* a}. \tag{3.82}$$

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 (3.77) we have

$$|\alpha\rangle = D(\alpha)|\varphi_0\rangle. \tag{3.83}$$

$D(\alpha)$ is therefore the unitary transformation which transforms the ground state $|\varphi_0\rangle$ into the quasi-classical state $|\alpha\rangle$. This was that cris derived but for only a position displacement.

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 (3.79) we have

$$\langle X\rangle = 5\sigma, \quad \text{and} \quad \langle P\rangle = \frac{10\hbar}{\sigma}.$$

Then,

$$\varphi_0(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-x^2/2\sigma^2} \Longrightarrow \langle x|D|\varphi_0\rangle = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{i\frac{x}{\hbar}\left(10\frac{\hbar}{\sigma}\right)} e^{-\frac{(x-5\sigma)^2}{2\sigma^2}}.$$

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,

$$\text{Orthonormalization relation} \qquad |\langle\alpha|\alpha'\rangle|^2 = e^{-|\alpha-\alpha'|^2}. \tag{3.84}$$

We see that **they are not orthogonal**, unless $\alpha = \alpha'$.

However, **they do satisfy the closure relation**:

$$\frac{1}{\pi}\iint |\alpha\rangle\langle\alpha|\, d\{\mathrm{Re}\,(\alpha)\}d\{\mathrm{Im}\,(\alpha)\} = \cdots = \sum_n |\varphi_n\rangle\langle\varphi_n| = 1.$$

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)

$$\begin{aligned}
|\psi(t)\rangle &= e^{-iE_nt/\hbar}|\alpha_0\rangle = e^{-i\omega t(a^\dagger a+1/2)}|\alpha_0\rangle = e^{-i\omega t/2}e^{-i\omega t\underbrace{a^\dagger a}_{N}}|\alpha_0\rangle = e^{-i\omega t/2}e^{-i\omega tN}|\alpha_0\rangle \\
&= e^{-i\omega t/2}e^{-i\omega tN}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle = e^{-i\omega t/2}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}e^{-i\omega tN}|n\rangle \\
&= e^{-i\omega t/2}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n}}(\alpha_0e^{-i\omega t})^n|n\rangle = e^{-i\omega t/2}|\alpha_0e^{-i\omega t}\rangle = e^{-i\omega t/2}|\alpha(t)\rangle.
\end{aligned}$$

Thus, we have found that

$$\text{Evolution of the quasi-classical state} \qquad \boxed{|\psi(t)\rangle = e^{-\frac{i\omega t}{2}}|\alpha(t) = \alpha_0e^{-i\omega t}\rangle}. \tag{3.85}$$

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 (3.79) and change α by $\alpha_0 e^{-i\omega t}$ to obtain:

$$\text{Mean values for } \alpha(t) \qquad \begin{array}{l} \langle X\rangle(t) = \sqrt{2}\sigma \text{Re}\left(\alpha(t)\right) \\ \langle P\rangle(t) = \frac{\sqrt{2}\hbar}{\sigma}\text{Im}\left(\alpha(t)\right) \\ \langle N\rangle = |\alpha|^2 \\ \langle H\rangle = \hbar\omega[|\alpha_0|^2 + \frac{1}{2}] \end{array} \tag{3.86}$$

And the corresponding uncertainties are:

$$\text{Uncertainties} \qquad \begin{array}{l} \Delta X = \frac{\sigma}{\sqrt{2}} \\ \Delta P = \frac{\hbar}{\sqrt{2}\sigma} \\ \Delta H = \hbar\omega|\alpha_0| \end{array} \tag{3.87}$$

The uncertainty relation holds:

$$\Delta X \Delta P = \frac{\hbar}{2}.$$

Using the above mean values, we express $\alpha(t)$ as:

$$\alpha(t) = \frac{1}{\sqrt{2}}\left[\frac{\langle X\rangle(t)}{\sigma} + i\frac{\sigma\langle P\rangle(t)}{\hbar}\right]. \tag{3.88}$$

Motion of the wave packet

Let us calculate the wave function $\psi(x,t)$. Using (3.85) 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.

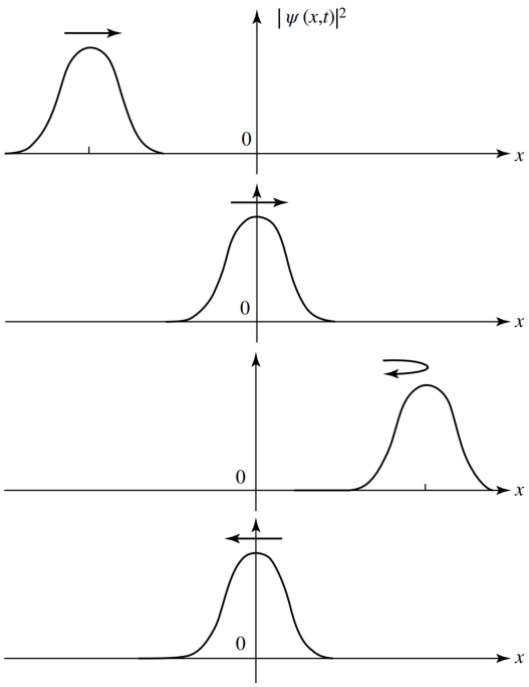


Figure 3.2 Motion of the Gaussian wave packet associated with $|\alpha\rangle$ state. Thanks to the form of $V(x)$, the wave packet oscillates without distortion.

Chapter 4

Theory of angular momentum

4.1 Introduction

We know the important role of angular momentum in cassical mechanics; the totl angular momentum of an isolated physical system is a **constant of motion**, even in some non-isolated systems. In other cases, when point particle is moving in a central potential (radial dependence only), the force on the particle is always directed towards the origin of the potential. Its moment with respect to this origin is zero, and the angular momentum theorem implies that:

$$\partial_t \mathcal{L} = 0.$$

The motion of the particle is therefore limited to a fixed plane, and satisfies the law of constant areas (Kepler's second law). All these properties have their equivalences in quantum mechanics.

With an angular momentum $\mathcal{L}$ of a classical system is associated an observable $\boldsymbol{L}$, actually a set of three observables L_x, L_y, L_z, which correspond to the three components of $\mathcal{L}$ in a Cartesia frame. We must also introduce typically quantum mechanical angular momenta, which have no classical equivalents.

We shall denote:

- **Orbital angular momentum L** is any angular momentum that has a classical equivalent.
- **Spin angular momentum S** is any intrinsic angular momentum of an elementary particle.
- **Total angular momentum J** is the sum of $\boldsymbol{L}$ and $\boldsymbol{S}$. We also used to refer to any angular momentum without specifying the type.

We will establish the general quanum mechanical properties associated with all AM, whatever their nature. These properties follow from the commutation relations satisfied by the three observables J_x, J_y, J_z, the compnents of an arbitrary AM $\boldsymbol{J}$. The origin of these commutation relations is the consequences of the quantization rules and the canonical relations.

4.2 Commutation relations characteristic of angular momentum

4.2.1 Orbital angular momentum

From the clasical conterpart of a spinless particle with $\mathcal{L}$, we apply the quantization rules to get the equivalent relation in the observables in the quantum mechanics framework.

For instance,

$$\mathcal{L}_x = yp_z - zp_y \overset{\text{Quantization rules}}{\longrightarrow} L_x = YP_z - ZP_y.$$

Then, in general we will have:

$$\boldsymbol{L} = \boldsymbol{R} \times \boldsymbol{P}. \tag{4.1}$$

Since we know the canonical relation for $\boldsymbol{R}, \boldsymbol{P}$, we can easily calculate the commutators of the operators L_x, L_y, L_z. For instance,

$$\begin{aligned}
[L_x, L_y] &= [YP_z - ZP_y, ZP_x - XP_z] = [YP_z, ZP_x] + [ZP_y, XP_z] \\
&= Y[P_z, Z]P_x + X[Z, P_z]P_y = -i\hbar YP_x + i\hbar XP_y \\
[L_x, L_y] &= i\hbar L_z.
\end{aligned}$$

Then, for the other cases we have the following commutation relations:

$$\text{Commutation relations for } \boldsymbol{L} \qquad [L_x, L_y] = i\hbar L_z,\ [L_y, L_z] = i\hbar L_x,\ [L_z, L_x] = i\hbar L_y. \tag{4.2}$$

This result can be generalized to a system of N spinless particles. The total AM of such a system is, in quantum mechanics,

$$\text{AM in a system of } N \text{ spinless particles} \qquad \boldsymbol{L} = \sum_{i=1}^{N} \boldsymbol{L}_i, \quad \boldsymbol{L}_i = \boldsymbol{R}_i \times \boldsymbol{P}_i\,. \tag{4.3}$$

Each of the individual AM $\boldsymbol{L}_i$ satisfies the commutation relations (4.2) and commutes with $\boldsymbol{L}_j$ when $j \neq i$ (state spaces of different particles).

4.2.2 Definition of angular momentum

The origin of these relations (4.2) lies in the geometric properties of rotations in three-dimensional space. This is why we shall adopt a more general point of view and define an angular momentum $\boldsymbol{J}$ as any set of three observables J_x, J_y, J_z that satisfies

$$\text{Commutation relations for } \boldsymbol{J} \qquad [J_x, J_y] = i\hbar J_z, \quad [J_y, J_z] = i\hbar J_x, \quad [J_z, J_x] = i\hbar J_y\,. \tag{4.4}$$

We then introduce the operator:

$$\text{Magnitude of } \boldsymbol{J} \qquad \boldsymbol{J}^2 = J_x^2 + J_y^2 + J_z^2 \tag{4.5}$$

the (scalar) square of the angular momentum $\boldsymbol{J}$. This operator is Hermitian, since the components are Hermitian. Moreover, $\boldsymbol{J}^2$ commutes with the these componentes:

$$[\boldsymbol{J}^2, \boldsymbol{J}] = \boldsymbol{0}\,. \tag{4.6}$$

For instance, for J_x:

$$\begin{aligned}
[\boldsymbol{J}^2, J_x] &= [J_x^2 + J_y^2 + J_z^2, J_x] \\
&= [J_y^2, J_x] + [J_z^2, J_x] \\
&= J_y[J_y, J_x] + [J_y, J_x]J_y + J_z[J_z, J_x] + [J_z, J_x]J_z \\
&= -i\hbar J_y J_z - i\hbar J_z J_y + i\hbar J_z J_y + i\hbar J_y J_z \\
[\boldsymbol{J}^2, J_x] &= 0.
\end{aligned}$$

AM theory in QM is founded **entirely** on the commutation relations (4.4). These relations imply that it is impossible to measure simumltaneously the three components of an angular momentum; however, $\boldsymbol{J}^2$ and any component of $\boldsymbol{J}$ are compatible.

4.2.3 Statement of the problem

In general, we must pick only a few of operators that forms the CSCO with the Hamiltonian as the components of an arbitrary AM $\boldsymbol{J}$ do not commute; they are not simultaneously diagonalizable. We shall therefore seek the system of eigenvectors common to $\boldsymbol{J}^2$ and J_z.

4.3 General theory of angular momentum

We will determine the spectrum of $\boldsymbol{J}^2$ and J_z for the general case and study their common eigenvectors.

4.3.1 Definitions and notation

The J_+ and J_- operators

It is more convenient to introduce the ladder operators for J to use in favor of J_x and J_y:

$$\text{Ladder operators} \qquad \begin{array}{l} J_+ = J_x + iJ_y \\ J_- = J_x - iJ_y \end{array} \longleftrightarrow \begin{array}{l} J_x = \frac{1}{2}(J_+ + J_-) \\ J_y = -\frac{i}{2}(J_+ - J_-) \end{array} . \tag{4.7}$$

They are not Hermitian; they are adjoints of each other. We will use the following operators: $J_+, J_-, J_z, \boldsymbol{J}^2$. These operators satisfy the commutation relation:

$$[J_z, J_+] = \hbar J_+, \quad [J_z, J_-] = -\hbar J_-, \quad [J_+, J_-] = 2\hbar J_z, \quad [\boldsymbol{J}^2, J_+] = [\boldsymbol{J}^2, J_-] = [\boldsymbol{J}^2, J_z] = 0. \tag{4.8}$$

Using (4.5) and the above relations, we can express $\boldsymbol{J}^2$ in the following form:

$$\boldsymbol{J}^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2 .$$

Notation for the eigenvalues of $\boldsymbol{J}^2$ and J_z

According to (4.5), $\boldsymbol{J}^2$ is the sum of the squares of three Hermitian operators. Consequently, for any ket $|\psi\rangle$, the matrix element $\langle\psi|\boldsymbol{J}^2|\psi\rangle$ is positive or zero:

$$\langle\psi|\boldsymbol{J}^2|\psi\rangle = \langle\psi|J_x^2|\psi\rangle + \langle\psi|J_y^2|\psi\rangle + \langle\psi|J_z^2|\psi\rangle = \|J_x|\psi\rangle\|^2 + \|J_y|\psi\rangle\|^2 + \|J_z|\psi\rangle\|^2 \geq 0.$$

This implies that all the eigenvalues of $\boldsymbol{J}^2$ are positive or zero. We shall write the eigenvalues of $\boldsymbol{J}^2$ in the form $j(j+1)\hbar^2$, with $j \geq 0$, so that they have dimensions of $\hbar^2$ and the $j(j+1)$ is a dimensionless number. As for the eigenvalues of J_z, which have the same dimensions as $\hbar$, they are traditionally written as $m\hbar$, with m a dimensionless number.

Eigenequations for $\boldsymbol{J}^2$ and J_z

We shall label the eigenvector common to $\boldsymbol{J}^2$ and J_z by the indices j and m. However, as they dont constitute a CSCO, it is necessary to introduce a third index k in order to distinguish between the different eigenvectors correposnding to the same eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ of $\boldsymbol{J}^2$ and J_z.

We shall therefore try to solve the simultaneously eigenequations:

$$\boldsymbol{J}^2|k,j,m\rangle = j(j+1)\hbar^2|k,j,m\rangle, \quad \text{and} \quad J_z|k,j,m\rangle = m\hbar|k,j,m\rangle. \tag{4.9}$$

4.3.2 Eigenvalues of $\boldsymbol{J}^2$ and J_z

We will prove three lemmas (as in the QHO) which will enable us to determine the spectrum of $\boldsymbol{J}^2$ and J_z.

Lemmas

a) **Properties of the eigenvalues of $\boldsymbol{J}^2$ and J_z**
If $j(j+1)\hbar^2$ and $m\hbar$ are the eigenvalues of $\boldsymbol{J}^2$ and J_z associated with the same eigenvector $|k,j,m\rangle$, then j and m satisfy the inequality:

$$-j \leq m \leq j. \tag{4.10}$$

b) **Properties of the vector $J_-|k,j,m\rangle$**
Let $|k,j,m\rangle$ be an eigenvector of $\boldsymbol{J}^2$ and J_z with the eigenvalues $j(j+1)\hbar^2$ and $m\hbar$.
   i) $m = -j \Longrightarrow J_-|k,j,-j\rangle = 0$.
   ii) If $m > -j$, $J_-|k,j,m\rangle$ is a non-null eigenvector of $\boldsymbol{J}^2$ and J_z with the eigenvalues $j(j+1)\hbar^2$ and $(m-1)\hbar$.

c) **Properties of the vector $J_+|k,j,m\rangle$**
Let $|k,j,m\rangle$ be an eigenvector of $\boldsymbol{J}^2$ and J_z with the eigenvalues $j(j+1)\hbar$ and $m\hbar$.
   i) $m = j \Longrightarrow J_+|k,j,j\rangle = 0$.
   ii) If $m < j$, $J_+|k,j,m\rangle$ is a non-null eigenvector of $\boldsymbol{J}^2$ and J_z with the eigenvalues $j(j+1)\hbar^2$ and $(m+1)\hbar$.

Determination of the spectrum of $\boldsymbol{J}^2$ and J_z

We shall show that the three lemmas above enable us to determine the possible values of j and m. The proove will be performed under iteration and is skipped.

Domain of the indices j,m

Let $\boldsymbol{J}$ be an arbitrary AM, obeying the commutation relations (4.4). If $j(j+1)\hbar^2$ and $m\hbar$ denote the eivengalues of $\boldsymbol{J}^2$ and J_z, then:

- The only possible values for j are postive integers of half-integers or zero: $0, 1/2, 1, 3, 2, 2, \cdots$.
- For a fixed j, the only values possible for m are the $(2j+1)$ numbers: $-j, -j+1, \cdots, j-1, j$.

Therefore, for a fixed j, the discretely indexed orthonormal basis $\{|j,m\rangle\}$ spans the $(2j+1)$-dimensional state space $\mathscr{E}_j$.

4.3.3 Standard $\{|k,j,m\rangle\}$ representations

We shall now study the eigenvectors common to $\boldsymbol{J}^2$ and J_z.

The basis state

Given a pair of eigenvalues, $j(j+1)\hbar^2$ and $m\hbar$, the set of eigenvectors associated with this pair of eigenvalues forms a vector subspace of $\mathscr{E}$ which we shall denote by $\mathscr{E}(j,m)$. We choose in $\mathscr{E}(j,m)$ an arbitrary orthonormal basis, $\{|k,j,m\rangle;\ k = 1,2,\cdots,g(j,m)\}$ with $g(j,m) \geq 1$ the dimension of this subspace.

The spaces $\mathscr{E}(k,j)$

Matrices representing the angular momentum operators

Let us give some exmamples of $(J_u)^{(j)}$ matrices:

i) $\boldsymbol{j=0}$
The subspaces $\mathscr{E}(k,j=0)$ are one-dimensional, since zero si the only possible value for m. The $(J_u)^0$ matrices reduces to numbers, which according to C-51, are zero.

ii) $\boldsymbol{j=1/2}$
The subspaces $\mathscr{E}(k,j=1/2)$ are two-dimensional $m\in\{1/2,-1/2\}$. If we choose the basis vector in this order, we find using C-51:

$$(J_z)^{(1/2)}=\frac{\hbar}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad (J_+)^{(1/2)}=\hbar\begin{bmatrix}0&1\\0&0\end{bmatrix},\quad (J_-)^{(1/2)}=\hbar\begin{bmatrix}0&0\\1&0\end{bmatrix},$$
$$(J_x)^{(1/2)}=\frac{\hbar}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad (J_y)^{(1/2)}=\frac{\hbar}{2}\begin{bmatrix}0&-i\\i&0\end{bmatrix},\quad (\boldsymbol{J}^2)^{(1/2)}=\frac{3}{4}\hbar^2\begin{bmatrix}1&0\\0&1\end{bmatrix}.$$

iii) $\boldsymbol{j=1}$
The subspaces $\mathscr{E}(k,j=1)$ are two-dimensional $m\in\{1,0,-1\}$. Similarly,

$$(J_z)^{(1)}=\frac{\hbar}{2}\begin{bmatrix}1&0&0\\0&0&0\\0&0&-1\end{bmatrix},\quad (J_+)^{(1)}=\hbar\begin{bmatrix}0&\sqrt{2}&0\\0&0&\sqrt{2}\\0&0&0\end{bmatrix},\quad (J_-)^{(1)}=\hbar\begin{bmatrix}0&0&0\\\sqrt{2}&0&0\\0&\sqrt{2}&0\end{bmatrix},$$
$$(J_x)^{(1)}=\frac{\hbar}{\sqrt{2}}\begin{bmatrix}0&1&0\\1&0&1\\0&1&0\end{bmatrix},\quad (J_y)^{(1)}=\frac{\hbar}{\sqrt{2}}\begin{bmatrix}0&-i&0\\i&0&-i\\0&i&0\end{bmatrix},\quad (\boldsymbol{J}^2)^{(1)}=2\hbar^2\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}.$$

iv) $\boldsymbol{j}$ **arbitrary**
The ladder operators can be written using C-51:

$$\langle k,j,m|J_x|k',j',m'\rangle=\frac{\hbar}{2}\delta_{kk'}\delta_{jj'}[\sqrt{j(j+1)-m'(m'+1)}\delta_{m,m'+1}+\sqrt{j(j+1)-m'(m'-1)}\delta_{m,m'-1}]$$
$$\langle k,j,m|J_y|k',j',m'\rangle=\frac{\hbar}{2i}\delta_{kk'}\delta_{jj'}[\sqrt{j(j+1)-m'(m'+1)}\delta_{m,m'+1}-\sqrt{j(j+1)-m'(m'-1)}\delta_{m,m'-1}].$$

$(J_x)^{(j)}$ is symmetrical and real, and $(J_y)^{(j)}$ is antisymmetrical and pure imaginary. Since the kets $|k,j,m\rangle$ are eigenvectors of $\boldsymbol{J}^2$, we have:

$$\langle k,j,m|\boldsymbol{J}^2|k',j',m'\rangle=j(j+1)\hbar^2\delta_{k'k}\delta_{jj'}\delta_{mm'}.$$

The matrix $(\boldsymbol{J}^2)^{(j)}$ is therefore proportinoal to the $(2j+1)\times(2j+1)$ unit matrix: its diagonal elements are all equal to $j(j+1)\hbar^2$.

- The OZ axis chosen as the quantization axis is **entirely arbitrary**. All directions are physically equivalent, and we should expect the eigenvalues of J_x and J_y to be the same as those of J_z. In general, inside a given subspace $\mathscr{E}(k,j)$, the eigenvalues of J_x and J_y (like those of $J_u=\boldsymbol{J}\cdot\boldsymbol{u}$) are $j\hbar,(j-1)\hbar,\cdots,(-j+1)\hbar,-j\hbar$. The corresponding eigenvectors [$(\boldsymbol{J}^2,J_x)$, $(\boldsymbol{J}^2,J_y)$, or $(\boldsymbol{J}^2,J_z)$] are linear combinations of the $|k,j,m\rangle$ with k and j fixed.

Eigenequations of $J_\pm$

An orthonormal basis $\{|k,j,m\rangle\}$ of the state space, composed of eigenvectors common to $\boldsymbol{J}^2$ and J_z:

$$\left.\begin{aligned}\boldsymbol{J}^2|k,j,m\rangle&=j(j+1)\hbar^2|k,j,m\rangle\\ J_z|k,j,m\rangle&=m\hbar|k,j,m\rangle\end{aligned}\right]\tag{4.11}$$

is called a **standard basis** if the action of $J_\pm$ on the basis vectors is given by:

$$\text{Eigenequation of } J_\pm \qquad J_\pm|k,j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm1)}|k,j,m\pm1\rangle\,. \tag{4.12}$$

And,

$$J_-|k,j,-j\rangle = 0, \quad J_+|k,j,j\rangle = 0. \tag{4.13}$$

4.4 Application to orbital angular momentum

We return now to the orbital angular momentum $\boldsymbol{L}$ of a spinless particle and see how the general theory developed applies to this particular case.

Using the $\{|\boldsymbol{r}\rangle\}$ representation, we shall show that the eigenvalues of the operator $\boldsymbol{L}^2$ are the numbers $l(l+1)\hbar^2$. Then, we shall indicate the eigenfunctions common to $\boldsymbol{L}^2$ and L_z and their principal properties.

4.4.1 Eigenvalues and eigenfunctions of L^2 and L_z

Eigenequation in the $\{|\boldsymbol{r}\rangle\}$ representation

In the $\{|\boldsymbol{r}\rangle\}$ representation, the observables $\boldsymbol{R}$ and $\boldsymbol{P}$ correspond respectively to multiplication by $\boldsymbol{r}$ and to the differential operator $(\hbar/i)\nabla$. The three components can therefore be written as

$$L_x = \frac{\hbar}{i}(y\partial_z - z\partial_y), \quad L_y = \frac{\hbar}{i}(z\partial_x - x\partial_z), \quad L_z = \frac{\hbar}{i}(x\partial_y - y\partial_x). \tag{4.14}$$

It is more convenient to work in spherical coordinates, since the various AM operators act only on the angular variables θ and ϕ, and not on r.

The conversion of a point M at $\boldsymbol{r} = (x,y,z)$ in the spherical coorindates $\boldsymbol{r} = (r,\theta,\phi)$ is therefore:

$$\text{Spherical coordinates} \qquad \begin{array}{l} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{array}, \quad \text{with} \quad \begin{array}{l} r \geq 0 \\ 0 \in [0,\pi] \\ \phi \in [0,2\pi] \\ d^3r = r^2\sin\theta dr d\theta d\phi \end{array}. \tag{4.15}$$

Using them in the AM operators yield

$$L_x = i\hbar\left(\sin\phi\partial_\theta + \frac{\cos\phi}{\tan\theta}\partial_\phi\right), \quad L_y = i\hbar\left(-\cos\phi\partial_\theta + \frac{\sin\phi}{\tan\theta}\partial_\phi\right), \quad L_z = \frac{\hbar}{i}\partial_\phi \tag{4.16}$$

$$\boldsymbol{L}^2 = -\hbar^2\left(\partial_\theta^2 + \frac{1}{\tan\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right), \quad L_+ = \hbar e^{i\phi}\left(\partial_\theta + i\cot\theta\partial_\phi\right), \quad L_- = \hbar e^{-i\phi}\left(-\partial_\theta + i\cot\theta\partial_\phi\right). \tag{4.17}$$

In the $\{|\boldsymbol{r}\rangle\}$ representation, the eigenfunctions associated with the eigenvalues $l(l+1)\hbar^2$ of $\boldsymbol{L}^2$ and $m\hbar$ of L_z are the solutions of the following partial differential equations:

$$\left.\begin{array}{r} -\left[\partial_\theta^2 + \frac{1}{\tan\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right]\psi(r,\theta,\phi) = l(l+1)\psi(r,\theta,\phi) \\ -i\partial_\phi\psi(r,\theta,\phi) = m\psi(r,\theta,\phi) \end{array}\right| \tag{4.18}$$

We already know that l is integral or half-integral and that, for fixed l, m can take only the values $-l,\cdots,l$. We also notice from the equations that r does not appear in any differential operator, se we can consider it to be a parameter and take into account only the $\theta-$ and $\phi-$dependence of ψ.

Thus, we denote by $Y_l^m(\theta,\phi)$ a common eigenfunction of $\boldsymbol{L}^2$ and L_z which corresponds to the eigenvalues $l(l+1)\hbar^2$ and $m\hbar$:

$$\begin{aligned}\boldsymbol{L}^2 Y_l^m(\theta,\phi) &= l(l+1)\hbar^2 Y_l^m(\theta,\phi)\\ L_z Y_l^m(\theta,\phi) &= m\hbar Y_l^m(\theta,\phi)\end{aligned} \tag{4.19}$$

These equations have only one solution for each pairt of allowed values of l and m, both indices are sufficient.

- Equation (4.19) gives the $\theta,\phi-$dependence of the eigenfuntions of $\boldsymbol{L}^2$ and L_z, after which we construct the complete eigenfunction:

$$\phi_{l,m}(r,\theta,\phi) = f(r)Y_l^m(\theta,\phi). \tag{4.20}$$

  The fact that $f(r)$ is arbitrary shows that $\boldsymbol{L}^2$ and L_z do not form a CSCO in the space $\mathscr{E}_r$ of functions of r.
- In order to normalize $\phi_{l,m}$ it is convenient to normalize Y_l^m and f **separately**:

$$\int_{r=0}^{\infty}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} |\psi_{m,l}(r,\theta,\phi)|^2\, r^2\sin\theta dr d\theta d\phi = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} |Y_l^m(\theta,\phi)|^2\, \sin\theta d\theta d\phi = \int_{r=0}^{\infty} r^2|f(t)|^2\, dr = 1. \tag{4.21}$$

Values of l and m

- **l and m must be integral**
  Using $L_z = \frac{\hbar}{i}\partial_\phi$ in (4.19) we have:

$$\frac{\hbar}{i}\partial_\phi Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi) \longrightarrow Y_l^m(\theta,\phi) = F_l^m(\theta)e^{im\phi}. \tag{4.22}$$

  We can cover all space by letting ϕ vary in $[0,2\pi]$. We must have by continuity of the solution,

$$Y_l^m(\theta,\phi=0) = Y_l^m(\theta,\phi=2\pi) \Longrightarrow e^{2im\pi} = 1. \tag{4.23}$$

  Therefore, in an orbital AM l and m must be integer.
- **All integral values ≥ 0 of l can be found**
  Given an integral value of l, we know from the prevous section that:

$$L_+ Y_l^l(\theta,\psi) = 0.$$

  Using (**??**) and (4.22) yields

$$\left[\partial_\theta - l\cot\theta\right] F_l^l(\theta) = 0.$$

  This first-order ODE can be integrated noting that $\cos\theta\, d\theta = d(\sin\theta)/\sin\theta$. The solution is:

$$F_l^l(\theta) = c_l(\sin\theta)^l.$$

  Thus, for each positive or zero integral value of l, there exists a function $Y_l^l(\theta,\phi)$ which is unique:

$$\text{Spherical harmonics} \qquad Y_l^l = c_l(\sin\theta)^l e^{il\phi}. \tag{4.24}$$

  Through repeated action fo L_-, we construct $Y_l^{l-1},\cdots,Y_l^m,\cdots,Y_l^{-l}$. We see then there corresponds to the pair of eigenvalues $l(l+1)\hbar^2$ and $m\hbar$ one and only one eigenfunction $Y_l^m(\theta,\phi)$, which can be computed from (4.24).

Fundamental properties of the spherical harmonics

We summarize some properties of spherical harmonics.

- **Recurrence relations**

$$\begin{aligned} e^{i\phi}\left[\partial_\theta - m\cot\theta\right]Y_l^m(\theta,\phi) &= \sqrt{l(l+1)-m(m+1)}Y_l^{m+1}(\theta,\phi) \\ e^{i\phi}\left[-\partial_\theta - m\cot\theta\right]Y_l^m(\theta,\phi) &= \sqrt{l(l+1)-m(m-1)}Y_l^{m-1}(\theta,\phi) \end{aligned} \tag{4.25}$$

- **Orthonormalization and closure relations**
  Normalization imposed on the spherical harmonics yields

$$\int_0^{2\pi}\int_0^{\pi}\sin\theta Y_{l'}^{m'*}(\theta,\phi)Y_l^m(\theta,\phi)\ \sin\theta d\theta d\phi = \delta_{l'l}\delta_{m'm}. \tag{4.26}$$

  Furtheremore, any function $f(\theta,\phi)$ can be expanded in terms of the spherical hermonics:

$$f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} c_{l,m}Y_l^m(\theta,\phi), \quad \text{with} \quad c_{l,m} = \int_0^{2\pi}\int_0^{\pi} f(\theta,\phi)Y_l^{m*}(\theta,\phi)\ d\theta d\phi. \tag{4.27}$$

  The spherical harmonics therefore constitute an orthonormal basis in the space $\mathscr{E}_\Omega$, which means the surface of a sphere with fixed value of r. This fact in expressed by the closure relation:

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^m(\theta,\phi)Y_l^{m*}(\theta',\phi') = \delta(\cos\theta-\cos\theta')\delta(\phi-\phi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\phi-\phi'). \tag{4.28}$$

- **Parity and complex conjugation**
  A reflection through the coordinate origin is expressed as $\boldsymbol{r} \longrightarrow -\boldsymbol{r}$ in cartesian coordinates, and as

$$\text{Reflection} \qquad \begin{aligned} r &\longrightarrow r \\ \theta &\longrightarrow \pi-\theta \\ \phi &\longrightarrow \pi+\phi \end{aligned} \tag{4.29}$$

  in spherical coordinates. It is simple to show that a reflection in Y_l^m yields:

$$\text{Reflection in spherical harmonics} \qquad Y_l^m(\pi-\theta,\pi+\phi) = (-1)^l Y_l^m(\theta,\phi)\,. \tag{4.30}$$

  Also, that a complex conjugation results in

$$\text{Complex conjugatino of spherical harmonics} \qquad [Y_l^m(\theta,\phi)]^* = (-1)^m Y_l^{-m}(\theta,\phi). \tag{4.31}$$

Standard bases of the wave function space of a spinless particle

We know that $\boldsymbol{L}^2$ and L_z do not constitute a CSCO in the wave function spcae of a spinless particle. We shall now indicate the form of the standard bases of this space. By repeated application of L_- on $\psi_{k,l,l}(\boldsymbol{r})$, we then construct the functions $\psi_{k,l,m}(\boldsymbol{r})$ which complete the standard basis for $m \neq l$. They satisfy the equations in and :

But we saw that all eigenfunctions common to $\boldsymbol{L}^2$ and L_z that correspond to given eigenvalues $l(l+1)\hbar^2$ and $m\hbar$ have the same angualr dependence in $Y_l^m(\theta,\phi)$, and only the radial dependence differs. From

the same above equations we deduce that the functions $\psi_{k,l,m}(\boldsymbol{r})$ of a standard basis of the wave function space of a spinless particle have the form:

$$\psi_{k,l,m}(\boldsymbol{r}) = R_{k,l}(r)Y_l^m(\theta,\phi). \tag{4.32}$$

Notice the dependence indices for each term of the right-side. The orthonormalization relation for the radial function is:

$$\int_0^\infty R_{k,l}^*(r)R_{k',l}(r)\ r^2dr = \delta_{kk'}. \tag{4.33}$$

Notice also the orthogonality is to respect to the k variable.

- If we want the basis function $\psi_{k,l,m}(\boldsymbol{r})$ to be continuous, only the radial functions corresponding to $l = 0$ can be non-zero at $r = 0$.

4.4.2 Physical considerations

Study of a $|k,l,m\rangle$ state

Calculations of the physical predictions concerning measurements of $\boldsymbol{L}^2$ and L_z

Chapter 5

Spin 1/2 and two-level systems

5.1 Spin 1/2 particle: quantization of the angular momentum

We will study a fundamental experiment that revealed the quantization of a simple physical quantity, the angular momentum. We will see that the component along Oz of the AM can take only certain values $(\pm\hbar/2)$, that is, is quantized.

A silver atom in the ground state is said to be a **spin 1/2 particle**. We shall alo study the exolution of a spin 1/2 particle in a uniform magneti field (Larmor precession).

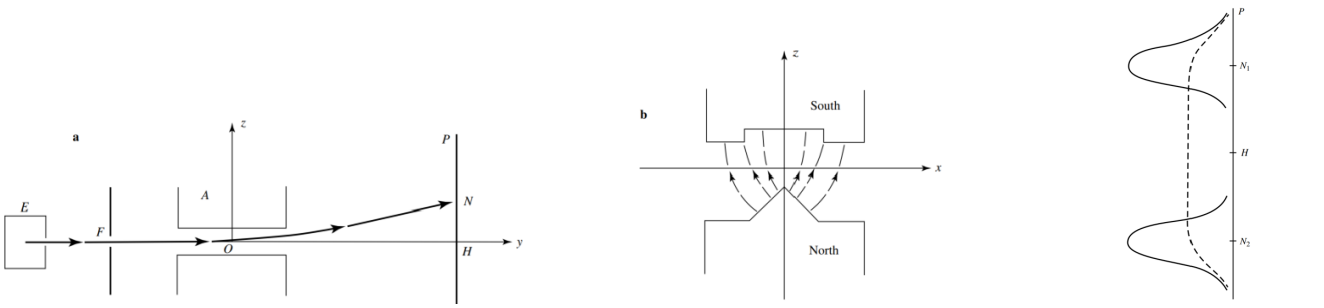
5.1.1 Experimental demonstration

We are going to describe and analyze the Stern-Gerlach experiment, which demonstrated the quantization of the componentes of the angular momentum.

The Stern-Gerlach apparatus

The experiment consists of studying the deflection of a beam of neutral paramgnetic atoms (in this case silver atoms). The leave a furnace E through a small opening and propagate in a straigth line in the high vacuum existing inside the apparatus. Then, the atomic beam traverses the electromagnet A and thus being deflected before reaching the plate P.

This B-field has a plane of symetry yOz that contains the initial direction Oy of the atomic beam. The B-field has no components along Oy, and its larges component is along Oz; it varies strongly with z. Since the B-field has a conserved flux $\nabla \cdot \boldsymbol{B} = 0$, it must also have a component along Ox which varies with the distance x from the plane of symmetry.



(a) Stern-gerlach apparatus **(b)** B-field distribution **(c)** Experimental results

Figure 5.1 The Stern-Gerlach experiment.

Classical calculations of the deflection

The neutral silver atoms posses a permanent magnetic moment $\boldsymbol{\mu}$ (they are paramgnetic atoms); the resulting forces are derived from the potential energy:

$$W_B = -\boldsymbol{\mu} \cdot \boldsymbol{B}. \tag{5.1}$$

For a given atomic level, the magnetic moment $\boldsymbol{\mu}$ and the angular momentum $\boldsymbol{J}$ are proportional:

$$\boldsymbol{\mu} = \gamma \boldsymbol{J}, \tag{5.2}$$

where γ is the **gyromagnetic ratio** of the level. Before the atoms traverse the electromagnet, the magnetic moments of the silver are oriented randomly (isotropically).

The resultat foces exerted on te atom is:

$$\boldsymbol{F} = \nabla(\boldsymbol{\mu} \cdot \boldsymbol{B}). \tag{5.3}$$

The angular momentum theorem can be written:

$$\partial_t \boldsymbol{L} = \boldsymbol{\Gamma} = \gamma \boldsymbol{L} \times \boldsymbol{B}. \tag{5.4}$$

The atom thus behaves like a gyroscope: $\partial_t \boldsymbol{L}$ is perpendicualr to $\boldsymbol{L}$, and the angular momentum turns about the magnetic field, the angle θ between $|bL$ and $\boldsymbol{B}$ remaining constant.

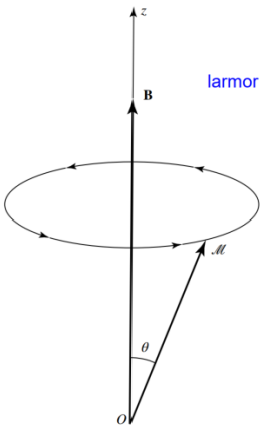


Figure 5.2 The effect of a uniform B-field $\boldsymbol{B}$ is to cause $\boldsymbol{\mu}$ to turn about $\boldsymbol{B}$ with a constant angular velocity (Larmor precession).

The rotational angular velocity is equal to the product of the gyromagnetic ratio γ and the modulus of the B-field.

To calculate the force $\boldsymbol{F}$, we can, to a very good aproximation, neglect in thte potential energy W the terms proportional to μ_x and μ_y and take μ_z to be constant. This is becuase the frequency of oscillation sue to rotation of $\boldsymbol{\mu}$ is so great that only the time-average values of μ_x and μ_y can play a role in W, and there are both zero.

Consequently, it is as if the atom were submitted to the sole force:

$$\boldsymbol{F}' = \nabla(\mu_z B_z) = \mu_z \nabla B_z. \tag{5.5}$$

The force on the atom is therefore parallel to Oz and proportional to μ_z. Consequently, because this force produced the deflection HN, measuring HN is equivalent to measuring μ_z and L_z.

Results and conclusions

The results of the experiment (performed in 1922) are in complete contradiction with the preceding predictions. We do not observe a single spot centered at H, but two spots centered at N_1 and N_2. The predictions of classical mechanics are therefore shown to be invalidated by the experiment.

It is possible, in order to describe the motion of the silver atoms, to construct wave packets whose width Δz and momentum dispersion Δp are negligible. They must satisfy the Heisenberg relation:

$$\Delta z \cdot \Delta p_z \geq \hbar.$$

Numerically, the mass M of a silver atom is $1.8\times10^{-25}\ kg$. Δz and the velocity uncertainty $\Delta v_z = \Delta p_z/M$ must be such that:

$$\Delta z \cdot \Delta v_z \geq \frac{\hbar}{M} \approx 10^{-9}. \tag{5.6}$$

Is is then easy to find uncertainties Δz and Δv_z which, while satisfying above, are negligible on the scale of the experiment being considered. Is is possible to reason in terms of quasi-pointlike wave packets moving along classical trajectories. Therefore, it is correct to claim that measurement of the deflection HN constitutes a measurement of μ_z or L_z.

Conclusion of the experiment

If we measure the component L_z of the intrinsic angular momentum of a silver atom in its ground state, we can find only one or the other of two values corresponding to the deflections HN_1 and HN_2. L_z is a **quantized** physical quantity whose discrete spectrum includes only two eigenvalues $(\pm\hbar/2)$.

5.1.2 Theorical description

We are now going to show how QM describes the degrees of freedom of a silver atom, that is, of a spin 1/2 particle. The idea is to give precise examples of kets and observables, to show how physical predictions can be extracted from them and how to distinguish clearly between the various stages of an experiment (preparation, evolution, measurement).

We must therefore define the state space and the observables corresponding to the components of $\boldsymbol{L}$: L_x, L_y, L_z, or more generally, $L_{\boldsymbol{u}} = L \cdot \boldsymbol{u}$, where $\boldsymbol{u}$ is an arbitrary unit vector.

The observale S_z and the spin state space

With L_z we must associate an observable S_z which has two eigenvalues $\pm\hbar/2$. We assume that these two eigenvalues are not degenrerate, ans we denot by $|\pm\rangle$ the respective orthonormal eigenvectors:

$$\text{Eigenequation of } S_z \qquad S_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle, \quad \text{with} \quad \begin{matrix}\langle+|+\rangle = \langle-|-\rangle = 1 \\ \langle\pm|\mp\rangle = 0\end{matrix} \tag{5.7}$$

S_z alone forms a CSCO, and the spin state space is the two-dimensional space $\mathscr{E}_s$ spanned by the eigenvectors $|\pm\rangle$. This is mathematically expressed by the closure relation:

$$\text{Closure relation of } \mathscr{E}_s \qquad |+\rangle\langle+| + |-\rangle\langle-| = \mathbb{1}. \tag{5.8}$$

The very most general vector in $\mathscr{E}_s$ is a linear superposition os these eigenvectors:

$$|\psi\rangle = \alpha|+\rangle + \beta|-\rangle, \quad \text{with} \quad |\alpha|^2 + |\beta|^2 = 1. \tag{5.9}$$

In the $\{|\pm\rangle\}$ basis, the matrix representing S_z is diagonal and is written as

$$S_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0 \\ 0 & -1\end{bmatrix}. \tag{5.10}$$

The other spin observables

With the L_x and L_y components of $\boldsymbol{L}$ will be associates the observables S_x and S_y. The three components of the angular momentum do not commute with each other but satisfy well-defined commutation relations. The matrices representing S_x and S_y in the basis of the eigenvectors $|\pm\rangle$ of S_z are the following:

$$S_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad S_y = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}. \tag{5.11}$$

We see that they can be expressed in terms of the **Pauli matrices** $\sigma_x, \sigma_y, \sigma_z$.

As fot the $L_{\boldsymbol{u}}$ component of $\boldsymbol{L}$ along the unit vector $\boldsymbol{u}$, charactrerized by the angles (θ, ϕ), it is written

$$L_{\boldsymbol{u}} = \boldsymbol{L}\cdot\boldsymbol{u} = L_x \sin\theta\cos\phi + L_y \sin\theta\sin\phi + L_z\cos\theta. \tag{5.12}$$

Using the previous definitions of S_x, S_y, S_z, we easily find the matrix that represents the correspondin observable $S_{\boldsymbol{u}} = \boldsymbol{S}\cdot\boldsymbol{u}$ in the $\{|\pm\rangle\}$ basis:

$$S_u = S_x\sin\theta\cos\phi + S_y\sin\theta\sin\phi + S_z\cos\theta = \frac{\hbar}{2}\begin{bmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{bmatrix}. \tag{5.13}$$

We now get the eigenvaleus of each observable defined. The S_x, S_y, S_u operators have the **same eigenvalues**, $+\hbar/2$ and $-\hbar/2$, as S_z. This is equivalent to rotate the Stern-Gerlach device, as all directions of space have the same properties, it must be invariant under rotations. The measurements of L_x, L_y, L_u can therefore yield only one of two results: $+\hbar/2$ or $-\hbar/2$.

As for the eigenvectors of S_x, S_y, S_u, we shall denote them rspectively by $|\pm\rangle_x, |\pm\rangle_y, |\pm\rangle_u$. The expansion of the eigenvectors of S_u in the $\{|\pm\rangle_z\}$ basis is:

Eigenstates of S_u in the $\{|\pm\rangle_z\}$ basis

$$\begin{aligned}|+\rangle_u &= \cos\frac{\theta}{2}e^{-i\phi/2}|+\rangle_z + \sin\frac{\theta}{2}e^{i\phi/2}|-\rangle_z\\ |-\rangle_u &= -\sin\frac{\theta}{2}e^{-i\phi/2}|+\rangle_z + \cos\frac{\theta}{2}e^{i\phi/2}|-\rangle_z\end{aligned} \tag{5.14}$$

We see that S_x is obtained when $(\theta, \phi) = (\pi/2, 0)$ while for S_y through $(\theta, \phi) = (\pi/2, \pi)$.

5.2 Illustration of the postules in the case of a spin 1/2

We are now to apply the postulaes of QM to a certain number of experiments on silver atoms.

5.2.1 Actual preparation of the various spin states

In order to make predictions about the results of a measurement, we must know the state of the system immediately before the measurement.

Preparation of the states $|\pm\rangle$

Let assume we have the hole at N_1. The atoms which are deflected downward contnue to condense about N_2, while some of those which are deflected upwards pass through N_1 of the plate.

Each of the atoms of the beam which propagates to the right of the plate is a physical system on which we have just performed a measurement of the observable S_z, the result being $+\hbar/2$: the atom is in the state $|+\rangle$.

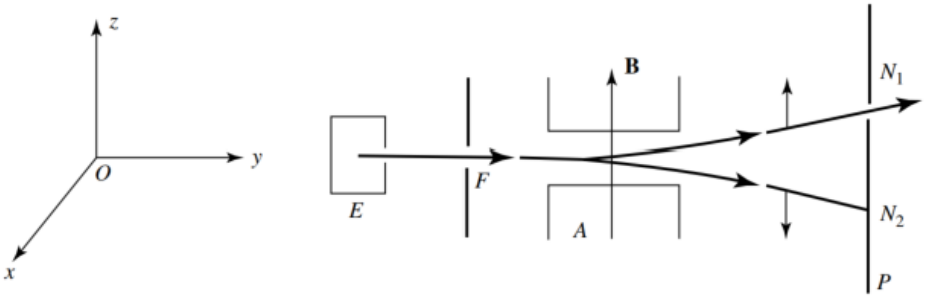


Figure 5.1 The atoms that pass through the hole made are all in the spin state $|+\rangle$. The Stern-Gerlach is then acting like a polarizer.

The device of the figure thus produces a beam of atoms which are all in the spin state $|+\rangle$, acting like a polarizer.

Preparation of the states $|\pm\rangle_x,\ |\pm\rangle_y,\ |\pm\rangle_z$

To prepare one of eigenstates of S_x (which is a CSCO), we must simply select, after a measurement of S_x, the atoms for which this measurement has yieldes the correspoding eigenvalue. If we rotate the device through an angle of $+\pi/2$ about Oy, we obtain a beam of atoms whose spin state is $|+\rangle_x$.

By placing the Stern-Gerlach device so that the axis of the magnetic field is parallel to an arbitrary unit vector $\boldsymbol{u}$, and piiercing the plate (at N_1 or N_2), we can prepare silver atoms in the spin state $|+\rangle_u$ or $|-\rangle_u$.

Preparation of the most general state

It is possible to prepare atoms whose spin state is described by the correpsondin ket $|\psi\rangle$?

Tere exists, for all $|\psi\rangle$, a unit vector $\boldsymbol{u}$ such that $|\psi\rangle$ is collinear with the ket $|+\rangle_{\boldsymbol{u}}$. We choose two complex numbers α, β that satisfy normalization equation in(5.9).

We find that there necessarily exists an angle θ such that

$$\cos\frac{\theta}{2} = |\alpha| \wedge \sin\frac{\theta}{2} = |\beta|, \quad \theta \in [0, \pi]. \tag{5.15}$$

Let us set

$$\begin{array}{l} \varphi = \arg\beta - \arg\alpha \\ \chi = \arg\beta + \arg\alpha \end{array} \implies \begin{array}{l} \arg\beta = \frac{1}{2}\chi + \frac{1}{2}\varphi \\ \arg\alpha = \frac{1}{2}\chi - \frac{1}{2}\varphi \end{array} \tag{5.16}$$

With this notation, the ket $|\psi\rangle$ is written as

$$|\psi\rangle = e^{i\chi/2}\left[\cos\frac{\theta}{2}e^{-i\varphi/2}|+\rangle + \sin\frac{\theta}{2}e^{i\varphi/2}|-\rangle\right]. \tag{5.17}$$

Consequently, to prepare silver atoms in the state $|\psi\rangle$, it suffices to place the Stern-Gerlach apparatus (with its plate pierced at N_1) so that its axis is directed along the vector $\boldsymbol{u}$.

5.2.2 Spin measurements

If we place two Stern-Gerlach magnets one after the other, we can verify experimentally the predictions of the postules. The first acts like ap olarizer, while the second is used to measure a specified component of the angular momentum $\boldsymbol{L}$: the analyzer.

First experiment

Assuming the axes of the two devices parallel to Oz. The first one prepares the aomt in the state $|+\rangle$ and the second one measure L_z.

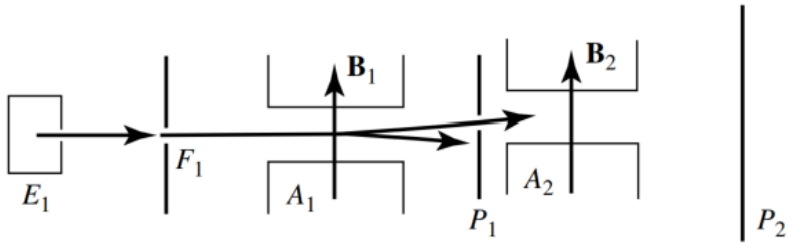


Figure 5.2 The result obtained is certain $+\hbar/2$.

Snce the state of the system under studiy is an eigenstat of S_z which we want to measure, the measurement result is **certain**: we find, without fail, the corresponding eigenvalue $+\hbar/2$. This is indeed what is observed experimentally: all the atoms strike the second plate in the vecinit of N_1, none hittin near N_2.

Second experiment

Let us place the axis of th first deviec along the unit vector $\boldsymbol{u}$, with $\theta, \phi = \pi$. $\boldsymbol{u}$ is therefore contained in the xOz plane. The axis of the second device rameins parallel to Oz.

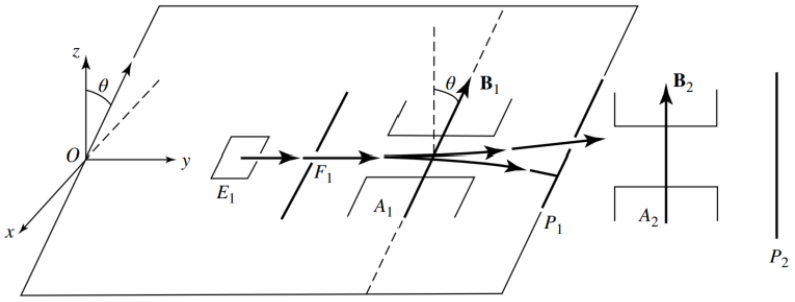


Figure 5.3 The possible results are $+\hbar/2$ with $\cos^2\theta$ of change and $-\hbar/2$ with $\sin^2\theta/2$.

According to (5.14), the spins state of the atoms when they leave the polarizer is:

$$|\psi\rangle = -\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle. \tag{5.18}$$

In this case, we find that certain atoms condense at N_1, and others at N_2. We can compute directly that the the probabilities of the eigenstates are, respectively $\cos^2\theta/2$ and $\sin^2\theta/2$. We observe experimentally that the intensity of the spots corresponds to numbers of aatoms which are proportional, to their respective probabilities.

The mean value of the results which would be obtained in a large number of identical experiments is $\langle S_z\rangle = \frac{\hbar}{2}\cos\theta$, which corresponds ot the classical result.

Third experiment

Let us take the second experiment, but with the analyzer rotated until its axis is directed along Ox, so that it measures the L_x componente of the AM.

We must expand the state $|\psi\rangle$ after the first device in terms of the eigenstates of S_x:

$$\begin{aligned} {}_x\langle +|\psi\rangle &= \tfrac{1}{\sqrt{2}}(\cos\tfrac{\theta}{2} + \sin\tfrac{\theta}{2}) = \cos(\tfrac{\pi}{4} - \tfrac{\theta}{2}) \\ {}_x\langle -|\psi\rangle &= \tfrac{1}{\sqrt{2}}(\cos\tfrac{\theta}{2} - \sin\tfrac{\theta}{2}) = \sin(\tfrac{\pi}{4} - \tfrac{\theta}{2}) \end{aligned} \tag{5.19}$$

The probability of find the eienvalue $+\hbar/2$ of S_x s therefore $\cos^2(\frac{\pi}{4} - \frac{\theta}{2})$ and that of finding $-\hbar/2$, $\sin^2(\frac{\pi}{4} - \frac{\theta}{2})$.

It is possible to verify these predictions by measuring th inensity of the two spots on the plate situated at the exit of the second Stern-Gerlach device.

Mean values

If we calculate the mean value of the possible results in the second experiment, we obtain:

$$\langle S_z\rangle = \frac{1}{N}\left[\frac{\hbar}{2}N\cos^2\frac{\theta}{2} - \frac{\hbar}{2}N\sin^2\frac{\theta}{2}\right] = \frac{\hbar}{2}\cos\theta. \tag{5.20}$$

This is indeed the value of the matrix element $\langle\psi|S_z|\psi\rangle$. Similarly, the average of the measurement results in the third experiment is

$$\langle S_x\rangle = \frac{1}{N}\left[\frac{\hbar}{2}N\cos^2(\frac{\pi}{2} - \frac{\theta}{2}) - \frac{\hbar}{2}N\sin^2(\frac{\pi}{4} - \frac{\theta}{2})\right] = \frac{\hbar}{2}\sin\theta. \tag{5.21}$$

The matrix element can be computed matricially:

$$\langle\psi|S_x|\psi\rangle = \frac{\hbar}{2}\begin{bmatrix}\cos\theta/2 & \sin\theta/2\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\cos\theta/2\\ \sin\theta/2\end{bmatrix} = \frac{\hbar}{2}\sin\theta. \tag{5.22}$$

The mean value of L_x is indeed equal to the matrix element, in the state $|\psi\rangle$, of the associated observable S_x.

There is an equivalence with the motion of classical mechanics. Using matrix computation, the mean values of S_x, S_y, S_z in the state $|+\rangle_u$ is:

$${}_u\langle +|S_x|+\rangle_u = \frac{\hbar}{2}\sin\theta\cos\phi, \quad {}_u\langle +|S_y|+\rangle_u = \frac{\hbar}{2}\sin\theta\sin\phi, \quad {}_u\langle +|S_z|+\rangle_u = \frac{\hbar}{2}\cos\theta. \tag{5.23}$$

These mean values are equal to the components of a classical agular momentum of modulus $\hbar/2$ oriented along the vector $\boldsymbol{u}$ with angles (θ, ϕ). However, recall that the only possible results of a measurements are $\pm\hbar/2$, not the above results of the mean values.

In the quantum sense, the motion of the atom is a linear superposition of the possible results, so both $\pm\hbar/2$ are traveling.

5.2.3 Evolution of a spin 1/2 particle in a uniform magnetic field

The interaction Hamiltonian and the Schrodinger equation

Consider a silver atom in a unifrom magnetic field $\boldsymbol{B}_0$, and choose the Oz axis along $\boldsymbol{B}_0$. The classical potential energy of the magnetic moment $\boldsymbol{\mu} = \gamma \boldsymbol{J}$ of this atom is then:

$$W = -\boldsymbol{\mu} \cdot \boldsymbol{B}_0 = -\mu_z B_0 = \underbrace{-\gamma B_0}_{\omega_0} J_z, \tag{5.24}$$

where ω_0 is the **Larmor frequency**. Since we are quantizing onl the internal degrees of freedom of the particle, J_z must be replaced by the operator S_z, and the clasical energy above becomes an operator: it is the Hamiltonian H which describes the evolution of the spin of the atom in the field $\boldsymbol{B}_0$:

$$H = \omega_0 S_z. \tag{5.25}$$

Since H is time-independent, we solve the respective eigenequation. We see that the eigenvectors of H are tose of S_z:

$$H|\pm\rangle = \pm\frac{\hbar\omega_0}{2}|\pm\rangle = E_\pm|\pm\rangle. \tag{5.26}$$

There are theerefore two energy levels, $E_\pm$. Their separation $\hbar\omega_0$ is proportional to the B-field; they define a single Bohr frequency:

$$\nu_{+-} = \frac{1}{\hbar}(E_+ - E_-) = \frac{\omega_0}{2\pi}. \tag{5.27}$$

- If $\boldsymbol{B}_0$ is parallel to the unit vector $\boldsymbol{u}$, the Hmailtonian (5.25) msut be replaced by its general form:

$$\text{General form Hamiltonian} \qquad H = \omega_0 \boldsymbol{S} \cdot \boldsymbol{u}\,. \tag{5.28}$$

- For silver atoms, $\gamma < 0$; ω_0 is therefore positive.

Larmor precession

Consider the spin at $t = 0$ in the state

$$|\psi(0)\rangle = \cos\frac{\theta}{2}e^{-i\phi/2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi/2}|-\rangle. \tag{5.29}$$

We saw that any state can be put in this form. To calculate the state at $t > 0$, we apply the evolution operator:

$$|\psi(t)\rangle = \cos\frac{\theta}{2}e^{-i\phi/2}e^{-iE_+t/\hbar}|+\rangle + \sin\frac{\theta}{2}e^{i\phi/2}e^{-iE_-t/\hbar}|-\rangle = \cos\frac{\theta}{2}e^{-\frac{i(\phi+\omega_0 t)}{2}}|+\rangle + \sin\frac{\theta}{2}e^{\frac{i(\phi+\omega_0 t)}{2}}|-\rangle.$$

The presence of $\boldsymbol{B}_0$ therefore introduces a phase shift between $|+\rangle$ and $|-\rangle$. The direction of $\boldsymbol{u}(t)$ along which the spin component if $+\hbar/2$ with certainty is defined by the polar angles:

$$\begin{aligned} \theta(t) &= \theta \\ \phi(t) &= \phi + \omega_0 t \end{aligned} \tag{5.30}$$

The angle between $\boldsymbol{u}(t)$ and Oz therefore remains constant, but $\boldsymbol{u}(t)$ revolves about Oz at an angular velocity of ω_0. THis effect is called the **Larmor precession**.

It can verified from $|\psi(t)\rangle$ that the probabilities of obtaining $+\hbar/2$ or $-\hbar/2$ in a measurement of this observables are time-indendent. These probabilities are equal, respectively, to $\cos^2\theta/2$ and $\sin^2\theta/2$. The mean value of S_z is also time-independent:

$$\langle\psi(t)|S_z|\psi(t)\rangle = \frac{\hbar}{2}\cos\theta. \tag{5.31}$$

Because S_x and S_y do not comute with H, we have that

$$\langle\psi(t)|S_x|\psi(t)\rangle = \frac{\hbar}{2}\sin\theta\cos(\phi+\omega_0 t), \quad \langle\psi(t)|S_y|\psi(t)\rangle = \frac{\hbar}{2}\sin\theta\sin(\phi+\omega_0 t). \tag{5.32}$$

We again find the Bohr frequencies $\omega_0/2\pi$ of the system. Moreover, the mean values above behave like the components of a classical AM of modulus $\hbar/2$ undergoing Larmos precession.

5.3 Two-level systems

There exist numerous other cases in physics which, to a first approximation, can be treated as a two-level system.

Assume that we want to evaluate the effect of an external perturbation in two levels. Then the intensity of the perturbation is sufficiently weak, it can be shown that its effect on the two state can eb computed, approximately, by ignoring all the other enegy levels of the system. All the calculations can then be performed in a two-dimensional subspace of the state space. We will study certian general properties of two-level systems.

5.3.1 Outline of the problem

Notation

Consider a physical system whose state space is two-dimensional. For a basis, we choose the system of the two eigenstates $|\varphi_1\rangle$ and $|\varphi_2\rangle$ of the Hamiltonian H_0 whose eigenvalues are, respectively, E_1 and E_2:

$$\text{Eigenequation in a two-level system} \qquad \begin{matrix} H_0|\varphi_1\rangle = E_1|\varphi_1\rangle \\ H_0|\varphi_2\rangle = E_2|\varphi_2\rangle \end{matrix} \tag{5.33}$$

Assume we want to take into account an external perturbation, initially neglected in H_0. The Hamltonian, eigenstates and eigenvalues become:

$$H = H_0 + W \Longrightarrow \begin{matrix} H|\psi_+\rangle = E_+|\psi_+\rangle \\ H|\psi_-\rangle = E_-|\psi_-\rangle \end{matrix}. \tag{5.34}$$

H_0 is called the unperturbed Hamiltonian and W, the perturbation or coupling. We also assume that W is time-independent. In the $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ basis of H_0, W is represented by a Hermitian matrix:

$$(W) = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}. \tag{5.35}$$

W_{11} ans W_{22} are real, and $W_{12} = (W_{21})^*$. In the absence of coupling, E_1 and E_2 are the possible energies of the system, and the states $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are stationary states.

Consequences of the coupling

- E_1 **and** E_2 **are no longer the possible energies of the system**
  An energy measurement will yield only one of the eigenvalues E_+ or E_-. We want to express these energies in terms of E_1, E_2 and the matrix elements W_{ij}.
- $|\varphi_1\rangle$ **and** $|\varphi_2\rangle$ **are no longer stationary states**
  Since $|\varphi_1\rangle$ and $|ket\varphi_2$ are not generally eigenstates of the total Hamiltonian H, they are no longer stationary states. W therefore induces **transitions** between the two unperturbed states.

Reduction to a ficticious spin 1/2

With every two-level system, can be associated a **ficticious spin 1/2** placed in a static field $\boldsymbol{B}$ and described by a Hamiltonian whose form is identical tothat of the initial two level system.

5.3.2 Static aspect: effect of coupling on the stationary states of the system

Expressions for the eigenstates and eigenvalues of H

In the $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ basis, the matrix representing H is written

$$H = \begin{bmatrix} E_1 + W_{11} & W_{12} \\ W_{21} & E_2 + W_{22} \end{bmatrix}. \tag{5.36}$$

The eigenvalues (after diagonalization) are:

Eigenvalues
$$E_\pm = \frac{1}{2}(E_1 + W_{11} + E_2 + W_{22}) \pm \frac{1}{2}\sqrt{(E_1 + W_{11} - E_2 - W_{22})^2 + 4|W_{12}|^2}. \tag{5.37}$$

The eigenvectors associated are:

Eigenstates
$$\begin{aligned} |\psi_+\rangle &= \cos\frac{\theta}{2}e^{-\phi/2}|\varphi_1\rangle + \sin\frac{\theta}{2}e^{i\phi/2}|\varphi_2\rangle \\ |\psi_+\rangle &= -\sin\frac{\theta}{2}e^{-\phi/2}|\varphi_1\rangle + \cos\frac{\theta}{2}e^{i\phi/2}|\varphi_2\rangle \end{aligned} \tag{5.38}$$

The angles θ and ϕ are defined by:

$$\tan\theta = \frac{2|W_{12}|}{E_1 + W_{11} - E_2 - W_{22}}, \quad \theta \in [0, \pi], \quad \text{and} \quad W_{21} = |W_{21}|e^{i\phi}. \tag{5.39}$$

Discussion

- **Graphical representation of the effect of coupling**
  We assume that $W_{11} = W_{22} = 0$, which reduces the eigenstates to:

$$E_\pm = \frac{1}{2}(E_1 + E_2) \pm \frac{1}{2}\sqrt{(E_1 - E_2)^2 + 4|W_{12}|^2}, \quad \text{and} \quad \tan\theta = \frac{2|W_{12}|}{E_1 + E_2}, \quad \theta \in [0, \pi].$$

  We introduce two other parameters, the **detuning** Δ and **mean energy** E_m:

$$E_m = \frac{1}{2}(E_1 + E_2), \quad \text{and} \quad \Delta = \frac{1}{2}(E_1 - E_2). \tag{5.40}$$

We see that changing E_m reduces to shifting the origin along the energy axis. Also, the eigenvectors do not depend on E_m, and we then care only about the influence of Δ. Substituting these new parameters in the eigenvalues yield:

$$E_\pm = E_m \pm \sqrt{\Delta^2 + |W_{12}|^2} = E_c \pm \frac{\hbar\Omega}{2}, \quad \Omega = \sqrt{\Delta^2 + |\Omega_0|^2}. \tag{5.41}$$

By plotting the four energies $E_{1,2}, E_\pm$, we obtain for $E_{1,2}$ two straight lines of slope ± 1. When Δ changes, $E_\pm$ describe two branches of a hyperbola whose asymptotes are the two straight lines associated with the unperturbed levels. The minimum separation is $2|W_{12}|$.

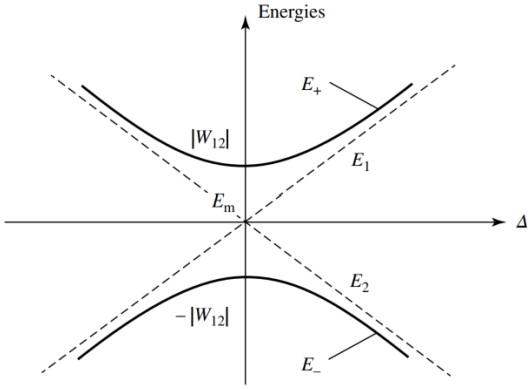


Figure 5.1 Variation of the energies $E_\pm$ as a function of the energy difference Δ. In absence of coupling, the levels behaves as the dashed lines. Under the effect of non-diagonal coupling, the two perturbed levels gives the solid lines.

- **Effect of the coupling on the energy levels**
  In the absence of coupling the energies $E_{1,2}$ cross at $\Delta = 0$. Under the effect fo non-diagonal coupling, the two level repel each other. The diagram in solid lines is therefore called an **anti-crossing diagram**. Moreover, we see that, for any Δ, we always have:

$$|E_+ - E_-| > |E_1 - E_2|. \tag{5.42}$$

  The coupling then separates the normal frequencies.

  Near the asymptotes, $|\Delta| \gg |W_{12}|$, and the energies are written in power series expansion. On the other hand, at the center of the hyperbola, $\Delta = 0$, and the energies reduces to the following:

$$\begin{aligned} |\Delta| \gg |W_{12}| : \qquad & E_\pm = E_m \pm \Delta\left(1 + \frac{1}{2}\left|\frac{W_{12}}{\Delta}\right|^2 + \cdots\right) \\ \Delta = 0 : \qquad & E_\pm = E_m \pm |W_{12}| \end{aligned}$$

  Therefore, the effect of the coupling is much more important when the two unperturbed levels have the same energy.

- **Effect of coupling on the eigenstates**
  Using the detuning and mean enegy value, we have:

$$\tan\theta = \frac{|W_{12}|}{\Delta} = \frac{|\Omega_0|}{\Delta} \tag{5.43}$$

When $\Delta \ll |W_{12}|$ (strong coupling), $\theta \approx \pi/2$. On the other hand, when $\Delta \gg |W_{12}|$ (weak coupling), $\theta \approx 0$.

At the center of the hyperbola ($\Delta = 0$), and near the symptotes ($\Delta \gg |W12|$) we have:

$$\begin{aligned} \Delta = 0: \quad & |\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left[\pm e^{-i\phi/2}|\varphi_1\rangle + e^{i\phi/2}|\varphi_2\rangle\right] \\ \Delta \gg |W_{12}|: \quad & \begin{aligned} |\psi_+\rangle &= e^{-i\phi/2}\left[|\varphi_1\rangle + e^{i\phi}\tfrac{|W_{12}|}{2\Delta}|\varphi_2\rangle + \cdots\right] \\ |\psi_-\rangle &= e^{i\phi/2}\left[|\varphi_2\rangle - e^{-i\phi}\tfrac{|W_{12}|}{2\Delta}|\varphi_1\rangle + \cdots\right] \end{aligned} \end{aligned}$$

We see that for weak coupling, the perturbed states differ very slightly from the unperturbed states. For instance $|\psi_+\rangle$ is equal to the state $|\varphi_1\rangle$ slightly contaminated b a small contribution from the state $|\varphi_2\rangle$. On the other hand, for a strong coupling, the states $|\psi_\pm\rangle$ are ery different from the state $|\varphi_{1,2}\rangle$.

5.3.3 Dynamical aspect: oscilattion of the system between the two unperturbed states

Evolution of the state vector

Let the state vector of the system at t be:

$$|\psi(t)\rangle = a_1(t)|\varphi_1\rangle + a_2(t)|\varphi_2\rangle$$

The evolution of $|\psi(t)\rangle$ in the presence of coupling W is governed by the Schrodinger equation:

$$i\hbar\partial_t|\psi(t)\rangle = (H_0+W)|\psi(t)\rangle \xrightarrow{\text{Projecting onto } \{|\varphi_{1,2}\rangle\}} \left.\begin{aligned} i\hbar\partial_t a_1(t) &= E_1 a_1(t) + W_{12}a_2(t) \\ i\hbar\partial_t a_2(t) &= W_{21}a_1(t) + E_2 a_2(t) \end{aligned}\right]$$

Is $|W_{12}| \neq 0$, these equations form a linear system of homogeneous coupled differential equations. The classical method involves looking the eigenpairs $(|\psi_\pm\rangle, E_\pm)$ of the operator $H = H_0 + W$ and decompose $|\psi(0)\rangle$ in terms of $|\psi_\pm\rangle$:

$$|\psi(0)\rangle = \lambda|\psi_+\rangle + \mu|\psi_-\rangle \Longrightarrow |\psi(t)\rangle = \lambda e^{-iE_+t/\hbar}|\psi_+\rangle + \mu e^{-iE_-t/\hbar}|\psi_-\rangle. \tag{5.44}$$

A system whose state vector is $|\psi(t)\rangle$ as above, oscillates between the two unperturbed states $|\varphi_1\rangle$ and $|\varphi_2\rangle$. To see this, we assume that at $t = 0$ the system is in $|\varphi_1\rangle$:

$$|\psi(0)\rangle = |\varphi_1\rangle \tag{5.45}$$

and compute the probability $P_{12}(t)$ of finding it in the state $|\varphi_2\rangle$ at time t.

Calculation of $P_{12}(t)$: Rabi's formula

Inverting (5.38) for $|\varphi_2\rangle$ yields:

$$|\psi(0)\rangle = |\varphi_1\rangle = e^{i\phi/2}\left[\cos\frac{\theta}{2}|\psi_+\rangle - \sin\frac{\theta}{2}|\psi_-\rangle\right] \longrightarrow |\psi(t)\rangle = e^{i\phi/2}\left[\cos\frac{\theta}{2}e^{-iE_+t/\hbar}|\psi_+\rangle - \sin\frac{\theta}{2}e^{-iE_-t/\hbar}|\psi_-\rangle\right] \tag{5.46}$$

The probability $P_{12}(t)$ is then, the projection of $|\psi(t)\rangle$ onto $|\varphi_2\rangle$:

$$\begin{aligned} P_{12}(t) &= |\langle\varphi_2|\psi(t)\rangle|^2 \\ &= \left| e^{i\phi/2}\left[\cos\frac{\theta}{2}e^{-iE_+t/\hbar}\langle\varphi_2|\psi_+\rangle - \sin\frac{\theta}{2}e^{-iE_-t/\hbar}\langle\varphi_2|\psi_-\rangle\right]\right|^2 \\ &= \left| e^{i\phi/2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}[e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}]\right|^2 \\ P_{12}(t) &= \sin^2\theta\sin^2\frac{(E_+ - E_-)t}{2\hbar}. \end{aligned}$$

Which can further expressed as

Rabi's oscillation

$$P_{12}(t) = \frac{4|W_{12}|^2}{4|W_{12}|^2 + (E_1 - E_2)^2}\sin^2\left[\sqrt{4|W_{12}|^2 + (E_1 - E_2)^2}\frac{t}{2\hbar}\right]. \tag{5.47}$$

This expression is called **Rabi's formula**.

Discussion

We see from (5.47) that $P_{12}(t)$ oscillates over time with frequency $(E_+ - E_-)/\hbar$, which is the unique Bohr frequency of the system. The maximum value $\sin^2\theta$ is achieves for all values of t such tat

$$t = \frac{(2k+1)\hbar}{2(E_+ - E_-)}, \quad k = 0, 1, \cdots. \tag{5.48}$$

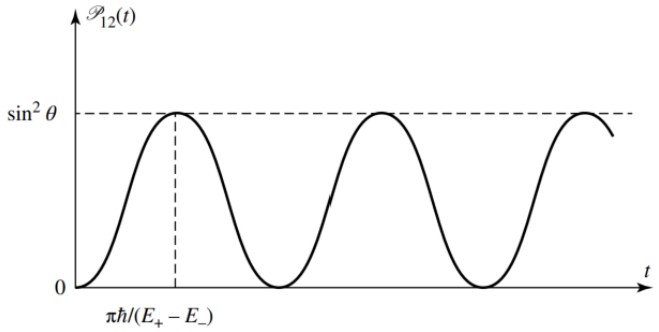


Figure 5.2 Evolution of $P_{12}(t)$ of finding the system in $|\varphi_2\rangle$ when initially was in $|\varphi_1\rangle$. When the states have the same unperturbed energy, the probability can attain the value 1.

- When $E_1 = E_2$, $(E_+ - E_-)/\hbar = 2|W_{12}|/\hbar$ and $\sin^2\theta$ takes on its greatest possible value 1 at times $t = (2k+1)\pi\hbar/2|W_{12}|$. The frequency is proportional to the coupling.
- When $E_1 - E_2$ increases, so does $(E_+ - E_-)/\hbar$ while $\sin^2\theta$ decreases. For weak coupling, $(E_+ - E_-) \approx (E_1 - E_2)$ and $\sin^\theta$ becomes very small. This is no surprising as the state $|\varphi_1\rangle$ is very close to the stationary state $|\psi_+\rangle$: the system, having statrted at $|\varphi_1\rangle$ evolves very little over time.

Chapter 6

Stationary perturbation theory

In real problems, the Hamiltonian are not that easy to solve analytically. In general, the equation is too complicated for us to be able to find its solutions in an analytic form.

There exists, however, **approximation methods** that enable us to obtain analytically approximate solutions of the basic eigenequation in certain cases. This technique is known as **stationary perturbation theory**.

In studying a phenomenon or a physical system, one begins by isolating the principal effects that are responsible for the main features of this phenomenon or this system. Once understood, one tries to explain the finer details by taking into account less important effects that were neglected in the first approximation. It is in treating these secondary effects that one commonly uses perturbation theory.

There is also another approximation method called the **variational method**.

6.1 Description of the method

6.1.1 Statement of the problem

Perturbation theory is applicable when the Hamiltonian H of the system being studied can be put in the form

$$\text{Hamiltonian of the system} \qquad H(\lambda) = H_0 + \underbrace{\lambda \hat{W}}_{W}, \quad \text{with} \quad \lambda \ll 1\,, \tag{6.1}$$

where the spectrum of H_0 is known, and where W is **much smaller** than H_0. This means that the matrix elements of W are much smaller than those of H_0. The operator H_0 is time-independent and is knwon as **unperturbed Hamiltonian**, while W is called the **perturbation**. When W is time-independent, we say we are dealing a *stationary perturbation*.

The problem then is to find the modifications produced in the enery levels of the system and its stationary states by the influence of W. Perturbation theory consists of expanding the eigenpairs of H in power of λ with a finite number of terms.

We assume the spectrum of H_0 is discrete, where eiganvalue E_p^0 and eigenstate $|\varphi_p^i\rangle$. We therefore have:

$$\text{Spectrum of } H_0 \qquad H_0|\varphi_p^i\rangle = E_p^0|\varphi_p^i\rangle, \quad \text{with} \quad \begin{array}{c}\langle\varphi_p^i|\varphi_p^i\rangle = \delta_{pp'}\delta_{ii'} \\ \displaystyle\sum_p \sum_i |\varphi_p^i\rangle\langle\varphi_p^i| = 1\end{array}\,. \tag{6.2}$$

Figure **??** represents possible forms of the variations of the eigenvalues $E(\lambda)$ of (6.1) with respect to λ. For a given value of λ, these vectors form a basis of the state space of $H(\lambda)$. The operator may have several degeneracies, as in E_3^0 and E_4^0. The perturbation is able to remove some degeneracies as for E_3^0.

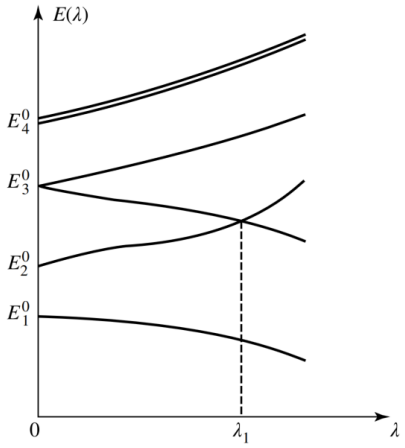


Figure 6.1 Variation of $E(\lambda)$ with respect to λ. For $\lambda = 0$, we obtain the spectrum of H_0. We see the two-fold of E_3^0 and E_4^0 where perturbation removes the degeneracy of E_3^0 but not that of E_4^0. Additional two-fold degeneracy appears at $\lambda = \lambda_1$.

6.1.2 Approximate solution of $H(\lambda)$

Lets define the eigenequation for the Hermitian operator $H(\lambda)$:

$$\text{Eigenequation of } H(\lambda) \qquad H(\lambda)|\psi(\lambda)\rangle = E(\lambda)|\psi(\lambda)\rangle\,. \tag{6.3}$$

We assume that $E(\lambda)$ and $|\psi(\lambda)\rangle$ can be expanded in powers of λ in the form:

$$E(\lambda) = \sum_{q=1}^{\infty} \lambda^q \varepsilon_q, \quad \text{and} \quad |\psi(\lambda)\rangle = \sum_{q=1}^{\infty} \lambda^q |q\rangle. \tag{6.4}$$

Substituting the above along with (6.1) in the eigenequation (6.3) yields

$$(H_0 + \lambda W) \left[\sum_{q=1}^{q} \lambda^q |q\rangle\right] = \left[\sum_{q'=1}^{q'} \lambda^{q'} \varepsilon_q\right] \left[\sum_{q=1}^{\infty} \lambda^q |q\rangle\right].$$

Equating the terms of the same power q:

$$\begin{aligned}
\text{0th-order}: &\quad H_0|0\rangle = \varepsilon_0|0\rangle && (6.5)\\
\text{1st-order}: &\quad (H_0 - \varepsilon_0)|1\rangle = (W - \varepsilon_1)|0\rangle = 0 && (6.6)\\
\text{2nd-order}: &\quad (H_0 - \varepsilon_0)|2\rangle + (W - \varepsilon_1)|1\rangle - \varepsilon_2|0\rangle = 0 && (6.7)\\
&\vdots\\
\text{qth-order}: &\quad (H_0 - \varepsilon_0)|q\rangle + (W - \varepsilon_1)|q-1\rangle - \varepsilon_2|q-2\rangle - \cdots - \varepsilon_q|0\rangle = 0 && (6.8)
\end{aligned}$$

We can choose the norm of $|\psi(\lambda)\rangle$ and its phase: we require it to be normalized, we choose its phase such that the scalar product $\langle 0|\psi(\lambda)\rangle$ is real. To 0th-order, this implies that the vector $|0\rangle$ must be normalized:

$$\langle 0|0\rangle = 1. \tag{6.9}$$

Its phase remain arbitrary, we will choose it after. To 1st order, the square of the nomro of $|\psi(\lambda)\rangle$ is written

$$\begin{aligned}
\langle\psi(\lambda)|\psi(\lambda)\rangle &= [\langle 0| + \lambda\langle 1|][|0\rangle + \lambda|1\rangle] + O(\lambda^2) && (6.10)\\
&= \langle 0|0\rangle + \lambda[\langle 1|0\rangle + \langle 0|1\rangle] + O(\lambda^2) && (6.11)\\
&= 1 + \lambda[\langle 1|0\rangle + \langle 0|1\rangle] + O(\lambda^2) = 1. && (6.12)
\end{aligned}$$

The choice of phase indicates that the scalar product $\langle 0|1\rangle$ is real since λ is real. Therefore,

$$\langle 0|1\rangle = \langle 1|0\rangle = 0. \tag{6.13}$$

Anologously,

$$\langle 0|2\rangle = \langle 2|0\rangle = -\frac{1}{2}\langle 1|1\rangle, \tag{6.14}$$

and in general:

$$\langle 0|q\rangle = \langle q|0\rangle = -\frac{1}{2}[\langle q-1|1\rangle + \langle q-2|2\rangle + \cdots + \langle 2|q-2\rangle + \langle 1|q-1\rangle]. \tag{6.15}$$

When we confine to second order in λ, the perturbation equations and the conditions, from above,

Second-order in λ

Equations	Conditions
$H_0\|0\rangle = \varepsilon_0\|0\rangle$	$\langle 0\|0\rangle = 1$
$(H_0 - \varepsilon_0)\|1\rangle = (W - \varepsilon_1)\|0\rangle = 0$	$\langle 0\|1\rangle = \langle 1\|0\rangle = 0$
$(H_0 - \varepsilon_0)\|2\rangle + (W - \varepsilon_1)\|1\rangle - \varepsilon_2\|0\rangle = 0$	$\langle 0\|2\rangle = \langle 2\|0\rangle = -\frac{1}{2}\langle 1\|1\rangle$

. (6.16)

From them, we now that $|0\rangle$ is an eigenvector of H_0 with eigenvalue ε_0, with the particular value E_n^0. Consider the set of eigenstates of $H(\lambda)$ corresponding to the various eigenvalues $E(\lambda)$ that approach E_n^0 when $\lambda \to 0$. They span a vector subspace whose dimension clearly cannot vary discontinuously when λ varies in the vecinity of zero. This dimension is consequently equal to the degeneracy g_n of E_n^0. We now consider the case of non-degenerae, and degenerate levels of H_0.

6.2 Perturbation of a non-degenerate case

Let be a non-denegerate eigenvalue E_n^0 of H_0, which is associated with the unique eigenvector $|\varphi_n\rangle$. We want to determine the modifications in this unperturbed energy in the corresponding statinary state produces by W.

For the eigenvalues of $H(\lambda)$ that approaches E_n^0 when $\lambda \to 0$ we ave

$$\varepsilon_0 = E_n^0 \Longrightarrow |0\rangle = |\varphi_n\rangle. \tag{6.17}$$

Thus, when $\lambda \to 0$ we again find the unperturbed state $|\varphi_n\rangle$ with the same phase. We call $E_n(\lambda)$ the eigenvalue of $H(\lambda)$ which when $\lambda \to 0$, approaches the eigenvalue E_n^0 of H_0, with eigenvector $|\psi_n(\lambda)\rangle$. We now compute the expansion of $E_n(\lambda)$ and $|\psi_n(\lambda)\rangle$ in powers of λ.

6.2.1 First-order corrections

We will determine the eigenvalue ε_1 and the eigenvector $|1\rangle$.

Energy correction

Projecting the first-order equation from (6.16) onto $|\varphi_n\rangle$ yields

$$\langle\varphi_n|(H_0-\varepsilon_0)|1\rangle + \langle\varphi_n|(W-\varepsilon_1)|0\rangle = \cancelto{0}{\langle\varphi_n|(\varepsilon_0-\varepsilon_0)|1\rangle} + \langle\varphi_n|(W-\varepsilon_1)|0\rangle = 0. \tag{6.18}$$

Considering equation (6.17), we have that:

$$\varepsilon_1 = \langle\varphi_n|W|0\rangle = \langle\varphi_n|W|\varphi_n\rangle. \tag{6.19}$$

The eigenvalue $E_n(\lambda)$ of H which corresponds to E_n^0 can be written, to first order in the perturbation as:

$$\text{First-order eigenvalue of } H \qquad \boxed{E_n(\lambda) = E_n^0 + \langle\varphi_n|W|\varphi_n\rangle + O(\lambda^2)}\,. \tag{6.20}$$

The first-order correction to a non-degenerate energy E_n^0 is simply equal to the averae value of the perturbation term W in the unperturbed state $|\varphi_n\rangle$.

Eigenvector correction

To exhaust all the information of the first-order perturbation equation (6.16), we must project it onto all the vectors of the $\{|\varphi_p^i\rangle\}$ basis other than $|\varphi_n\rangle$. Using (6.17):

$$\langle\varphi_p^i|(H_0-E_n^0)|1\rangle + \langle\varphi_p^i|(W-\cancelto{0}{\varepsilon_1})|\varphi_n\rangle = 0, \quad p \neq n \qquad \text{Orthogonality}$$
$$(E_p^0 - E_n^0)\langle\varphi_p^i|1\rangle + \langle\varphi_p^i|W|\varphi_n\rangle =$$

THe index i is for any possible degeneration in the energies E_p^0 other than E_n^0. This expression gives the coefficients of the desired expansion of the vector $|1\rangle$ on all the unperturbed basis states, except $|\varphi_n\rangle$:

$$\langle\varphi_p^i\rangle = \frac{1}{E_n^0 - E_p^0}\langle\varphi_p^i|W|\varphi_n\rangle, \quad p \neq n. \tag{6.21}$$

The las coefficient which we lack, $\langle\varphi_n|1\rangle = \langle 0|1\rangle$, is zero by the second condition of (6.16). We therefore know the vector $|1\rangle$ since we know its expansion on the $\{|\varphi_p^i\rangle\}$ basis:

$$|1\rangle = \sum_{p\neq n}\sum_i \frac{\langle\varphi_p^i|W|\varphi_n\rangle}{E_n^0 - E_p^0}|\varphi_p^i\rangle. \tag{6.22}$$

Thus, to first order in the perturbation, the eigenvector $|\varphi_n(\lambda)\rangle$ of H corresponding to the unperturbed state $|\varphi_n\rangle$ can be written as:

First-order eigenvector of H

$$|\psi_n(\lambda)\rangle = |\varphi_n\rangle + \sum_{p\neq n}\sum_i \frac{\langle\varphi_p^i|W|\varphi_n\rangle}{E_n^0 - E_p^0} + O(\lambda^2)\,. \tag{6.23}$$

It is a linear combination of all unperturbed states other than $|\varphi_n\rangle$: the perturbation W is said to produce a mixing of the state $|\varphi_n\rangle$ with the other iegenstates of H_0. The contribution of a given state $|\varphi_p^i\rangle$ is zero if the perturbation has no matrix element between $|\varphi_n\rangle$ and $|\varphi_p^i\rangle$.

First-order correction constraint

The first order correction of the state vector is small only if the non-diagonal matrix elements of W are much smaller than the corresponding unperturbed energy differences.

6.2.2 Second-order corrections

The process is analogous to the first-order, with the use of the second equation in (6.16).

Energy correction

We project second equation of (6.16) onto the vector $|\varphi_n\rangle$, using the conditions:

$$\langle\varphi_n|\cancelto{0\text{ Orthogonality}}{(H_0 - E_n^0)}|2\rangle + \langle\varphi_n|(W - \varepsilon_1)\cancelto{0\text{ Orhtogonality}}{|1\rangle} - \varepsilon_2\langle\varphi_n|\varphi_n\rangle = 0 \Longrightarrow \varepsilon_2 = \langle\varphi_n|W|1\rangle.$$

Using the expression for $|1\rangle$ from the first-order section, we have that:

$$\varepsilon_2 = \sum_{p\neq n}\sum_i \frac{|\langle\varphi_p^i|W|\varphi_n\rangle|^2}{E_n^0 - E_p^0}. \tag{6.24}$$

This enables us to write the energy $E_n(\lambda)$ to second order in the perturbation in the form:

Second-order eigenvalue of H

$$E_n(\lambda) = E_n^0 + \langle\varphi_n|W|\varphi_n\rangle + \sum_{p\neq n}\sum_i \frac{|\langle\varphi_p^i|W|\varphi_n\rangle|^2}{E_n^0 - E_p^0} + O(\lambda^3)\,. \tag{6.25}$$

To second-order, the closer the state $|\varphi_p^i\rangle$ to $|\varphi_n\rangle$, and th estronger the coupling $|\langle\varphi_p^i|W|\varphi_n\rangle|$, the more these two levels repel each other.

Eigenvector correction

By projecting the second equation (6.16) onto the set of basis vectors $|\varphi_p^i\rangle$ different from $|\varphi_n\rangle$, and by using conditions we can obtain the expression for the ket $|2\rangle$ and therefore the eigenvector to second order. It is not present in CT nor FG.

In general, we retain one more term in the energy expansion than in that of the eigenvector. This is because when projecting the second-order equation onto $|\varphi_n\rangle$, one makes the first term go to zero, which gives ε_q in terms of the corrections of order $q-1, q-2, \cdots$ of the eigenvector.

Upper limit of ε_2

If we limit the energy expansion to first order in λ, we can obtain an approximate idea of the error involver by evaluating the second-order term. We denote by $\Delta E =$ the absolute value of the difference between the energy E_n^0 of the level being studied and that of the closest level. We have:

$$\Delta E \leq |E_n^0 - E_p^0|, \quad \forall n. \tag{6.26}$$

This gives us an upper limit for the absolute value of ε_2:

$$\begin{aligned}
|\varepsilon_2| \leq & \frac{1}{\Delta E} \sum_{p\neq n} \sum_i |\langle \varphi_p^i | W | \varphi_n \rangle|^2 \\
= & \frac{1}{\Delta E} \sum_{p\neq n} \sum_i \langle \varphi_n | W | \varphi_p^i \rangle \langle \varphi_p^i | W | \varphi_n \rangle \\
= & \frac{1}{\Delta E} \langle \varphi_n | W \left[\sum_{p\neq n} \sum_i |\varphi_p^i\rangle\langle\varphi_p^i| \right] W | \varphi_n \rangle \\
\overset{(a)}{=} & \frac{1}{\Delta E} \langle \varphi_n | W \left[1 - |\varphi_n\rangle\langle\varphi_n| \right] W | \varphi_n \rangle \\
= & \frac{1}{\Delta E} \left[\langle \varphi_n | W^2 | \varphi_n \rangle - (\langle \varphi_n | W | \varphi_n \rangle)^2 \right]
\end{aligned}$$

In (a), we have used the fact that inside the brakets, we have the projector onto the basis $\{|\varphi_p^i\rangle\}$ minus a single elements $|\varphi_n\rangle$.

Finally, we multiply both sides by λ^2 to obtain an upper limit for the second-order term in the expansin of $E_n(\lambda)$, in the form:

$$\text{Upper limit for second-order term in } E_n(\lambda) \qquad \boxed{|\lambda^2 \varepsilon_2| \leq \frac{1}{\Delta E} (\Delta W)^2}. \tag{6.27}$$

This indicates the order of magnitude of the error on the energy resulting from taking only the first-order correction into account.

6.3 Perturbation of a degenerate level

Now assume that the level E_n^0 whose perturbatino we want to study is g_n-degenerate, with $\mathscr{E}_n^0$ the eigen-subspace of H_0. In this case, the choice $\varepsilon_0 = E_n^0$ does not suffice to determine the vector $|0\rangle$, since the 0th-order equation (6.16) can be satisfied by any linear combinarion of the g_n vectors $|\varphi_n^i\rangle$.

Under the action of W, the level E_n^0 generally gives rise to several distinct **sublevels** $f_n \in [0, g_n]$. If $f_n < g_n$, some of these sublevels are degenerate, since the total number of orthogonal eigenvectors of H associated with the f_n sublevels is always equal to g_n.

To determine ε_1 and $|0\rangle$, we project 1st-order equation (6.16) onto the g_n basis vectors $|\varphi_n^i\rangle$. Since these are eigenvectors of H_0 with eigenvalue $\varepsilon_0 = E_n^0$, we obtain

$$\varepsilon_1 \langle \varphi_n^i | 0 \rangle = \langle \varphi_n^i | W | 0 \rangle = \sum_p \sum_{i'} \langle \varphi_n^i | W | \varphi_p^{i'} \rangle \langle \varphi_p^{i'} | 0 \rangle \overset{(a)}{=} \sum_{i'=1}^{g_n} \langle \varphi_n^i | W | \varphi_n^{i'} \rangle \langle \varphi_n^{i'} | 0 \rangle.$$

In (a), the vector $|0\rangle$ belongs to the eigensubspace with E_n^0, is orthogonal to all the basis vectors $|\varphi_p^{i'}\rangle,\ p \neq n$; it only produces a single term for $p = n$.

We arrange the g_n^2 numbers $\langle \varphi_n^i | W | \varphi_n^{i'} \rangle$ (n fixed, $i, i' = 1, \cdots, g_n$) in a $g_n \times g_n$ matrix of row index i and collumn index i'. This matrix is denoted by W^n and is the part which corresponds to $\mathscr{E}_n^0$. The column vector of elements $\langle \varphi_n^i | 0 \rangle$ is an eigenvector of W^n with the eigenvalue ε_1.

This equation can also be transformed into a vector equation inside $\mathscr{E}_n^0$. The equivalent vector equation is then:

$$\text{Eigenequation of } W^{(n)} \text{ (in } \mathscr{E}_n^0) \qquad \boxed{W^{(n)}|0\rangle = \varepsilon_1 |0\rangle}\,. \tag{6.28}$$

To calculate the eigenvalues (to first order) and the eigenstates (to zeroth order) of the Hamiltonian corresponding to a degenerate uperturbed state E_n^0, diagonalize the matrix W^n, which represents the perturbation W inside the eigensubspace $\mathscr{E}_n^0$ associated with E_n^0.

Let $\varepsilon_1^j,\ j = 1, \cdots, f_n^{(1)}$ be the various distinct roots of the characteristic equation of $W^{(n)}$. Since $W^{(n)}$ is Hermitian, its eigenvalues are all real, and the sum of their degree of degeneracy is equal to g_n ($f_n^{(1)} \leq g_n$). Each eigenvalue introduces a different energy correction. Therefore, under W, the degeneracy level splits, to first order, into $f_n^{(1)}$ distintc sublevels, whose energies can be written as:

$$\text{First-order eigenvalue of } W^{(n)} \qquad \boxed{E_{n,j}(\lambda) = E_n^0 + \lambda \varepsilon_j^i, \quad j = 1, \cdots, f_n^{(1)} \leq g_n}\,. \tag{6.29}$$

If $f_n^{(1)} = g_n$, we say that, to first order, W completely removes the degeneracy of the level E_n^0. When $f_n^{(1)} < g_n$, the degeneracy, to first order, is only partially removed (or not at all if $f_n^{(1)} = 1$).

We now choose ε_1^j of $W^{(n)}$. If it is non-degenerate, the corresponding $|0\rangle$ is uniquely determined by (6.28). There then exist a single eigenvalue $E(\lambda)$ of $H(\lambda)$ which is equal to $E_n^0 + \lambda \varepsilon_1^j$, to first order, and this eigenvalue is non-degenerate. On the other hand, if ε_1^j is q-degenerate, (6.28) indicates that only that $|0\rangle$ belongs to the corresponding q-dimensional subspace $\mathcal{F}_j^{(1)}$.

This property of ε_1^j can reflect two different situations:

- There is only one exact energy $E(\lambda)$ that is equal, to first order, to $E_n^0 + \lambda \varepsilon_1^j$, and that this energy is q-degenerate. A q-dimensional eigensubspace then corresponds to the eigenvalue $E(\lambda)$, so that the degeneracy of the approximate eigenvalues will never be removes, to any order of λ.

  This often arises when H_0 and W possess common symmetry properties. The degeneracy then remains to all order in the perturbation theory.

- Several different energies $E(\lambda)$ are equal, to first order, to $E_n^0 + \lambda \varepsilon_1^j$. The subspace $\mathcal{F}_j^{(1)}$ obtained to first order is only the direct sum of the limits, for $\lambda \to 0$, of several eigensubspaces associated with these various energies $E(\lambda)$. That is, all the eigenvectors of $H(\lambda)$ corresponding to these energies

certainly approach kets of $\mathcal{F}_j^{(1)}$, but, inversely, a particular ket of $\mathcal{F}_j^{(1)}$ is not necessarily the limits $|0\rangle$ of an eigenket of $H(\lambda)$. Going to higher order terms allows one, not only to improve the accuracy of the energies, but also to determine the zeroth-order kets $|0\rangle$.

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