Notes of Quantum Mechanics

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Preface

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1.1 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.

1.2 Statements of the postulates

1.2.1 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**.

1.2.2 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 $\{|u_n^i\rangle\}$:

$$A|u_n^i\rangle = a_n|u_n^i\rangle,\ i = 1, 2, \cdots, g_n \Longrightarrow |\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i|u_n^i\rangle. \tag{1.1}$$

The probability now becomes

$$P(a_n) = \sum_{i=1}^{g_n} |c_n^i|^2 = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2. \tag{1.2}$$

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:

$$P(\alpha_1 < \alpha < \alpha_2) = \langle\psi|P_{\alpha_1,\alpha_2}|\psi\rangle = \int_{\alpha_1}^{\alpha_2} |\langle v_\alpha|\psi\rangle|^2\, d\alpha\,, \quad P_{\alpha_1,\alpha_2} = \int_{\alpha_1}^{\alpha_2} |v_\alpha\rangle\langle v_\alpha|\, d\alpha. \tag{1.3}$$

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

$$\begin{array}{ll} \text{Discrete case} & \text{Continuous case} \\ P(a_n) = \dfrac{1}{\langle\psi|\psi\rangle}\displaystyle\sum_{i=1}^{g_n}|c_n^i|^2 & \rho(\alpha) = \dfrac{1}{\langle\psi|\psi\rangle}|c(\alpha)|^2. \end{array} \tag{1.4}$$

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.

1.2.3 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:

$$\text{State of collapse} \qquad |\psi\rangle \overset{(a_n)}{\Longrightarrow} |u_n\rangle. \tag{1.5}$$

- 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 (1.1)):

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

And the state of collapse just after the measurement is

$$\text{State of collapse} \qquad |\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{1}{\sqrt{\sum_{i=1}^{g_n} |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle. \tag{1.6}$$

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:

$$|\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}} \tag{1.7}$$

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

1.2.4 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:

$$ih\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle\ , \tag{1.8}$$

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

1.2.5 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.

1.3 The physical interpretation of the postulates

1.3.1 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 (1.4)):

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

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

$$\langle x|p\rangle = (2\pi\hbar)^{-1/2} e^{\frac{ipx}{\hbar}}. \tag{1.9}$$

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:

$$dP(p) = |\langle p|\psi\rangle|^2 \, dp = |\tilde{\psi}(p)|^2 \, dp. \tag{1.10}$$

1.3.2 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.

1.3.3 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

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle \tag{1.11}$$

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

$$\lim_{N\to\infty} \frac{N(a_n)}{N} = P(a_n), \quad \text{and} \quad \sum_n N(a_n) = N. \tag{1.12}$$

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

$$\langle A\rangle_\psi = \lim_{N\to\infty} \frac{1}{N} \sum_n a_n N(a_n) = \sum_n a_n P(a_n). \tag{1.13}$$

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:

$$\lim_{N\to\infty} \frac{dN(\alpha)}{N} = dP(\alpha). \tag{1.14}$$

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

$$\langle A\rangle_\psi = \lim_{N\to\infty} \frac{1}{N} \int \alpha \; dN(\alpha) = \int \alpha \; dP(\alpha). \tag{1.15}$$

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

$$\text{Mean value of } A \qquad \boxed{\langle A\rangle_\psi = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}}. \tag{1.16}$$

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

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

1.3.4 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

$$\text{RMS deviation} \qquad \boxed{\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}}\,. \tag{1.17}$$

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

$$\text{Heisenberg relations} \qquad \begin{array}{l} \Delta X \cdot \Delta P_x \geq \frac{\hbar}{2} \\ \Delta Y \cdot \Delta P_y \geq \frac{\hbar}{2} \\ \Delta Z \cdot \Delta P_z \geq \frac{\hbar}{2} \end{array}\,. \tag{1.18}$$

1.3.5 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

$$P(a_n) = \sum_{p,i} |c_{n,p,i}|^2. \tag{1.19}$$

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

$$P_{a_n}(b_p) = \frac{1}{\sum_{p,i} |c_{n,p,i}|^2} \sum_i |c_{n,p,i}|^2. \tag{1.20}$$

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,

$$P(a_n, b_p) = P(a_n)P_{a_n}(b_p) = \sum_i |c_{n,p,i}|^2. \tag{1.21}$$

The state of the system becomes imediately after the second measuremet

$$|\psi''_{n,p}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{1.22}$$

$|\psi''_{n,p}\rangle$ 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

$$P(b_p, a_n) = \sum_i |c_{n,p,i}|^2, \quad \text{and} \quad |\psi''_{p,n}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{1.23}$$

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:

$$P(a_n, b_p) = P(b_p, a_n) = \sum_i |c_{n,p,i}|^2 = \sum_i |\langle a_n, b_p, i|\psi\rangle|^2, \quad \text{and} \tag{1.24}$$

$$|\psi''_{n,p}\rangle = |\psi''_{p,n}\rangle = \frac{1}{\sqrt{\sum_i |c_{n,p,i}|^2}} \sum_i c_{n,p,i}|a_n, b_p, i\rangle. \tag{1.25}$$

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

1.4 Physical implications of the Schrodinger equation

Recall the Schrodinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi\rangle. \tag{1.26}$$

1.4.1 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 (1.26) is linear and homogeneous, then their slutions are linearly superposable:

$$|\psi(t_0)\rangle = \lambda_1|\psi_1(t_0)\rangle + \lambda_2|\psi_2(t_0)\rangle \Longrightarrow |\psi(t)\rangle = \lambda_1|\psi_1(t)\rangle + \lambda_2|\psi_2(t)\rangle. \tag{1.27}$$

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

$$\langle\psi(t)|\psi(t)\rangle = \int d^3r\ |\psi(\boldsymbol{r},t)|^2 = \langle\psi(t_0)|\psi(t_0)\rangle = 1. \tag{1.28}$$

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

$$\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle. \tag{1.29}$$

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 $$\boxed{\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[A, H(t)]\rangle + \langle\frac{\partial A}{\partial t}\rangle}\ . \tag{1.30}$$

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 (1.30) to the observables $\boldsymbol{R}$ and $\boldsymbol{P}$, assuming a scalar stationary potential $V(\boldsymbol{r})$:

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

We also have

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

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

$$\text{Ehrenfest's theorem} \qquad \boxed{\begin{array}{l} \frac{d}{dt}\langle \boldsymbol{R} \rangle = \frac{1}{m}\langle \boldsymbol{P} \rangle \\ \frac{d}{dt}\langle \boldsymbol{P} \rangle = -\langle \nabla V(\boldsymbol{R}) \rangle \end{array}}. \tag{1.31}$$

classical limits of the Ehrenfest's theorem

1.4.2 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):

$$H|\varphi_{n,\tau}\rangle = E_n|\varphi_{n,\tau}\rangle. \tag{1.32}$$

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 $|\varphi_{n,\tau}\rangle$:

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

This equation can be integrated to give

$$c_{n,\tau}(t) = c_{n,\tau}(t_0)e^{-E_n(t-t_0)/\hbar}. \tag{1.33}$$

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 $e^{-iE_n(t-t_0)/\hbar}$:

$$|\psi(t)\rangle = \sum_n \sum_\tau c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{1.34}$$

  or, in the continuous case,

$$|\psi(t)\rangle = \sum_\tau \int dE\ c_\tau(E, t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{1.35}$$

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:

$$\text{Constant of the motion } A \qquad \boxed{\frac{\partial A}{\partial t} = 0 \wedge [A, H] = 0}\,. \tag{1.36}$$

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,

$$P(a_p, t) = P(a_p, t_0). \tag{1.37}$$

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 $|\psi(t)\rangle$ (1.34). 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

1.5 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**.

1.6 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

$$\text{Evolution operator} \qquad \boxed{|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle}\,, \tag{1.38}$$

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

1.6.1 General properties

From (1.38) we know that

$$U(t_0,t_0) = \mathbb{1}. \tag{1.39}$$

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

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = H(t)U(t,t_0)|\psi(t_0)\rangle \Longrightarrow i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)U(t,t_0). \tag{1.40}$$

This a first-order differential equation completely defined $U(t,t_0)$. Equations (1.39) and (1.40) can be condenses into a single integral form:

$$U(t,t_0) = \mathbb{1} = \int_{t_0}^{t} H(t')U(t',t_0)\,dt. \tag{1.41}$$

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:

$$U(t,t')U(t',t'') = U(t,t'') \tag{1.42}$$

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

$$\mathbb{1} = U(t',t)U(t,t') \Longrightarrow U(t',t) = U^{-1}(t,t'). \tag{1.43}$$

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**:

$$\text{Infinitesimal evolution operator} \qquad \boxed{U(t+dt,t) = \mathbb{1} - \frac{i}{\hbar}H(t)\ dt}. \tag{1.44}$$

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.

1.6.2 Case of conservative systems

When the operator H does not depend on time, equation (1.40) can be integrated easily:

$$U(t,t_0) = e^{-iH(t-t_0)/\hbar}. \tag{1.45}$$

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

$$U(t,t_0)|\varphi_{n,\tau}\rangle = e^{-iH(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle = e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle. \tag{1.46}$$

1.7 One-dimensional Gaussian wave packet (G1)

1.8 Particle in an infinite potential well

1.8.1 Introduction (H1)

1.8.2 Distribution of the momentum values in a stationary state

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

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{1.47}$$

and to the wave functions

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, \tag{1.48}$$

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

$$\bar{P}_n(p)\ dp = |\bar{\varphi}_n(p)|^2\ dp, \quad \text{with} \tag{1.49}$$

$$\begin{aligned}
\bar{\varphi}_n(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_0^a \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}e^{-ipx/\hbar}\ dx \\
&= \frac{1}{2i\sqrt{n\hbar a}}\int_0^a \left[e^{(\frac{n\pi}{a}-\frac{p}{\hbar})x} - e^{-i(\frac{n\pi}{a}+\frac{p}{\hbar})x}\right]\ dx \\
&= \frac{1}{2i}\sqrt{\frac{a}{\pi\hbar}}e^{i(\frac{n\pi}{a}-\frac{pa}{2\hbar})}\left[F(p-\frac{n\pi\hbar}{a}) + (-1)^{n+1}F(p+\frac{n\pi\hbar}{a})\right], \quad \text{with} \quad F(p) = \frac{\sin(pa/2\hbar)}{pa/2\hbar}.
\end{aligned} \tag{1.50}$$

The function inside the brakets in equation (1.50) 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

$$\text{Mean value of the momentum in the energy state } E_n \qquad \langle P\rangle_n = \int_{-\infty}^{\infty}\bar{P}_n(p)p\ dp = 0. \tag{1.51}$$

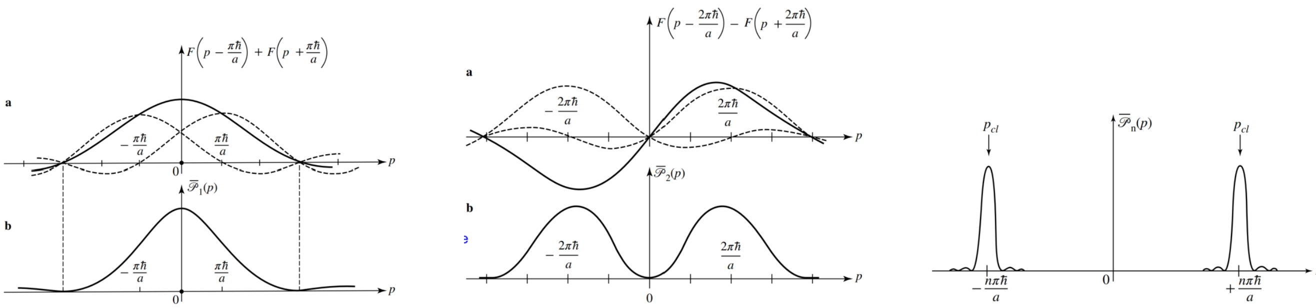
In the same way, we can compute $\langle P^2\rangle_n$. Using the fact that in the $\{|x\rangle\}$ representation P acts like $-i\hbar\partial_x$ and performing an integration by parts, we obtain:

$$\langle P^2\rangle_n = \hbar^2\int_0^a\left|\frac{d\varphi_n}{dx}\right|^2\ dx = \hbar^2\int_0^a\frac{2}{a}\left(\frac{n\pi}{a}\right)^2\cos^2\frac{n\pi x}{a}\ dx = \left(\frac{n\pi x}{a}\right)^2. \tag{1.52}$$

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.

1.8.3 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

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

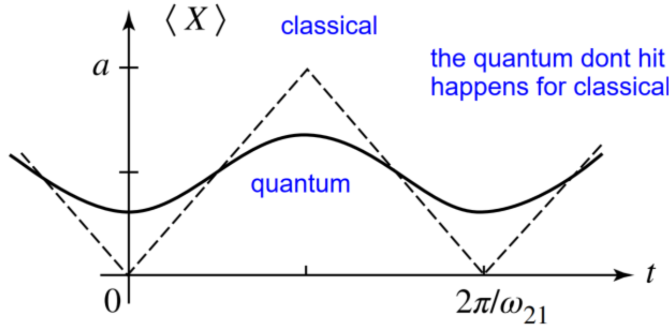


Figure 1.2 Time variation of $\langle X \rangle$ corresponding to the wave packet's motion. QM predicts that the center of the wave packet will turn back before hitting the wall

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,

$$\Delta H \Delta t = \frac{3}{2}E_1\frac{\hbar}{3E_1} = \frac{\hbar}{2}. \tag{1.53}$$

1.8.4 Perturbation created by a position measurement

1.9 Shcrodinger and Heisenberg pictures

1.9.1 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:

Effective state of the second frame $$|\psi_E(t)\rangle = F(t)|\psi(t)\rangle, \quad F(t_0) = \mathbb{1} \,. \tag{1.54}$$

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:

Effective Schrodinger equation and Hamiltonian $$\begin{aligned} &i\hbar\partial_t|\psi_E(t)\rangle = H_E(t)|\psi_E(t)\rangle \\ &H_E(t) = F(t)H(t)F^\dagger(t) - i\hbar F(t)\left(\partial_t F^\dagger(t)\right) \end{aligned} \tag{1.55}$$

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

1.9.2 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.

1.9.3 Schrodinger picture

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

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

$$\langle A_S(t)\rangle(t) = \langle\psi_S(t)|A_S(t)|\psi_S(t)\rangle \longrightarrow \frac{d}{dt}\langle A_S\rangle = \frac{1}{i\hbar}\langle[A_S, H_S]\rangle + \langle\frac{\partial A_S}{\partial t}\rangle \,. \tag{1.56}$$

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 $\partial_t\boldsymbol{R} = \partial_t\boldsymbol{P} = 0$:

Ehrenfest's equations $$\begin{aligned} &\frac{d}{dt}\langle\boldsymbol{R}\rangle = \frac{1}{m}\langle\boldsymbol{P}\rangle \\ &\frac{d}{dt}\langle\boldsymbol{P}\rangle = -\langle\nabla V(\boldsymbol{R})\rangle \end{aligned} \quad , \quad \langle V(\boldsymbol{R})\rangle = \left[\langle\partial_X V(\boldsymbol{R})\rangle, \langle\partial_Y V(\boldsymbol{R})\rangle, \langle\partial_Z V(\boldsymbol{R})\rangle\right] \,. \tag{1.57}$$

1.9.4 Heisenberg picture

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

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

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

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

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

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

Heisenberg picture quantities and dynamics

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

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

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

1.9.5 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

$$\text{Time-dependent S picture Hamiltonian} \qquad \boxed{H_S(t) = H_0 + W(t)}\,, \tag{1.58}$$

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

Transformed state vector and operator
$$\begin{aligned} |\psi_I(t)\rangle &= U_0^\dagger(t,t_0)|\psi_S(t)\rangle \\ A_I(t) &= U_0^\dagger(t,t_0)A_S(t)U_0(t,t_0) \end{aligned} \tag{1.59}$$

The effective Schrodinger equation in the interaction picture is

$$i\hbar\partial_t|\psi_I(t)\rangle = H_E(t)|\psi_I(t)\rangle, \quad \text{where} \quad H_E(t) = U_0^\dagger(t,t_0)W(t)U(t,t_0) \tag{1.60}$$

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

1.10 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**.

1.10.1 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 $|\psi_k\rangle$.

1.10.2 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

$$\text{Density operator} \qquad \boxed{\rho(t) = |\psi(t)\rangle\langle\psi(t)|}\,. \tag{1.61}$$

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

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

Secondly, the mean value of A is

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

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

$$\begin{aligned} \text{Time evolution of } \rho(t) \qquad \partial_t\rho(t) &= (\partial_t|\psi(t)\rangle)\langle\psi(t)| + |\psi(t)\rangle(\partial_t\langle\psi(t)|) \\ &= \frac{1}{i\hbar}H(t)|\psi(t)\rangle\langle\psi(t)| - \frac{1}{i\hbar}|\psi(t)\rangle\langle\psi(t)| \\ \partial_t\rho(t) &= \frac{1}{i\hbar}[H(t),\rho(t)]. \end{aligned} \tag{1.62}$$

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

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

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

$$\rho^\dagger(t) = \rho(t), \quad \underbrace{\rho^2(t) = \rho(t), \quad \text{Tr}\left[\rho^2(t)\right] = 1}_{\text{Only for pure case}}. \tag{1.63}$$

1.10.3 A statistical mixture of states (non-pure case)

Definition of the density operator

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

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

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

$$P(a_n) = \sum_k p_k P_k(a_n) = \sum_k p_k \text{Tr}\left[\rho_k P_n\right] = \text{Tr}\left[\sum_k p_k \rho_k P_n\right] = \text{Tr}\left[\rho P_n\right]. \tag{1.64}$$

We see that the linearity of the formulas whih 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:

$$\langle A\rangle = \sum_n a_n P(a_n) = \text{Tr}\left[\rho \sum_n a_n P_n\right] = \text{Tr}\left[\rho A\right]. \tag{1.65}$$

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

$$\rho(t) = \sum_k p_k \rho_k(t), \quad \text{with} \quad \rho_k(t) = |\psi_k(t)\rangle\langle\psi_k(t)|. \tag{1.66}$$

According to the pure case, $\rho_k(t)$ obeys the evolution equation (1.62). Thus,

$$\text{Time evolution of } \rho(t) \qquad \boxed{i\hbar\partial_t \rho(t) = [H(t), \rho(t)]}\,. \tag{1.67}$$

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 diagonal 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

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

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 ($\rho_{nn}\rho_{pp} \ge |\rho_{np}|^2$).

1.10.4 Separate description of part of a physical system. Concept of a partial trace

Chapter 2

The quantum harmonic oscillator

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2.1 Introduction

2.1.1 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:

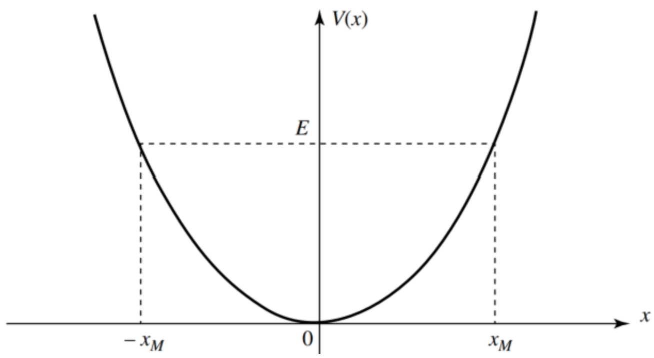

Figure 2.1 Potential energy $V(x)$ of a 1D harmonic oscillator.

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

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.

2.1.2 The harmonic oscillator in classical mechanics

The motion of the particle is governed by the dynamics equation

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx} = -kx \longrightarrow x = x_M \cos(\omega t - \varphi). \tag{2.1}$$

The kinetic energy of the particle is

$$T = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{p^2}{2m}, \tag{2.2}$$

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

$$F_x = -\frac{dV}{dx} = -2b(x - x_0) - 3c(x - x_0)^2 + \cdots \tag{2.3}$$

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**.

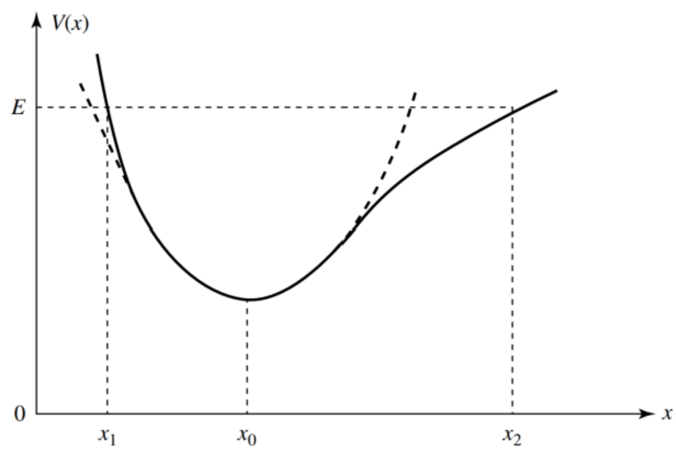

Figure 2.2 Any potential can be approximated by a parabolic potential. In $V(x)$, a classical particle of energy E oscillates between x_1 and x_2.

2.1.3 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.**

2.2 Eigenvalues of the Hamiltonian

2.2.1 Notation

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

$$\text{Dimensionless observables} \qquad \boxed{\hat{X}=\frac{X}{\sigma},\quad \hat{P}=\frac{\sigma P}{\hbar},\quad \text{where} \quad \sigma=\sqrt{\frac{\hbar}{m\omega}}=\text{Oscillator length }(m)}\,.$$

are dimensionless. With these new operators, the canonical commutation is

$$\text{Canonical commutation} \qquad \boxed{[\hat{X},\hat{P}]=i} \tag{2.4}$$

and the Hamiltonian can be put in the form

$$H=\hbar\omega\hat{H},\quad \text{with} \quad \hat{H}=\frac{1}{2}(\hat{X}+\hat{P}). \tag{2.5}$$

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

$$\begin{aligned} a&=\frac{1}{\sqrt{2}}(\hat{X}+i\hat{P}) \\ a^\dagger&=\frac{1}{\sqrt{2}}(\hat{X}-i\hat{P}) \end{aligned} \quad\Longleftrightarrow\quad \begin{aligned} \hat{X}&=\frac{1}{\sqrt{2}}(a^\dagger+a) \\ \hat{P}&=\frac{i}{\sqrt{2}}(a^\dagger-a) \end{aligned}\,. \tag{2.6}$$

The commutator of a and $a^\dagger$ is

$$[a, a^\dagger] = \frac{1}{2}[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}] = \frac{i}{2}[\hat{P}, \hat{X}] - \frac{i}{2}[\hat{X}, \hat{P}] = 1 \longrightarrow \boxed{[a, a^\dagger] = 1}\,. \tag{2.7}$$

If we do $aa^\dagger$ we obtain

$$a^\dagger a = \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P}) = \frac{1}{2}(\hat{X}^2 + \hat{P}^2 + i\hat{X}\hat{P} - i\hat{P}\hat{X}) = \frac{1}{2}(\hat{X}^2 + \hat{P}^2 - 1).$$

Comparing with $\hat{H}$ we see that

$$\boxed{\hat{H} = a^\dagger a + \frac{1}{2} = aa^\dagger - \frac{1}{2}}\,.$$

We see that we canot put $\hat{H}$ in a product of linear terms, due to the non-commutatitivty of $\hat{X}$ and $\hat{P}$ ($1/2$ term).

We introduce another operator:

$$\text{Operator } N \qquad \boxed{N = a^\dagger a}\,. \tag{2.8}$$

This operator is Hermitian

$$N^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = N. \tag{2.9}$$

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

$$\hat{H} = N + \frac{1}{2} \tag{2.10}$$

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

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a \longrightarrow \boxed{[N, a] = -a} \tag{2.11}$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger [a, a^\dagger] + [a^\dagger, a^\dagger]a = a^\dagger \longrightarrow \boxed{[N, a^\dagger] = a^\dagger}\,. \tag{2.12}$$

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

$$\text{Eigenequation of } N \qquad \boxed{N|\varphi_\nu^i\rangle = \nu|\varphi_\nu^i\rangle}\,. \tag{2.13}$$

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

$$H|\varphi_\nu^i\rangle = (\nu + 1/2)\hbar\omega|\varphi_n u^i\rangle. \tag{2.14}$$

The solution of the eigenequation of N will be based on the commutation relation $[a, a^\dagger] = 1$.

2.2.2 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 $a|\varphi_n u^i\rangle$

$$\|a|\varphi_\nu^i\rangle\|^2 = \langle\varphi_\nu^i|a^\dagger a|\varphi_\nu^i\rangle = \langle\varphi_\nu^i|N|\varphi_\nu^i\rangle = \nu\langle\varphi_\nu^i|\varphi_\nu^i\rangle \geq 0 \Longrightarrow \boxed{\nu \geq 0}.$$

- **Properties of the vector $a|\varphi_\nu^i\rangle$**
  i) $\nu = 0 \Longrightarrow a|\varphi_{\nu=0}^i\rangle = 0$. If $\nu = 0$ is an eigenvalue of N, all eigenvectors $|\varphi_0^i\rangle$ associated with this eigenvalue satisfy the relation

$$a|\varphi_0^i\rangle = 0. \tag{2.15}$$

  Anyn vector which satisfy this relation is therefore an eigenvector of N with the eigenvalue $\nu = 0$.
  ii) $\nu > 0 \Longrightarrow a|\varphi_\nu^i\rangle$ is a non-zero eigenvector of N with eigenvalue $\nu - 1$.

$$\begin{aligned} [N,a]|\varphi_\nu^i\rangle &= -a|\varphi_\nu^i\rangle \\ Na|\varphi_\nu^i\rangle &= aN|\varphi_\nu^i\rangle - a|\varphi_\nu^i\rangle \quad \Longrightarrow \quad \boxed{N[a|\varphi_\nu^i\rangle] = (\nu-1)[a|\varphi_\nu^i\rangle]}. \\ N[a|\varphi_\nu^i\rangle] &= a\nu|\varphi_\nu^i\rangle - a|\varphi_\nu^i\rangle \end{aligned}$$

- **Properties of the vector $a^\dagger|\varphi_\nu^i\rangle$**
  i) $a^\dagger|\varphi_\nu^i\rangle$ is always non-zero. We study it with the square of the norm:

$$\|a^\dagger|\varphi_\nu^i\rangle\|^2 = \langle\varphi_\nu^i|aa^\dagger|\varphi_\nu^i\rangle = \langle\varphi_\nu^i|(N+1)|\varphi_\nu^i\rangle = (\nu+1)\langle\varphi_\nu^i|\varphi_\nu^i\rangle.$$

  As $\nu \geq 0$ by lemma 1, the ket $a^\dagger|\varphi_\nu^i\rangle$ always has non-zero norm and, consequently, is never zero.
  ii) $a^\dagger|\varphi_\nu^i\rangle$ is an eigenvector of N with eigenvalue $N+1$. We do it analoguisly to lemma IIb):

$$\begin{aligned} [N,a^\dagger]|\varphi_\nu^i\rangle &= a^\dagger|\varphi_\nu^i\rangle \\ Na^\dagger|\varphi_\nu^i\rangle &= a^\dagger N|\varphi_\nu^i\rangle + a^\dagger|\varphi_\nu^i\rangle \quad \Longrightarrow \quad \boxed{N[a^\dagger|\varphi_\nu^i\rangle] = (\nu+1)[a^\dagger|\varphi_\nu^i\rangle]}. \\ N[a^\dagger|\varphi_\nu^i\rangle] &= \nu a^\dagger|\varphi_\nu^i\rangle + a^\dagger|\varphi_\nu^i\rangle \end{aligned}$$

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

$$\text{Eigenvalue of } H \qquad \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n \in \mathbb{N}_0^+}. \tag{2.16}$$

In QM, the energy of the harmonic oscillator is **quantized**. The smallest value (ground state) is $\hbar\omega/2$.

Interpretation of the a and $a^\dagger$ operators

We have seen that, given $|\varphi_n^i\rangle$ with eigenvalue E_n, application of a gives an eigenvector associated with E_{n-1} while application of $a^\dagger$ yields the energy E_{n+1}.

Thats why $a^\dagger$ is said to be a **creation operator** and a an **annihilation operator**; their action on an eigenvector of N makes an energy quantum $\hbar\omega$ appear or dissapear.

2.2.3 Degeneracy of the eigenvalues

The grounds state is non-degenerate

The eigenstates of H associated with $E_0 = \hbar\omega/2$ (or eigenvector of N associated with $n = 0$), according to lemma II, must all satisfy the equation

$$a|\varphi_0^i\rangle = 0.$$

To find the degeneracy of the E_0 level, all we must do is see how many li kets satisfy the above. We can write the above equation using the definition of $\hat{X}, \hat{P}$ and a in terms of them, in the form

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

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

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

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

$$\varphi_0^i(x) = ce^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{2.17}$$

The various solutions of the ODE are all proportional to each other. Consequently, there exists only one ket $|\varphi_0\rangle$ that satisfies the initial equation: the ground sate $E_0 = \hbar\omega/2$ is not degenerate.

All the states are non-degenerate

We use recurrence to show that all other states are also non-degenerate. We need to prove that if E_n is non degenerate, the level E_{n+1} is not either.

Lets assume there exists only one vector $|\varphi_n\rangle$ such that

$$N|\varphi_n\rangle = n|\varphi_n\rangle.$$

Then consider an eigenvector $|\varphi_{n+1}^i\rangle$ corresponding to the eigenvalue $n+1$

$$N|\varphi_{n+1}^i\rangle = (n+1)|\varphi_{n+1}^i\rangle.$$

We know that the ket $a|\varphi_{n+1}^i\rangle$ is not zero and that it is an eigenvector of N with eigenvalue n. Since this ket is not degenerae by hypothesis, there exists a number c^i such that

$$a|\varphi_{n+1}^i\rangle = c^i|\varphi_n\rangle/a^\dagger \longrightarrow a^\dagger a|\varphi_{n+1}^i\rangle = N|\varphi_{n+1}^i\rangle = (n+1)|\varphi_{n+1}^i\rangle = c^i a^\dagger|\varphi_n\rangle.$$

We have,

$$|\varphi_{n+1}^i\rangle = \frac{c^i}{n+1}a^\dagger|\varphi_n\rangle.$$

We see that all kets $|\varphi^i_{n+1}\rangle$ 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.

2.3 Eigenstates of the Hamiltonian

2.3.1 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 $c_1 = 1$:

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2 = 1 \Longrightarrow |\varphi_1\rangle = a^\dagger|\varphi_0\rangle. \tag{2.18}$$

We can do the same to constrcut $|\varphi_2\rangle$ from $|\varphi_1\rangle$ and get c_2 and so on. In general, if we know $|\varphi_{n-1}\rangle$ (normalized), then the normalized vector $|\varphi_n\rangle$ is written

$$|\varphi_n\rangle = c_n a^\dagger|\varphi_{n-1}\rangle, \quad \text{so that} \quad c_n = \frac{1}{\sqrt{n}}.$$

In fact, we can express all $|\varphi_n\rangle$ in terms of $|\varphi_0\rangle$ by recursion:

$$\text{Excited states in terms of the ground state} \qquad \boxed{|\varphi_n\rangle = \frac{1}{\sqrt{n}}(a^\dagger)^n|\varphi_0\rangle}. \tag{2.19}$$

Orthonormalization and closure relations

Since H is Hermitian, the kets $|\varphi_n\rangle$ corresponding to different values of n are orthogonal so that they satisfy the orthonormalization relation:

$$\langle\varphi_n'|\varphi_n\rangle = \delta_{nn'}.$$

In addition, H is an obsrvable; the set of the $|\varphi_n\rangle$ therefore constitutes a basis in $\mathscr{E}_x$, which is expressed by the closure relation

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = \mathbb{1}.$$

Action of the various operators

The observables X and P are linear combinations of the operators a and $a^\dagger$. Therefore, all physical quantities can be expressed in terms of the latters. The action of a and $a^\dagger$ on the vectors of the $\{|\varphi_n\rangle\}$ basis is

$$\text{Action of } a \text{ and } a^\dagger \qquad \begin{array}{lcl} a^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle & \xrightarrow{\text{Adjoint}} & \langle\varphi_n|a = \sqrt{n+1}\langle\varphi_{n+1}| \\ a|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle & & \langle\varphi_n|a^\dagger = \sqrt{n}\langle\varphi_{n-1}| \end{array} \tag{2.20}$$

Note that a decreases or increases n by one unit depending on wheter it acts on the $|\varphi_n\rangle$ or on the bra $\langle\varphi_n|$, similarly for $a^\dagger$. The expressions for X and P are then:

$$X|\varphi_n\rangle = \sqrt{\frac{\hbar}{m\omega}}\frac{1}{\sqrt{2}}(a^\dagger + a)|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n+1}|\varphi_{n+1}\rangle + \sqrt{n}|\varphi_{n-1}\rangle] \tag{2.21}$$

$$P|\varphi_n\rangle = \sqrt{m\hbar\omega}\frac{i}{\sqrt{2}}(a^\dagger - a)|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}[\sqrt{n+1}|\varphi_{n+1}\rangle - \sqrt{n}|\varphi_{n-1}\rangle] \tag{2.22}$$

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

$$\langle\varphi_{n'}|a|\varphi_n\rangle = \sqrt{n}\delta_{n',n-1} \tag{2.23}$$

$$\langle\varphi_{n'}|a^\dagger|\varphi_n\rangle = \sqrt{n+1}\delta_{n',n+1} \tag{2.24}$$

$$\langle\varphi_{n'}|X|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \tag{2.25}$$

$$\langle\varphi_{n'}|P|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}[\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}] \tag{2.26}$$

The matrices representing a and $a^\dagger$ are Hermitian conjugates of each other, while matrices representing X and P are both Hermitian.

Eigenstates of a

Does a have eigenstates? that is, can we express any vector as

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle?$$

We begin with $a|\alpha\rangle = \alpha|\alpha\rangle$ in the left side:

$$a|\alpha\rangle = a\mathbb{1}|\alpha\rangle = a\sum_{n=0}^{\infty}|n\rangle\langle n|\alpha\rangle = \cancelto{0}{a|0\rangle} c_0 + \sum_{n=1}^{\infty} c_n a|\alpha\rangle = \sum_{n=1}^{\infty}\sqrt{n}|n-1\rangle c_n = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle.$$

On the right side, we have

$$\alpha|\alpha\rangle = \alpha\mathbb{1}|\alpha\rangle = \alpha\sum_{n=0}^{\infty}|n\rangle\langle n|\alpha\rangle = \alpha\sum_{n=0}^{\infty} c_n|n\rangle.$$

Equating both side results:

$$\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = \alpha \sum_{n=0}^{\infty} c_n|n\rangle / \langle m|$$
$$\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}\langle m|n\rangle = \alpha \sum_{n=0}^{\infty} c_n\langle m|n\rangle$$
$$c_{m+1}\sqrt{m+1} = \alpha c_m$$

from which we get

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle.$$

We normalize it:

$$\begin{aligned}\langle\alpha|\alpha\rangle = 1 &= \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m\alpha^n}{\sqrt{m!}\sqrt{n!}} c_0^* c_0\langle m|n\rangle \\ &= \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n}!|c_0|^2 \\ &= |c_0|^2 e^{|\alpha|^2} = 1 \longrightarrow c_0 = e^{-\frac{|\alpha|^2}{2}}.\end{aligned}$$

Therefore, we finally get:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{2.27}$$

2.3.2 Wave functions associated with the stationary states

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

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

To obtain the functions $\varphi_n(x)$, all we need to do is use expression (2.19) and the fact that in $\{|x\rangle\}$ $a^\dagger$ is represented by

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]. \tag{2.28}$$

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

$$\varphi_n(x) = \langle x|\varphi_n(x)\rangle = \frac{1}{\sqrt{n!}}\langle x|(a^\dagger)^n|\varphi_0\rangle = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right]^n \varphi_0(x). \tag{2.29}$$

That is,

Excited state
$$\varphi_n(x) = \underbrace{\left[\frac{1}{2^n n!}\left(\frac{\hbar}{m\omega}\right)^n\right]^{1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\frac{m\omega}{\hbar}x - \frac{d}{dx}\right]^n}_{\text{Hermite polynomial}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}. \tag{2.30}$$

When n increases, the region of the Ox axis in which $\varphi_n(x)$ takes on non-negligible values becomes larger. It follows that the mean value of the potential energy grows with n. In addition, the number of zeros of $\varphi_n(x)$ is n, this mplies that the mean kinetic energy of the particle increases with n.

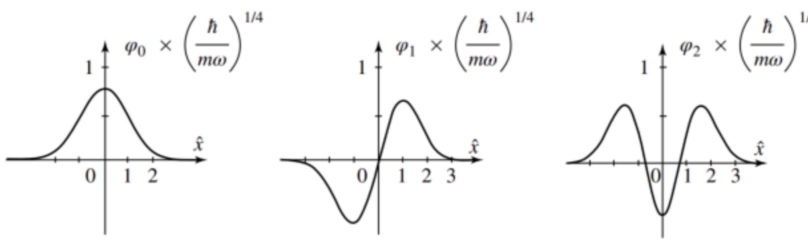

Figure 4: Wave functions associated with the first three levels of a harmonic oscillator.

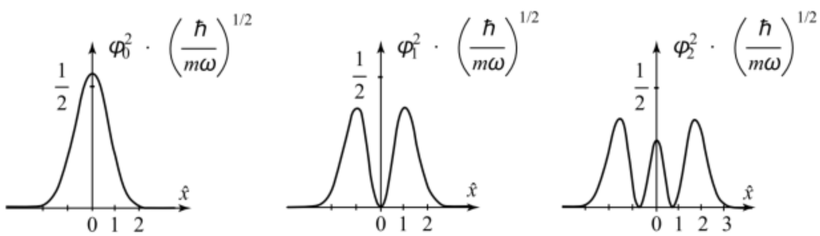

Figure 5: Probability densities associated with the first three levels of a harmonic oscillator.

2.4 Discussion

2.4.1 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 (2.22), which show that neither X nor P has diagonal matrix elements:

$$\langle\varphi_n|X|\varphi_n\rangle = \langle\varphi_n|P|\varphi_n\rangle = 0. \tag{2.31}$$

To obtain the rms deviations, we must calculate the mean value of X^2 and P^2. First, we note that

$$\begin{aligned} X^2 &= \frac{\hbar}{2m\omega}(a^\dagger + a)(a^\dagger + a) = \frac{\hbar}{2m\omega}(a^{\dagger 2} + aa^\dagger + a^\dagger a + a^2) \\ P^2 &= -\frac{m\hbar\omega}{2}(a^\dagger - a)(a^\dagger - a) = -\frac{m\hbar\omega}{2}(a^{\dagger 2} - aa^\dagger - a^\dagger a + a^2) \end{aligned}$$

The terms a^2 and $a^{\dagger 2}$ do not contribute to the diagonal matrix elements, since $a^2|\varphi_n\rangle$ is proportional to $|\varphi_{n-2}\rangle$ and $a^{\dagger 2}|\varphi_n\rangle$ to $|\varphi_{n+2}\rangle$; both are orthogonal to $|\varphi_n\rangle$. The rest of the terms yields:

$$\langle\psi_n|(a^\dagger a + aa^\dagger)|\varphi_n\rangle = \langle\varphi_n|(2a^\dagger a + 1)|\varphi_n\rangle = 2n + 1.$$

Therefore, we have:

$$(\Delta X)^2 = \langle\varphi_n|X|\varphi_n\rangle - \langle\varphi_n|X^2|\varphi_n\rangle = \langle\varphi_n|X^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega} = \sigma^2\left(x + \frac{1}{2}\right). \tag{2.32}$$

$$(\Delta P)^2 = \langle\varphi_n|P|\varphi_n\rangle - \langle\varphi_n|P^2|\varphi_n\rangle = \langle\varphi_n|P^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega = \frac{\hbar^2}{\sigma^2}\left(x + \frac{1}{2}\right). \tag{2.33}$$

The product is therefore

$$\text{Uncertainty relation} \qquad \boxed{\Delta X \Delta P = \left(n + \frac{1}{2}\right)\hbar\,.} \tag{2.34}$$

We see that the lower bound is attained for $n = 0$, that is, for the ground state.

2.4.2 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.

2.4.3 Time evolution of the mean values

Consider thw state at $t = 0$

$$|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n(0)|\varphi_n\rangle.$$

Its state $|\psi(t)\rangle$ at t can be obtained by using the evolution operator for conservative systems:

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-iE_nt/\hbar}|\varphi_n\rangle = \sum_{n=0}^{\infty} c_n(0)e^{-i(n+1/2)\omega t}|\varphi_n\rangle. \tag{2.35}$$

The mean value of any physical quantity A is

$$\langle\varphi(t)|A|\varphi(t)\rangle = \sum_{m,n=0}^{\infty} c_m^*(0)c_n(0)A_{mn}e^{i(m-n)\omega t}, \quad \text{with} \quad A_{mn} = \langle\varphi_m|A|\varphi_n\rangle.$$

The time evolution of the mean values involves only the frequency $\omega/2\pi$ and its various harmonics, which constitutes the Bohr frequencies of the harmonics oscillator.

If we consider X and P, we know that the only non-zero elements X_{mn} and P_{mn} are those for which $m = n \pm 1$. Consequently, the mean values of X and P include only terms in $e^{\pm\omega t}$. Moreover, the form of the harmonics oscillator potential implies that for all $|ket\varphi_n$ the mean values of X and P rigorously satisfy the classical equations of motion. Using Ehrenfest theorem:

$$\begin{array}{lcl} \dfrac{d}{dt}\langle X\rangle = \dfrac{1}{i\hbar}\langle[X,H]\rangle = \dfrac{\langle P\rangle}{m} & \xrightarrow{\int dt} & \langle X\rangle(t) = \langle X\rangle(0)\cos\omega t + \dfrac{1}{m\omega}\langle P\rangle(0)\sin\omega t \\ \dfrac{d}{dt}\langle P\rangle = \dfrac{1}{i\hbar}\langle[P,H]\rangle = -m\omega^2\langle X\rangle & & \langle P\rangle(t) = \langle P\rangle(0)\cos\omega t + m\omega\langle X\rangle(0)\sin\omega t \end{array} \tag{2.36}$$

- In a stationary state $|\varphi_n\rangle$, the behavior of the harmonic oscillator is totally different from that predicted by classical mechanics. The mean values of all the observables are constant over time.

2.5 Stationary states in the $\{|x\rangle\}$ representation

2.5.1 Hermite polynomials

Definition

Let be the Gaussian function

$$F(z) = e^{-z^2} \tag{2.37}$$

The successive derivatives are

$$F'(z) = -2ze^{-z^2}, \quad F''(z) = (4z^2 - 2)e^{-z^2}, \quad \cdots, \quad F^{(n)}(z) = (-1)^n H_n(z)e^{-z^2},$$

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

$$\text{Hermite polynomial} \qquad \boxed{H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}}\,. \tag{2.38}$$

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

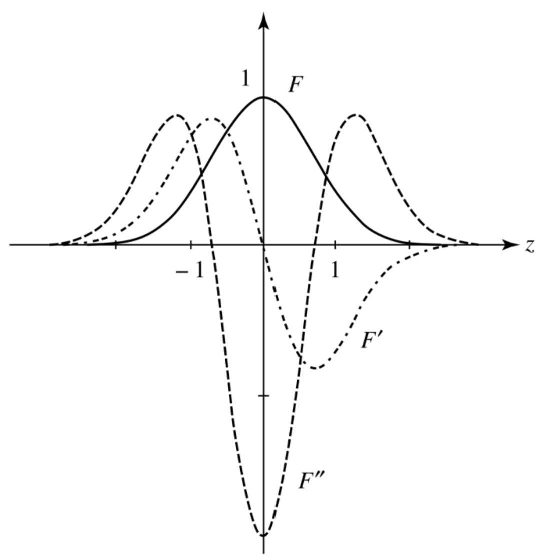

Figure 2.1 Shape of the Gaussian function $F(z)$ and its first and second derivatives.

Generating function

Recurrence relations; differential equation

2.5.2 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

$$\begin{aligned}\langle x|a|\varphi_0\rangle = \langle x|\frac{1}{\sqrt{2}}\left(\frac{x}{\sigma}+\frac{ip\sigma}{\hbar}\right)|\varphi_0\rangle = 0\\ \frac{1}{\sqrt{2}}\left(\frac{x}{\sigma}+\sigma\frac{\partial}{\partial x}\right)\varphi_0(x) =\\ \frac{\partial\varphi_0(x)}{\partial x} = -\frac{x}{\sigma^2}\varphi_0(x).\end{aligned}$$

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:

Excited state in $\{|x\rangle\}$
$$\boxed{\varphi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-\beta^2x^2/2}H_n(\beta x)}\,. \tag{2.39}$$

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 $a^\dagger$ (2.20) in the $\{|x\rangle\}$ representation. The action of them in this representation is

$$a \longrightarrow \frac{\beta}{\sqrt{2}}\left[x+\frac{1}{\beta^2}\frac{d}{dx}\right] \qquad a^\dagger \longrightarrow \frac{\beta}{\sqrt{2}}\left[x-\frac{1}{\beta^2}\frac{d}{dx}\right]. \tag{2.40}$$

Then equation (2.20) becomes:

Action of $a, a^\dagger$ in $\{|x\rangle\}$
$$\boxed{\begin{aligned}\frac{\beta}{\sqrt{2}}\left[x+\frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) = \sqrt{n}\varphi_{n-1}(x)\\ \frac{\beta}{\sqrt{2}}\left[x-\frac{1}{\beta^2}\frac{d}{dx}\right]\varphi_n(x) = \sqrt{n+1}\varphi_{n+1}(x)\end{aligned}} \tag{2.41}$$

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 $\hat{x} = \beta x$):

$$\begin{aligned}&2\hat{x}H_n(\hat{x}) = 2nH_{n-1}(\hat{x})+H_{n+1}(\hat{x})\\ &2\left[-\hat{x}H_n(\hat{x})+\frac{d}{d\hat{x}}H_n(\hat{x})\right] = 2nH_{n-1}(\hat{x})-H_{n+1}(\hat{x})\end{aligned}$$

2.6 The isotropic three-dimensional harmonic oscillator

2.7 Coherent states of the harmonic oscillator

Formula sheet

2.7.1 Useful formulas

Closure relation (discrete)	$\sum_k \sum_{i=1}^{g_k} \lvert v_k^i\rangle\langle v_k^i\rvert = \mathbb{1}$	Closure relation (continuous)	$\int_\beta d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert = \mathbb{1}$
Glauber Formula	$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$	Generalized uncertainty relation	$\Delta A \Delta B \geq \frac{1}{2}\lvert\langle[A,B]\rangle\rvert$
Function of an operator	$F(A) = \sum_{n=0}^{\infty} f_n (A-a)^n$		$\Delta Q = \sqrt{\langle Q^2\rangle - \langle Q\rangle^2}$
Eigenequation of $F(A)$	$F(A)\lvert\psi\rangle = F(\lambda)\lvert\psi\rangle$		
Transformation $\{u\} \to \{v\}$	$\mathbb{M}_{jk} = \langle u_j \vert v_k\rangle$	$\lvert\psi\rangle_{\{u\}} = \mathbb{M}\lvert\psi\rangle_{\{v\}}$ $A_{\{u\}} = \mathbb{M}A_{\{v\}}\mathbb{M}^\dagger$	$\lvert\psi\rangle_{\{v\}} = \mathbb{M}^\dagger\lvert\psi\rangle_{\{u\}}$ $A_{\{v\}} = \mathbb{M}^\dagger A_{\{u\}}\mathbb{M}$

2.7.2 Basis

Quantity	Discrete basis (sum over j, k)	Continuous basis (integrate over β, β')
$\mathbb{1}$	$= \sum \lvert v_k\rangle\langle v_k\rvert$	$= \int d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\rvert$
$\lvert\psi\rangle = \mathbb{1}\lvert\psi\rangle$	$= \sum \lvert v_k\rangle\langle v_k\vert\psi\rangle$	$= \int d\beta\ \lvert\omega_\beta\rangle\langle\omega_\beta\vert\psi\rangle$
$\langle\varphi\rvert = \langle\varphi\rvert\mathbb{1}$	$= \sum \langle\varphi\vert v_k\rangle\langle v_k\rvert$	$= \int d\beta\ \langle\varphi\vert\omega_\beta\rangle\langle\omega_\beta\rvert$
$A = \mathbb{1}A\mathbb{1}$	$= \sum\sum \lvert v_j\rangle\langle v_j\vert A\vert v_k\rangle\langle v_k\rvert$	$= \iint d\beta\ d\beta'\ \lvert\omega_\beta\rangle\langle\omega_\beta\vert A\vert\omega_{\beta'}\rangle\langle\omega_{\beta'}\rvert$

Quantity	X representation	P_x representation
X	x	$i\hbar\,\partial/\partial p$
P_x	$-i\hbar\,\partial/\partial x$	p
$\lvert x'\rangle$	$\langle x\vert x'\rangle = \delta(x-x')$	$\langle p\vert x'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(-ix'p/\hbar)$
$\lvert p'\rangle$	$\langle x\vert p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ixp'/\hbar)$	$\langle p\vert p'\rangle = \delta(p-p')$
$\lvert\psi\rangle$	$\langle x\vert\psi\rangle = \psi(x)$	$\langle p\vert\psi\rangle = \tilde{\psi}(p)$

Fourier transforms for 3D wavefunctions

$\tilde{\psi}(\boldsymbol{p}) = \mathscr{F}[\psi(\boldsymbol{r})] = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int_{-\infty}^{\infty} d^3\boldsymbol{r}\ e^{-i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\psi(\boldsymbol{r})$	$\psi(\boldsymbol{r}) = \mathscr{F}^{-1}\left[\tilde{\psi}(\boldsymbol{p})\right] = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int_{-\infty}^{\infty} d^3\boldsymbol{p}\ e^{i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\tilde{\psi}(\boldsymbol{p})$
$\mathscr{F}\left[\psi^{(n)}(x)\right] = \left(\frac{ip}{\hbar}\right)^n \tilde{\psi}(p)$	$\tilde{\psi}^{(n)}(p) = \mathscr{F}\left[\left(-\frac{ix}{\hbar}\right)^n \psi(x)\right]$
$\tilde{\psi}(p-p_0) = \mathscr{F}\left[e^{ip_0x/\hbar}\psi(x)\right]$	$e^{-ipx_0/\hbar}\tilde{\psi}(p) = \mathscr{F}[\psi(x-x_0)]$
$\mathscr{F}[\psi(cx)] = \tilde{\psi}(p/c)/\lvert c\rvert$	$\int_{-\infty}^{\infty} dx\ \varphi^*(x)\psi(x) = \int_{-\infty}^{\infty} dp\ \tilde{\varphi}^*(p)\tilde{\psi}(p)$
$\psi(x)$ real: $[\tilde{\psi}(p)]^* = \tilde{\psi}(-p)$	$\psi(x)$ imaginary: $[\tilde{\psi}(p)]^* = -\tilde{\psi}(-p)$
$\Delta x \Delta p \geq \hbar$	

Commutators

Key points

- When a matrix has a block form, we can compute the eigenvalues in each block submatrix.
- The eigenpairs allows you to diagonalize $A = V\Lambda V^{-1}$ in the eigenbasis, where $V = [\boldsymbol{u}_1\vert\boldsymbol{u}_2\vert\cdots]$, $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \cdots)$, and $A\lvert\boldsymbol{u}_i\rangle = \lambda_i\lvert\boldsymbol{u}_i\rangle$. In the eigenbasis we can do $F(A) = VF(\Lambda)V^{-1}$.
- When A is Hermitian, V is unitary: $V^{-1} = V^\dagger$.

$[A,B]=-[B,A]$	$[A+B,C+D]=[A,C]+[A,D]+[B,C]+[B,D]$
$[A,B]^\dagger=[B^\dagger,A^\dagger]$	$[F(A),A]=0$
$[AB,CD]=A[B,C]D+AC[B,D]+[A,C]DB+C[A,D]B$	$[A,B]=0 \Longrightarrow [F(A),B]=[A,F(B)]=[F(A),F(B)]=0$
$[A,[B,C]]+[B,[C,A]]+[C,[A,B]]=0$	$[A,[A,B]]=[B,[A,B]]=0 \Longrightarrow [A,F(B)]=[A,B]\frac{dF(B)}{dB}$
$e^Ae^B=e^{A+B}e^{\frac{1}{2}[A,B]}$ $([A,[A,B]]=[B,[A,B]]=0)$	$[A,[A,B]]=[B,[A,B]]=0 \Longrightarrow [F(A),B]=[A,B]\frac{dF(A)}{dA}$
$[X,P]=i\hbar$	$[H,X]=-\frac{i\hbar}{m}P$
$[H,P]=i\hbar\frac{dV(X)}{dX}$	$\langle\varphi_n\|[A,H]\|\varphi_n\rangle=0,\ \forall A$

- If the matrix is diagonal, the exponential acts directly onto the elements.
- The evolution operator is $U=e^{-iHt/\hbar}$ and it evolves the state by matrix multiplication $U|\psi\rangle$.
- The eigenequation show you the relation of the eigenvectors that must be considered to construct the eigenvectors of the eigenbasis: $A|u_i\rangle=\lambda|u_j\rangle$. Its matrix representation is λ in the ji position.
- You can reduce the dimension of an operator to its eigensubspace when only acting inside it.
- To know the action of an operator you can stimulate it by applying $|\psi\rangle$ or $\langle\psi|$.
- In the operation $|u_i\rangle\langle u_j|$, the element will be located at ij in the matrix.
- Conservative=H time-independent, Stationary state=$|\psi\rangle$ projects in a single eigenstate of H.
- Constant of motion=A time-independent and $[A,H]=0$.

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