

Notes of Quantum Mechanics

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Preface

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1.1 Introduction

1.1.1 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:

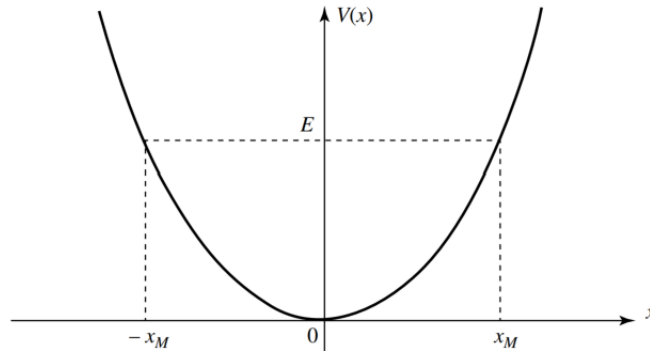


Figure 1.1 Potential energy $V(x)$ of a 1D harmonic oscillator.

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

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.

1.1.2 The harmonic oscillator in classical mechanics

The motion of the particle is governed by the dynamics equation

$$m \frac{d^2x}{dt^2} = -\frac{dV}{dx} = -kx \longrightarrow x = x_M \cos(\omega t - \varphi). \quad (1.1)$$

The kinetic energy of the particle is

$$T = \frac{1}{2}m \left(\frac{dx}{dt} \right)^2 = \frac{p^2}{2m}, \quad (1.2)$$

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

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

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

$$V(x) = \underbrace{V(x_0)}_a + \underbrace{V'(x_0)(x - x_0)}_b + \underbrace{\frac{1}{2!}V^{(2)}(x_0)(x - x_0)^2}_c + \frac{1}{3!}V^{(3)}(x_0)(x - x_0)^3 + \dots$$

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

$$F_x = -\frac{dV}{dx} = -2b(x - x_0) - 3c(x - x_0)^2 + \dots \quad (1.3)$$

The point $x = x_0$ is a stable equilibrium for the particle: $F_x(x_0) = 0$. In addition, 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**.

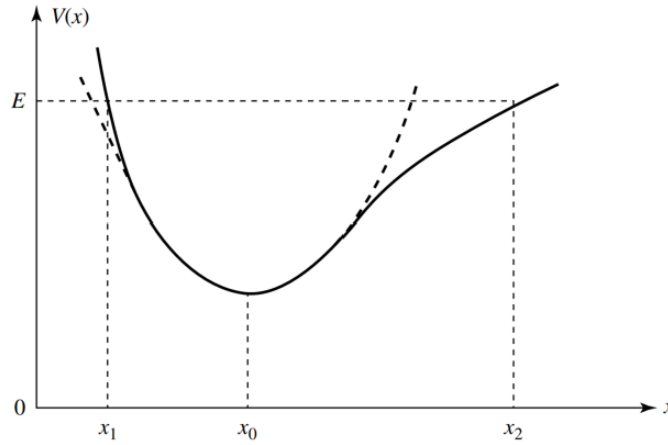


Figure 1.2 Any potential can be approximated by a parabolic potential. In $V(x)$, a classical particle of energy E oscillates between x_1 and x_2 .

1.1.3 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

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

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 states are necessarily either even or odd.
- **The energy spectrum is discrete.**

1.2 Eigenvalues of the Hamiltonian

1.2.1 Notation

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

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

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

$$\text{Canonical commutation} \quad [\hat{X}, \hat{P}] = i \quad (1.4)$$

and the Hamiltonian can be put in the form

$$H = \hbar\omega \hat{H}, \quad \text{with} \quad \hat{H} = \frac{1}{2}(\hat{X}^2 + \hat{P}^2). \quad (1.5)$$

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 introduction of operators proportional to $\hat{H} \pm i\hat{P}$ enables us to simplify considerably our search for eigenvalues and eigenvectors of \hat{H} . We therefore set

$$\begin{aligned} a &= \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) & \hat{X} &= \frac{1}{\sqrt{2}}(a^\dagger + a) \\ a^\dagger &= \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}) & \hat{P} &= \frac{i}{\sqrt{2}}(a^\dagger - a) \end{aligned} \quad \Longleftrightarrow \quad (1.6)$$

The commutator of a and a^\dagger is

$$[a, a^\dagger] = \frac{1}{2}[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}] = \frac{i}{2}[\hat{P}, \hat{X}] - \frac{i}{2}[\hat{X}, \hat{P}] = 1 \longrightarrow [a, a^\dagger] = 1. \quad (1.7)$$

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

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

We see that we cannot put \hat{H} in a product of linear terms, due to the non-commutativity of \hat{X} and \hat{P} (1/2 term).

We introduce another operator:

$$\text{Operator } N \quad N = a^\dagger a. \quad (1.8)$$

This operator is Hermitian

$$N^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = N. \quad (1.9)$$

And its relation with \hat{H} is

$$\hat{H} = N + \frac{1}{2} \quad (1.10)$$

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

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a \longrightarrow [N, a] = -a \quad (1.11)$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger [a, a^\dagger] + [a^\dagger, a^\dagger]a = a^\dagger \longrightarrow [N, a^\dagger] = a^\dagger. \quad (1.12)$$

The study of the harmonic oscillator is based on these operators a , a^\dagger , and N . The eigenequation for N is

$$\text{Eigenequation of } N \quad N|\varphi_\nu^i\rangle = \nu|\varphi_\nu^i\rangle. \quad (1.13)$$

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

$$H|\varphi_\nu^i\rangle = (\nu + 1/2)\hbar\omega|\varphi_\nu^i\rangle. \quad (1.14)$$

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

1.2.2 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 at the square of the norm of the vector $a|\varphi_\nu^i\rangle$

$$\|a|\varphi_\nu^i\rangle\|^2 = \langle\varphi_\nu^i|a^\dagger a|\varphi_\nu^i\rangle = \langle\varphi_\nu^i|N|\varphi_\nu^i\rangle = \nu\langle\varphi_\nu^i|\varphi_\nu^i\rangle \geq 0 \implies \nu \geq 0.$$

- **Properties of the vector $a|\varphi_\nu^i\rangle$**

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

$$a|\varphi_0^i\rangle = 0. \quad (1.15)$$

Any vector which satisfies this relation is therefore an eigenvector of N with the eigenvalue $\nu = 0$.

- $\nu > 0 \implies a|\varphi_\nu^i\rangle$ is a non-zero eigenvector of N with eigenvalue $\nu - 1$.

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

- **Properties of the vector $a^\dagger|\varphi_\nu^i\rangle$**

- $a^\dagger|\varphi_\nu^i\rangle$ 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.

- $a^\dagger|\varphi_\nu^i\rangle$ is an eigenvector of N with eigenvalue $N + 1$. We do it analogously to lemma 1b):

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

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

$$\text{Eigenvalue of } H \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad n \in \mathbb{N}_0^+. \quad (1.16)$$

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.

1.2.3 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

$$\varphi_0^i(x) = ce^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} \quad (1.17)$$

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

All the states are non-degenerate

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

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

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

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

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

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

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

We have,

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

We see that all kets $|\varphi_{n+1}^i\rangle$ associated with the eigenvalue $n + 1$ are proportional to $a^\dagger|\varphi_n\rangle$. They are proportional to each other: the eigenvalue $n + 1$ is not degenerate.

Since the eigenvalue $n = 0$ is not degenerate, the eigenvalue $n = 1$ is not either, nor is $n = 2$, etc.: all the eigenvalues of N and, consequently, all those of H , are non-degenerate. Now, we can just write $|\varphi_n\rangle$ for the eigenvector of H associated with E_n .

1.3 Eigenstates of the Hamiltonian

1.3.1 The $\{\varphi_n\}$ representation

Since none of the eigenvalues of N (H) is degenerate, N (H) alone constitutes a CSCO in \mathcal{E}_c .

The basis vectors in terms of $|\psi_0\rangle$

We assume that the vector $|\varphi_0\rangle$ which satisfies $a|\varphi_0\rangle = 0$, 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 be 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 $c_1 = 1$:

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2 = 1 \implies |\varphi_1\rangle = a^\dagger|\varphi_0\rangle. \quad (1.18)$$

We can do the same to construct $|\varphi_2\rangle$ 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:

$$\text{Excited states in terms of the ground state} \quad |\varphi_n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |\varphi_0\rangle. \quad (1.19)$$

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 observable; the set of the $|\varphi_n\rangle$ therefore constitutes a basis in \mathcal{E}_x , which is expressed by the closure relation

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

Equating both side results:

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

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:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (1.27)$$

1.3.2 Wave functions associated with the stationary states

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

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

To obtain the functions $\varphi_n(x)$, all we need to do is use expression (1.19) and the fact that in $\{|x\rangle\}$ a^\dagger is represented by

$$\frac{1}{\sqrt{2}} \left[\sqrt{\frac{m\omega}{\hbar}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} \right]. \quad (1.28)$$

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

$$\varphi_n(x) = \langle x | \varphi_n(x) \rangle = \frac{1}{\sqrt{n!}} \langle x | (a^\dagger)^n | \varphi_0 \rangle = \frac{1}{\sqrt{n!}} \frac{1}{\sqrt{2^n}} \left[\sqrt{\frac{m\omega}{\hbar}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} \right]^n \varphi_0(x). \quad (1.29)$$

That is,

$$\text{Excited state} \quad \varphi_n(x) = \underbrace{\left[\frac{1}{2^n n!} \left(\frac{\hbar}{m\omega} \right)^n \right]^{1/2} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \left[\frac{m\omega}{\hbar} x - \frac{d}{dx} \right]^n}_{\text{Hermite polynomial}} e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2}. \quad (1.30)$$

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 implies that the mean kinetic energy of the particle increases with n .

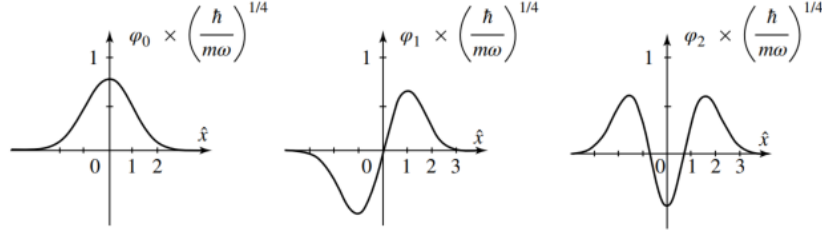


Figure 4: Wave functions associated with the first three levels of a harmonic oscillator.

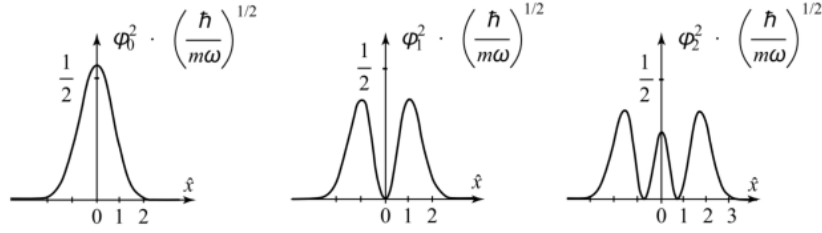


Figure 5: Probability densities associated with the first three levels of a harmonic oscillator.

1.4 Discussion

1.4.1 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 (1.22), which show that neither X nor P has diagonal matrix elements:

$$\langle \varphi_n | X | \varphi_n \rangle = \langle \varphi_n | P | \varphi_n \rangle = 0. \quad (1.31)$$

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:

$$(\Delta X)^2 = \langle \varphi_n | X | \varphi_n \rangle - \langle \varphi_n | X^2 | \varphi_n \rangle = \langle \varphi_n | X^2 | \varphi_n \rangle = \left(n + \frac{1}{2}\right) \frac{\hbar}{m\omega} = \sigma^2 \left(x + \frac{1}{2}\right). \quad (1.32)$$

$$(\Delta P)^2 = \langle \varphi_n | P | \varphi_n \rangle - \langle \varphi_n | P^2 | \varphi_n \rangle = \langle \varphi_n | P^2 | \varphi_n \rangle = \left(n + \frac{1}{2}\right) m\hbar\omega = \frac{\hbar^2}{\sigma^2} \left(x + \frac{1}{2}\right). \quad (1.33)$$

The product is therefore

$$\text{Uncertainty relation} \quad \Delta X \Delta P = \left(n + \frac{1}{2}\right) \hbar. \quad (1.34)$$

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

1.4.2 Properties of the ground state

In classical mechanics, the lowest energy of the harmonic oscillator is obtained when the particle is at rest. In QM, the minimum energy state is $|\varphi_0\rangle$, whose energy is not zero, and the associated wave function has a certain spatial extension, characterized by the rms deviation $\Delta X = \sqrt{\hbar/2m\omega}$. The ground state corresponds to a compromise 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.

1.4.3 Time evolution of the mean values

Consider the state at $t = 0$

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

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

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n(0) e^{-iE_n t/\hbar} |\varphi_n\rangle = \sum_{n=0}^{\infty} c_n(0) e^{-i(n+1/2)\omega t} |\varphi_n\rangle. \quad (1.35)$$

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 harmonic 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 $e^{\pm i\omega t}$. Moreover, the form of the harmonic oscillator potential implies that for all $|\varphi_n\rangle$ the mean values of X and P rigorously satisfy the classical equations of motion. Using Ehrenfest theorem:

$$\begin{aligned} \frac{d}{dt} \langle X \rangle &= \frac{1}{i\hbar} \langle [X, H] \rangle = \frac{\langle P \rangle}{m} & \xrightarrow{\int dt} \quad \langle X \rangle(t) &= \langle X \rangle(0) \cos \omega t + \frac{1}{m\omega} \langle P \rangle(0) \sin \omega t \\ \frac{d}{dt} \langle P \rangle &= \frac{1}{i\hbar} \langle [P, H] \rangle = -m\omega^2 \langle X \rangle & \langle P \rangle(t) &= \langle P \rangle(0) \cos \omega t + m\omega \langle X \rangle(0) \sin \omega t \end{aligned} \quad (1.36)$$

- 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.

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

1.5.1 Hermite polynomials

Definition

Let be the Gaussian function

$$F(z) = e^{-z^2} \quad (1.37)$$

The successive derivatives are

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

If we have $F^{(n-1)}$, its differentiation will yields $F^{(n)}$ and we can obtain the above general equation:

$$H_n(z) = \left(2z - \frac{d}{dz}\right) H_{n-1}(z), \quad (1.38)$$

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

$$\text{Hermite polynomial} \quad H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}. \quad (1.39)$$

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

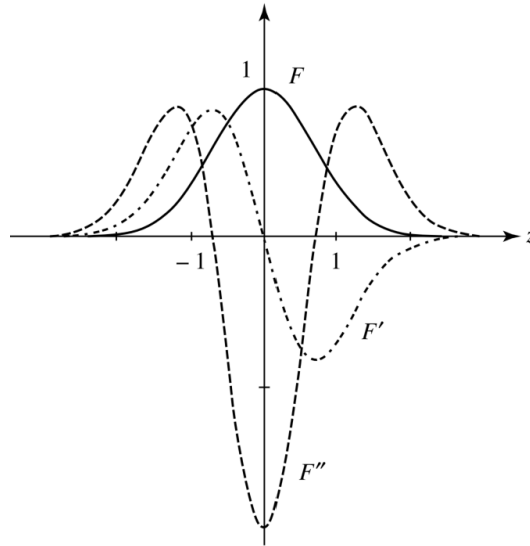


Figure 1.1 Shape of the Gaussian function $F(z)$ and its first and second derivatives.

Generating function

Consider the function

$$F(z + \lambda) = e^{-(z+\lambda)^2} \stackrel{\text{Taylor}}{=} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} F^{(n)}(z) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (-1)^n H_n(z) e^{-z^2}.$$

Multiplying this relation by e^{z^2} and replacing λ by $-\lambda$ we obtain:

$$\text{Generating function of Hermite polynomials} \quad e^{z^2} F(z - \lambda) = e^{-\lambda^2 + 2\lambda z} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} H_n(z). \quad (1.40)$$

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

Recurrence relations; differential equation

We can obtain other recurrence relation by using the equation (1.40). For instance, differentiating equation (1.40) with respect to z and using its expansion:

$$\frac{d}{dz} H_n(z) = 2n H_{n-1}(z). \quad (1.41)$$

If we differentiate with respect to λ , we get

$$H_n(z) = 2z H_{n-1}(z) - 2(n-1) H_{n-2}(z). \quad (1.42)$$

Finally, we can obtain an ODE differentiating equation (1.41) and using (1.38):

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

Thus,

$$\text{ODE satisfied by Hermite polynomials} \quad \left[\frac{d^2}{dz^2} - 2z \frac{d}{dz} + 2n \right] H_n(z) = 0. \quad (1.43)$$

1.5.2 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

$$\varphi_0(x) = c e^{-\frac{x^2}{2\sigma^2}} \xrightarrow{\text{normalization}} \varphi_0(x) = \left(\frac{1}{\pi\sigma^2} \right)^{1/4} e^{-\frac{x^2}{2\sigma^2}}.$$

The general form is the following:

$$\text{Excited state in } \{|x\rangle\} \quad \varphi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\beta^2 x^2/2} H_n(\beta x). \quad (1.44)$$

The shape of $\varphi_n(x)$ is therefore analogous to that of the n th-order derivative of the Gaussian function $F(x)$. Moreover, $\varphi_n(x)$ is of parity $(-1)^n$ and possesses 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 (1.20) in the $\{|x\rangle\}$ representation. The action of them in this representation is

$$a \longrightarrow \frac{\beta}{\sqrt{2}} \left[x + \frac{1}{\beta^2} \frac{d}{dx} \right] \quad a^\dagger \longrightarrow \frac{\beta}{\sqrt{2}} \left[x - \frac{1}{\beta^2} \frac{d}{dx} \right]. \quad (1.45)$$

Then equation (1.20) becomes:

$$\begin{aligned} \text{Action of } a, a^\dagger \text{ in } \{|x\rangle\} \quad & \frac{\beta}{\sqrt{2}} \left[x + \frac{1}{\beta^2} \frac{d}{dx} \right] \varphi_n(x) = \sqrt{n} \varphi_{n-1}(x) \\ & \frac{\beta}{\sqrt{2}} \left[x - \frac{1}{\beta^2} \frac{d}{dx} \right] \varphi_n(x) = \sqrt{n+1} \varphi_{n+1}(x) \end{aligned} \quad (1.46)$$

Taking the sum and difference:

$$\begin{aligned} x\beta\sqrt{2}\varphi_n(x) &= \sqrt{n}\varphi_{n-1}(x) + \sqrt{n+1}\varphi_{n+1}(x) \\ \frac{\sqrt{2}}{\beta} \frac{d}{dx} \varphi_n(x) &= \sqrt{n}\varphi_{n-1}(x) - \sqrt{n+1}\varphi_{n+1}(x) \end{aligned}$$

Replacing in them the function $\varphi_n(x)$ of equation x yields two recursive equations for $H(x)$ (setting $\hat{x} = \beta x$):

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

1.6 The isotropic three-dimensional harmonic oscillator

The main idea is the same, but here there is an extension of the problem.

The spinless particle of mass m is subjected to a central force

$$\mathbf{F} = -k\mathbf{r}. \quad (1.47)$$

This force is derived from the potential energy:

$$V(\mathbf{r}) = \frac{1}{2}k\mathbf{r}^2 = \frac{1}{2}m\omega^2\mathbf{r}^2, \quad \omega = \sqrt{\frac{k}{m}}. \quad (1.48)$$

The classical Hamiltonian is therefore:

$$\text{Classical Hamiltonian} \quad \mathcal{H}(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2 \mathbf{r}^2. \quad (1.49)$$

Using the quantization rules, we get the Hamiltonian operator:

$$\text{Hamiltonian operator} \quad H = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega^2 \mathbf{R}^2. \quad (1.50)$$

Since the Hamiltonian is time-independent, we shall solve its eigenequation $H|\psi\rangle = E|\psi\rangle$, where $|\psi\rangle \in \mathcal{E}_{\mathbf{r}}$ the state space of the particle in three-dimensional space.

Isotropic QHO

Due to $V(\mathbf{r})$ only depends on the distance $r = |\mathbf{r}|$ of the particle from the origin (invariant to rotations), this harmonic oscillator is said to be **isotropic**.

$$V(\mathbf{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (1.51)$$

It is defined by a single frequency $\omega = \omega_x = \omega_y = \omega_z$.

1.6.1 Separation of variables in cartesian coordinates

We assume the state space is a separable function so that:

$$\mathcal{E}_{\mathbf{r}} = \mathcal{E}_x \otimes \mathcal{E}_y \otimes \mathcal{E}_z. \quad (1.52)$$

The expression for the Hamiltonian is therefore

$$H = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega(Z^2 + Y^2 + Z^2) = H_x + H_y + H_z, \quad \text{with} \quad H_k = \frac{P_k^2}{2m} + \frac{1}{2}m\omega^2 R_k^2. \quad (1.53)$$

Each operator acts in its own state space \mathcal{E}_k . H_x, H_y, H_z commute, and also with the sum H . Consequently, the eigenequation can be solved by seeking the eigenvectors of H that are also eigenvectors of H_x, H_y, H_z :

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

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

$$|\psi_{n_x, n_y, n_z}\rangle = |\varphi_{n_x}\rangle |\varphi_{n_y}\rangle |\varphi_{n_z}\rangle. \quad (1.54)$$

According to the above Hamiltonian and the eigenequations, we have

$$H|\psi_{n_x, n_y, n_z}\rangle = E_{n_x, n_y, n_z}|\psi_{n_x, n_y, n_z}\rangle = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega|\psi_{n_x, n_y, n_z}\rangle. \quad (1.55)$$

The eigenvectors of H are seen to be the **tensor product** of the eigenvectors of H_x, H_y, H_z while the eigenvalues of H to be the **sum** of eigenvalues of these operators. The energy levels E_n of the isotropic 3D QHO are of the form:

$$\text{Energy levels} \quad E_n = \left(n + \frac{3}{2}\right) \hbar\omega, \quad n = n_x + n_y + n_z \in \mathbb{N}_0^+. \quad (1.56)$$

The a operators are defined analogously:

$$\text{Operator } a \text{ and } a^\dagger \quad \begin{aligned} a_j &= \frac{1}{\sqrt{2}} \left(\frac{R_j}{\sigma_j} + \frac{iP_j\sigma_j}{\hbar} \right) \\ a_j^\dagger &= \frac{1}{\sqrt{2}} \left(\frac{R_j}{\sigma_j} - \frac{iP_j\sigma_j}{\hbar} \right) \end{aligned}, \quad \text{with} \quad [a_i, a_j^\dagger] = \delta_{ij}. \quad (1.57)$$

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

$$a_x |\psi_{n_x, n_y, n_z}\rangle = (a_x |\varphi_{n_x}\rangle) |\varphi_{n_y}\rangle |\varphi_{n_z}\rangle = \sqrt{n_x} |\varphi_{n_x-1}\rangle |\varphi_{n_y}\rangle |\varphi_{n_z}\rangle = \sqrt{n_x} |\varphi_{n_x-1, n_y, n_z}\rangle \quad (1.58)$$

$$a_x^\dagger |\psi_{n_x, n_y, n_z}\rangle = (a_x^\dagger |\varphi_{n_x}\rangle) |\varphi_{n_y}\rangle |\varphi_{n_z}\rangle = \sqrt{n_x + 1} |\varphi_{n_x+1}\rangle |\varphi_{n_y}\rangle |\varphi_{n_z}\rangle = \sqrt{n_x + 1} |\varphi_{n_x+1, n_y, n_z}\rangle. \quad (1.59)$$

And for the other dimensions is analogous. We also know that

$$|\varphi_{n_x}\rangle = \frac{1}{\sqrt{n_x!}} (a_x^\dagger)^{n_x} |\varphi_0\rangle, \quad a_x \in \mathcal{E}_x : \quad a_x |\varphi_0\rangle = 0.$$

In \mathcal{E}_y and \mathcal{E}_z we have something similar. Consequently, we can write

$$\text{Excited state} \quad |\psi_{n_x, n_y, n_z}\rangle = \frac{1}{\sqrt{n_x! n_y! n_z!}} (a_x^\dagger)^{n_x} (a_y^\dagger)^{n_y} (a_z^\dagger)^{n_z} |\psi_{0,0,0}\rangle, \quad (1.60)$$

where $|\psi_{0,0,0}\rangle$ is the tensor product of the ground states of each dimension:

$$a_x |\psi_{0,0,0}\rangle = a_y |\psi_{0,0,0}\rangle = a_z |\psi_{0,0,0}\rangle = 0.$$

Finally, the associated wave functions is of the form

$$\langle \mathbf{r} | \psi_{n_x, n_y, n_z} \rangle = \langle z | \langle y | \langle x | \varphi_{n_z} \rangle | \varphi_{n_y} \rangle | \varphi_{n_x} \rangle = \varphi_{n_x}(x) \varphi_{n_y}(y) \varphi_{n_z}(z), \quad (1.61)$$

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

$$\langle \mathbf{r} | \psi_{0,0,0} \rangle = \left(\frac{1}{\pi\sigma^2} \right)^{3/4} e^{-\frac{1}{2\sigma^2}(x^2+y^2+z^2)}, \quad \omega = \omega_x = \omega_y = \omega_z. \quad (1.62)$$

1.6.2 Degeneracy of the energy levels

We have that $\{H_x, H_y, H_z\}$ constitutes a CSCO in \mathcal{E}_r (Others CSCOs are $\{H_x, H_y, H\}, \{X, P_y, H_z\}$) so that there exists a unique ket $|\psi_{n_x, n_y, n_z}\rangle$ corresponding to a given set of eigenvalues for H_x, H_y, H_z . However, H alone does not form a CSCO since the energy levels E_n are **degenerate**. Choosing an eigenvalue of H , $E_n = (n + 3/2)\hbar\omega$, all the kets $\{|\psi_{n_x, n_y, n_z}\rangle\}$ basis that satisfy

$$n_x + n_y + n_z = n$$

are eigenvectors of H with eigenvalue E_n . The degree of degeneracy g_n of E_n is equal to the number of different sets $\{n_x, n_y, n_z\}$ satisfying the above equation. It is equal then to

$$\text{Degree of degeneracy of } E_n \quad g_n = \frac{(n+1)(n+2)}{2}. \quad (1.63)$$

Therefore, only the ground state $E_n = 3\hbar\omega/2$ is non-degenerate.

Ejemplo 1.1

Measurements of energies

- a) Measurement with H and result is $\hbar\omega(1 + 3/2)$, then $n_x + n_y + n_z = 1$.
- b) Measurement with H_x and result is $n_x = 0$, then $n_y + n_z = 1$.
- c) Measurement with H_z and result is $n_z = 1$, then $n_y = 0$.

Therefore, the state is

$$|0, 0, 1\rangle = |n_x = 0, n_y = 0, n_z = 1\rangle.$$

1.7 Coherent states of the harmonic oscillator

We know that quantum mechanics must yield the same results as classical mechanics in the limiting case where the harmonic oscillator has an energy much greater than the quantum $\hbar\omega$.

It is possible to construct quantum mechanics states leading to physical predictions which are almost identical to the classical ones, at least for a macroscopic oscillator? Such quantum systems do exist: they are coherent linear superpositions of all the states $|\varphi_n\rangle$. We shall call them **quasi-classical states** or coherent states of the harmonic oscillator.

It is important to understand, in the framework of quantum mechanics, how to move gradually from the case in which the results given by the classical approximation are sufficient to the case in which quantum effects are preponderant.

The position, momentum, and energy of a harmonic oscillator are described in QM by operators which do not commute. It is not possible to construct a state in which they are all perfectly well-defined.

Therefore, we shall only look for a state vector such that for all t , the mean values $\langle X \rangle$, $\langle P \rangle$, and $\langle H \rangle$ are as close as possible to the corresponding classical values: the compromise is then that none of these three observables is perfectly known. Nevertheless, the rms deviation ΔX , ΔY , and ΔH are, in the macroscopic limit, completely negligible.

1.7.1 Quasi-classical states

Introducing α_0 to characterize a classical motion

The classical quantities of motion of a 1D harmonic oscillator of mass m and angular frequency ω are

$$\text{Equations of motion for CHO} \quad \begin{aligned} \frac{d}{dt}x(t) &= \frac{1}{m}p(t) \\ \frac{d}{dt}p(t) &= -m\omega^2x(t) \end{aligned}. \quad (1.64)$$

The classical state of the HO is determined at time t when we know its position $x(t)$ and its momentum $p(t)$. We shall therefore combine them into a single complex number $\alpha(t)$ given by:

$$\text{Displacement coordinate} \quad \alpha(t) = \frac{1}{\sqrt{2}} \left(\frac{x(t)}{\sigma} + i \frac{\sigma p(t)}{\hbar} \right) \quad (-). \quad (1.65)$$

Then, the equations of motions turn to

$$\frac{d}{dt}\alpha(t) = -i\omega\alpha(t) \longrightarrow \alpha(t) = \alpha_0 e^{-i\omega t}, \quad \alpha_0 = \alpha(0) \quad (1.66)$$

We can plot this evolution in a geometrical representation of the evolution of the state of the system through the **phase-space diagram** as shown in the following figure. According to the solution of the

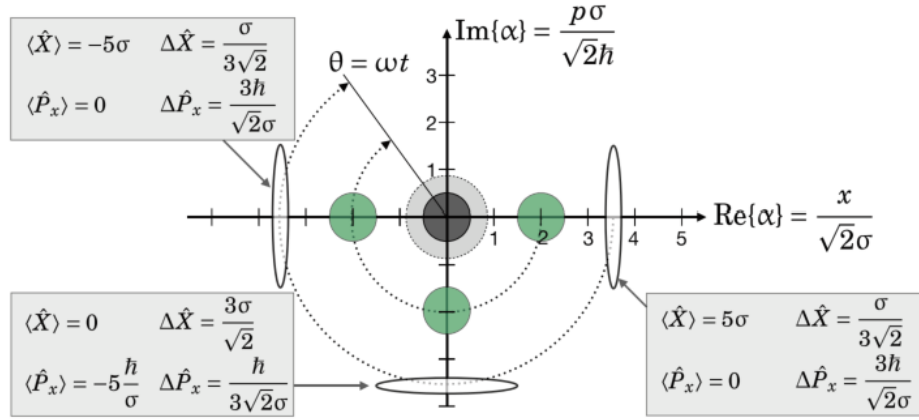


Figure 1.1 Illustration of four HO states in the phase-space diagram: black=ground state, gray=first excited state, ovals=squeezed state, green=coherent state.

ODE, we have

$$x(t) = \frac{1}{\sqrt{2}}(\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t}), \quad p(t) = -\frac{i}{\sqrt{2}}(\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t}). \quad (1.67)$$

As for the classical energy \mathcal{H} of the system, it is constant in time and equal to:

$$\mathcal{H} = \frac{1}{2m}p(0)^2 + \frac{1}{2}m\omega^2 x(0)^2 = \frac{\hbar\omega}{2} \left[\left(\frac{x(0)}{\sigma} \right)^2 + \left(\frac{\sigma p(0)}{\hbar} \right)^2 \right] = \hbar\omega |\alpha_0|^2.$$

For a macroscopic oscillator, the energy \mathcal{H} is much greater than the quantum $\hbar\omega$, so

$$\text{Macroscopic regime} \quad |\alpha_0| \gg 1. \quad (1.68)$$

Conditions defining quasi-classical states

We are looking for a quantum mechanical state for which at every instant the mean values $\langle X \rangle$, $\langle P \rangle$, and $\langle H \rangle$ are practically equal to the values of x , p , and \mathcal{H} which correspond to a given classical motion.

The time evolution of the matrix element $\langle a \rangle(t) = \langle \psi(t) | a | \psi(t) \rangle$ is given by

$$i\hbar \partial_t \langle a \rangle(t) = \langle [a, H] \rangle(t)$$

The commutator is $[a, H] = [a, a^\dagger a] = \hbar\omega a$, which implies that the solution of the above ODE is

$$\langle a \rangle(t) = \langle a \rangle(0)e^{-i\omega t}. \quad (1.69)$$

The evolution of $\langle a^\dagger \rangle(t)$ satisfies the adjoint equation:

$$\langle a^\dagger \rangle(t) = \langle a^\dagger \rangle(0)e^{i\omega t} = \langle a \rangle^*(0)e^{i\omega t}.$$

The equation (1.69) is analogous to equation (1.66). We can substitute $\langle a \rangle(t)$ and $\langle a^\dagger \rangle(t)$ in the mean value of X and P to get:

$$\langle X \rangle(t) = \frac{1}{\sqrt{2}}(a + a^\dagger) = \frac{1}{\sqrt{2}}[\langle a \rangle(0)e^{-i\omega t} + \langle a \rangle^*(0)e^{i\omega t}] \quad (1.70)$$

$$\langle P \rangle(t) = \frac{i}{\sqrt{2}}(a^\dagger - a) = \frac{i}{\sqrt{2}}[\langle a \rangle^*(0)e^{i\omega t} - \langle a \rangle(0)e^{-i\omega t}] \quad (1.71)$$

It is necessary and sufficient to set at $t = 0$ the condition $\langle a \rangle(0) = \alpha_0$, which resembles to the classical motion. The normalized state vector $|\psi(t)\rangle$ of the oscillator must therefore satisfy the condition

$$\text{First condition} \quad \langle \psi(0) | a | \psi(0) \rangle = \alpha_0.$$

We must now require the mean value

$$\langle H \rangle = \hbar\omega \langle a^\dagger a \rangle(0) + \frac{\hbar\omega}{2} \quad (1.72)$$

to be equal to the classical energy \mathcal{H} . Given that for a classical oscillator $|\alpha_0|$ is much greater than 1, we shall neglect the term $\hbar\omega/2$ with respect to $\hbar\omega|\alpha_0|^2$. The second condition on the state vector can now be written:

$$\text{Second condition} \quad \langle \psi(0) | a^\dagger a | \psi(0) \rangle = |\alpha_0|^2. \quad (1.73)$$

The two conditions are sufficient to determine the normalized state vector $|\psi(0)\rangle$.

Quasi-classical states are eigenvectors of the operator a

If a normalized vector $|\psi(0)\rangle$ satisfy the relation

$$a|\psi(0)\rangle = \alpha_0|\psi(0)\rangle, \quad (1.74)$$

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

$$\text{Eigenvector of } a \text{ with eigenvalue } \alpha \quad a|\alpha\rangle = \alpha|\alpha\rangle. \quad (1.75)$$

1.7.2 Properties of the $|\alpha\rangle$ states

Expansion of $|\alpha\rangle$ on the basis of the stationary states $|\varphi_n\rangle$

Let us determine the ket $|\alpha\rangle$ which is a solution of (1.74) by using an expansion on $|\varphi_n\rangle$:

$$|\alpha\rangle = \sum_n c_n(\alpha) |\varphi_n\rangle.$$

We then have

$$a|\alpha\rangle = \sum_n c_n(\alpha) \sqrt{n} |\varphi_{n-1}\rangle$$

and, substituting this into (1.75) yields

$$c_{n+1}(\alpha) = \frac{\alpha}{\sqrt{n+1}} c_n(\alpha).$$

This relation enable us to determine by recurrence all the coefficient $c_n(\alpha)$ in terms of $c_0(\alpha)$:

$$c_n(\alpha) = \frac{\alpha^n}{\sqrt{n!}} c_0(\alpha). \quad (1.76)$$

When $c_0(\alpha)$ is fixed, all the $c_n(\alpha)$ are also fixed. The vectoeer $|\alpha\rangle$ is therefore unique. We shall choose $c_0(\alpha)$ real, positive and normalized with $|\alpha\rangle$, which determines it completely:

$$\sum_n |c_n(\alpha)|^2 = |c_0(\alpha)|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = |c_0(\alpha)|^2 e^{|\alpha|^2} = 1. \quad (1.77)$$

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

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |\varphi_n\rangle. \quad (1.78)$$

This result was also obtained by Cris displacing the $|\varphi_0\rangle$ from the origin by x_0 (lecture 14). It began with $|\psi\rangle = S(x_0)|\varphi_0\rangle$ and got some expression. Then, we replaced $|\psi\rangle$ by $|\alpha\rangle$ with the corresponding transformation: $\alpha = x_0/(\sqrt{2}\sigma)$.

Possible values of the energy in an $|\alpha\rangle$ state

Assuming an oscillator in the state $|\alpha\rangle$, we see from (1.78) that a measurement of the energy can yield the result $E_n = (n + 1/2)\hbar\omega$ with the probability:

$$\text{Probability of having } E_n \quad P_n(\alpha) = |\langle\alpha|\varphi_n\rangle|^2 = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2}. \quad (1.79)$$

The probability obtained corresponds to a **Poisson distribution**. We have from its a recurrence relation:

$$P_n(\alpha) = \frac{|\alpha|^2}{n} P_{n-1}(\alpha).$$

$P_n(\alpha)$ reaches its maximum when n is the integral part of $|\alpha|^2$.

Calculation of mean values and uncertainties

The mean value can be obtaines expressing them in terms of the a operators, and using (1.78):

$$\begin{aligned} \langle X \rangle_\alpha &= \langle \alpha | X | \alpha \rangle = \sqrt{2}\sigma \text{Re}(\alpha), & \langle X^2 \rangle_\alpha &= \frac{\sigma^2}{2} [(\alpha + \alpha^*)^2 + 1] \\ \langle P \rangle_\alpha &= \langle \alpha | P | \alpha \rangle = \frac{\sqrt{2}\hbar}{\sigma} \text{Im}(\alpha), & \langle P^2 \rangle_\alpha &= \frac{m\hbar\omega}{2} [1 - (\alpha - \alpha^*)^2] \\ \langle N \rangle_\alpha &= \langle \alpha | N | \alpha \rangle = |\alpha|^2, & \langle N^2 \rangle_\alpha &= - \\ \langle H \rangle_\alpha &= \langle \alpha | H | \alpha \rangle = \hbar\omega [|\alpha|^2 + \tfrac{1}{2}], & \langle H^2 \rangle_\alpha &= \hbar^2\omega^2 [|\alpha|^4 + 2|\alpha|^2 + \tfrac{1}{4}] \end{aligned} \quad (1.80)$$

Therefore, we have:

$$\Delta X_\alpha = \frac{\sigma}{\sqrt{2}}, \quad \Delta P_\alpha = \frac{\hbar}{\sqrt{2}\sigma}, \quad \Delta N_\alpha = |\alpha|, \quad \Delta H_\alpha = \hbar\omega|\alpha|. \quad (1.81)$$

The XP uncertainty relation is therefore:

$$\Delta X_\alpha \Delta P_\alpha = \frac{\hbar}{2}. \quad (1.82)$$

The displacement operator $D(\alpha)$

Let be the operator define by

$$\text{Displacement operator} \quad D(\alpha) = T(\langle X \rangle) S(\langle P \rangle) e^{i\langle X \rangle \langle P \rangle / \hbar} = e^{\alpha a^\dagger - \alpha^* a}. \quad (1.83)$$

This operator is unitary since

$$D^\dagger(\alpha) = e^{\alpha^* a - \alpha a^\dagger} \implies D(\alpha) D^\dagger(\alpha) = D^\dagger(\alpha) D(\alpha) = 1.$$

The argument of the exponential can be defined with the commutator $[\alpha a^\dagger, -\alpha^* a] = \alpha^* \alpha$ so that using the Glauber formula for exponential yields:

$$D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a}$$

Now, the action of $D(\alpha)$ into a ket $|\varphi_0\rangle$ can be considered by parts. First,

$$e^{-\alpha^* a} |\varphi_0\rangle = \left[1 - \alpha^* a + \frac{\alpha^{*2}}{2!} a^2 + \dots \right] |\varphi_0\rangle = |\varphi_0\rangle.$$

Because it returns the same ket, we are left with the second exponential:

$$D(\alpha) |\varphi_0\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |\varphi_0\rangle = e^{-|\alpha|^2/2} \sum_n \frac{(\alpha a^\dagger)^n}{n!} |\varphi_0\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |\varphi_n\rangle.$$

Comparing with (1.78) we have

$$|\alpha\rangle = D(\alpha) |\varphi_0\rangle. \quad (1.84)$$

$D(\alpha)$ is therefore the unitary transformation which transforms the ground state $|\varphi_0\rangle$ into the quasi-classical state $|\alpha\rangle$.

Ejemplo 1.2

Translation with D

Let be

$$D(\alpha) = e^{\frac{1}{\sqrt{2}}(5+10i)a^\dagger - \frac{1}{\sqrt{2}}(5-10i)a}.$$

We identify $\alpha = 5 + 10i$ and $\alpha^* = 5 - 10i$. Using the result of mean values (1.80) we have

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

Then,

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

Scalar product of two $|\alpha\rangle$ states. Closure relation

The $|\alpha\rangle$ states are eigenvectors of the non-Hermitian operator a . There is therefore no obvious reason for these states to satisfy orthogonality and closure relation.

The scalar product between $|\alpha\rangle$ and $|\alpha'\rangle$ is:

$$\langle\alpha|\alpha'\rangle = \sum_n c_n^*(\alpha) c_n(\alpha') = e^{-|\alpha|^2/2} e^{-|\alpha'|^2/2} \sum_n \frac{(\alpha^* \alpha')^n}{n!} = e^{-|\alpha|^2/2} e^{-|\alpha'|^2/2} e^{\alpha^* \alpha'}.$$

That is,

$$\text{Orthonormalization relation} \quad |\langle\alpha|\alpha'\rangle|^2 = e^{-|\alpha-\alpha'|^2}. \quad (1.85)$$

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

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

$$\frac{1}{\pi} \iint |\alpha\rangle \langle\alpha| d\{\text{Re}(\alpha)\} d\{\text{Im}(\alpha)\} = \dots = \sum_n |\varphi_n\rangle \langle n| = 1.$$

1.7.3 Time evolution of a quasi-classical state

Given the initial state $|\psi(0)\rangle = |\alpha_0\rangle$, How do its physical properties evolve over time?

A quasi-classical state always remains an eigenvector of a

We use the time evolution assuming conservative system (Hamiltonian time-independent)

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

Thus, we have found that

$$\text{Evolution of the quasi-classical state} \quad |\psi(t)\rangle = e^{-\frac{i\omega t}{2}} |\alpha(t)\rangle = \alpha_0 e^{-i\omega t}. \quad (1.86)$$

We see that a quasi-classical state remains an eigenvector of a for all time, with an eigenvalue $\alpha_0 e^{-i\omega t}$ which is nothing more than $\alpha(t)$ obtained at the beginning.

Evolution of physical properties

We use equation (1.80) and change α by $\alpha_0 e^{-i\omega t}$ to obtain:

$$\begin{aligned} \text{Mean values for } \alpha(t) \quad & \begin{aligned} \langle X \rangle(t) &= \sqrt{2\sigma} \text{Re}(\alpha(t)) \\ \langle P \rangle(t) &= \frac{\sqrt{2\hbar}}{\sigma} \text{Im}(\alpha(t)) \\ \langle N \rangle &= |\alpha|^2 \\ \langle H \rangle &= \hbar\omega[|\alpha_0|^2 + \frac{1}{2}] \end{aligned} \end{aligned} \quad (1.87)$$

And the corresponding uncertainties are:

$$\begin{aligned} \text{Uncertainties} \quad \Delta X &= \frac{\sigma}{\sqrt{2}} \\ \Delta P &= \frac{\hbar}{\sqrt{2}\sigma} \\ \Delta H &= \hbar\omega|\alpha_0| \end{aligned} \quad (1.88)$$

The uncertainty relation holds:

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

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

$$\alpha(t) = \frac{1}{\sqrt{2}} \left[\frac{\langle X \rangle(t)}{\sigma} + i \frac{\sigma \langle P \rangle(t)}{\hbar} \right]. \quad (1.89)$$

Motion of the wave packet

Let us calculate the wave function $\psi(x, t)$. Using (1.86) and (76), we have:

$$\psi(x, t) = e^{i\theta_\alpha} \left(\frac{1}{\pi\sigma^2} \right)^{1/4} e^{-i\omega t/2} e^{-\frac{x\langle P \rangle(t)}{\hbar}} e^{-\left[\frac{x - \langle x \rangle(t)}{2\Delta X} \right]^2}.$$

At t , the wave packet is still Gaussian. Thus, it remains minimum for all time. The following figure shows the motion of the wave packet, performing periodic oscillation without becoming distorted. In free particle, this type of wave packet would become distorted as it propagates, but here the potential compensates that spreading so that the shape is always the same.

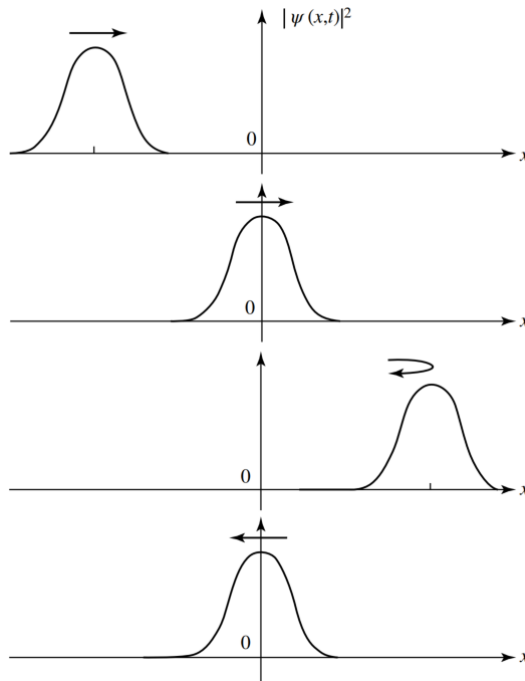


Figure 1.2 Motion of the Gaussian wave packet associated with $|\alpha\rangle$ state. Thanks to the form of $V(x)$, the wave packet oscillates without distortion.

Formula sheet

1.7.4 Useful formulas

Closure relation (discrete)	$\sum_k \sum_{i=1}^{g_k} v_k^i\rangle \langle v_k^i = \mathbb{1}$	Closure relation (continuous)	$\int_{\beta} d\beta \omega_{\beta}\rangle \langle \omega_{\beta} = \mathbb{1}$
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} \langle [A, B] \rangle $
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 $F(A)$	$F(A) \psi\rangle = F(\lambda) \psi\rangle$		
Transformation $\{u\} \rightarrow \{v\}$	$\mathbb{M}_{jk} = \langle u_j v_k \rangle$	$ \psi\rangle_{\{u\}} = \mathbb{M} \psi\rangle_{\{v\}}$ $A_{\{u\}} = \mathbb{M} A_{\{v\}} \mathbb{M}^{\dagger}$	$ \psi\rangle_{\{v\}} = \mathbb{M}^{\dagger} \psi\rangle_{\{u\}}$ $A_{\{v\}} = \mathbb{M}^{\dagger} A_{\{u\}} \mathbb{M}$

1.7.5 Basis

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

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

Fourier transforms for 3D wavefunctions

$\tilde{\psi}(\mathbf{p}) = \mathcal{F}[\psi(\mathbf{r})] = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int_{-\infty}^{\infty} d^3\mathbf{r} e^{-i\mathbf{r}\cdot\mathbf{p}/\hbar} \psi(\mathbf{r})$	$\psi(\mathbf{r}) = \mathcal{F}^{-1}[\tilde{\psi}(\mathbf{p})] = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int_{-\infty}^{\infty} d^3\mathbf{p} e^{i\mathbf{r}\cdot\mathbf{p}/\hbar} \tilde{\psi}(\mathbf{p})$
$\mathcal{F}[\psi^{(n)}(x)] = \left(\frac{ip}{\hbar}\right)^n \tilde{\psi}(p)$	$\tilde{\psi}^{(n)}(p) = \mathcal{F}\left[\left(-\frac{ix}{\hbar}\right)^n \psi(x)\right]$
$\tilde{\psi}(p - p_0) = \mathcal{F}[e^{ip_0x/\hbar} \psi(x)]$	$e^{-ipx_0/\hbar} \tilde{\psi}(p) = \mathcal{F}[\psi(x - x_0)]$
$\mathcal{F}[\psi(cx)] = \tilde{\psi}(p/c)/ c $	$\int_{-\infty}^{\infty} dx \varphi^*(x) \psi(x) = \int_{-\infty}^{\infty} dp \tilde{\varphi}^*(p) \tilde{\psi}(p)$
$\psi(x)$ 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 $V = [\mathbf{u}_1|\mathbf{u}_2|\dots]$, $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots)$, and $A|\mathbf{u}_i\rangle = \lambda_i|\mathbf{u}_i\rangle$. In the eigenbasis we can do $F(A) = VF(\Lambda)V^{-1}$.
- When A is Hermitian, V is unitary: $V^{-1} = V^{\dagger}$.

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