Chapter 4

Continuous Degrees of Freedom

In the previous Chapters we have focused on the theoretical description of discrete degrees of freedom. These typically arise in the case of spin wave functions, when measurements only result in a discrete and finite set of possibilities. There are however very important cases in which observables are intrinsically continuous, even in the quantum case. This is the case for example of quantities such as position and momenta of particles. While it is always possible to think about these cases as specific limit of finite-dimensional vector spaces, it is more natural to extend the previous formalism to account for intrinsically continuous degrees of freedom.

4.1 Bra-Ket formalism for Continuous Degrees of Freedom

The formalism in this case is very close to what already discussed about finite vector spaces. We consider for example some continuous degree of freedom described by the operator ξ, so that it possesses a set of eigenvalues ξ and eigenvectors $|\xi\rangle$ satisfying:

$$\hat{\xi}\,|\xi'\rangle = \xi'\,|\xi'\rangle \tag{4.1.1}$$

notice that in this case there will be infinitely many kets $|\xi'\rangle$ satisfying this relationship, each of those with some associated eigenvalue.

Other than this important distinction, we also need to generalize our formalism to accommodate for orthonormality relationships and closure relationships that are well suited for continuous variables. Table 4.1 summarizes the main correspondences, that should be fairly intuitive to understand.

Since, in general, the variable ξ' associated to the eigen-kets is continuous, we can identify the expansion coefficients of an arbitrary quantum state in this basis as a complex-valued function (also known as "wave function" or "state function"):

$$\Psi(\xi) \equiv \langle \xi | \Psi \rangle \tag{4.1.2}$$

with the property of being L2, integrable, i.e. it can be correctly normalized in a way that

Property	Discrete case	Continuous case
Operator	$\hat{A}$	$\hat{\xi}$
Eigenvalues	$\hat{A}\|A_i\rangle = a_i\|A_i\rangle$	$\hat{\xi}\|\xi'\rangle = \xi'\|\xi'\rangle$
Completeness	$\sum_i \|A_i\rangle\langle A_i\| = \hat{1}$	$\int d\xi'\|\xi'\rangle\langle\xi'\| = \hat{1}$
State Expansion	$\|\Psi\rangle = \sum_i \|A_i\rangle\langle A_i\|\Psi\rangle$	$\|\Psi\rangle = \int d\xi'\|\xi'\rangle\langle\xi'\|\Psi\rangle$
State Normalization	$\sum_i \|\langle\xi_i\|\Psi\rangle\|^2 = 1$	$\int d\xi'\|\langle\xi'\|\Psi\rangle\|^2 = 1$
Orthonormality	$\langle A_i\|A_j\rangle = \delta_{ij}$	$\langle\xi'\|\xi''\rangle = \delta(\xi' - \xi'')$
Operators Matrix Elements	$\langle A_i\|\hat{A}\|A_j\rangle = \delta_{ij}a_j$	$\langle\xi'\|\hat{\xi}\|\xi''\rangle = \delta(\xi' - \xi'')\xi'$

Table 4.1: Correspondence between discrete and continuous kets formalism.

$$\int d\xi\, |\Psi(\xi)|^2 = 1 \tag{4.1.3}$$

Notice that this property is a fundamental property of wave functions, and it is a direct consequence of the Born rule $P(\xi) = |\Psi(\xi)|^2$. For example if we had to compute the probability P_δ of measuring a value ξ within the interval $\xi \in (\xi_0, \xi_0 + \delta)$, we would use the standard rule of probability theory:

$$P_\delta(\xi_0) = \int_{\xi_0}^{\xi_0+\delta} d\xi\, |\Psi(\xi)|^2 \approx \delta|\Psi(\xi_0)|^2 \tag{4.1.4}$$

Notice that this also marks a slight but important difference with respect to the case of discrete variables, since the amplitude $|\langle\xi_0|\Psi\rangle|^2$ is not the probability of obtaining the measurement value ξ_0, as it would be in the discrete case, but rather the probability density of obtaining ξ_0. Strictly speaking, for a continuous variable the probability of obtaining exactly ξ_0 is infinitesimally small in the window δ around it, thus it is zero in the limit $\delta \to 0$. In most of the applications we will never compute point-wise probability densities to evaluate physical quantities, but rather integrals over finite windows of values.

4.2 The Position Operator

Let us now focus on the common case in which we are interested in measuring or just characterizing theoretically the position of a given particle (say, an electron). For simplicity, we first focus on the case in which the particle is constrained to be in one dimension. In this case, the eigen-kets are just one-dimensional coordinates:

$$\hat{x}\,|x'\rangle = x'\,|x'\rangle \tag{4.2.1}$$

As much as done when considering the measurement postulates for spin systems, a very similar situation is found when considering continuous variables. Specifically, we can imagine that we can measure the position of our particle taking a snapshot of it. Every time we take a picture of this particle, we will see a spot in our picture at a given position x', and the wave-function collapses into the corresponding eigenstate

$$|\Psi\rangle \to |x'\rangle\langle x'|\Psi\rangle. \tag{4.2.2}$$

We can easily extend this description also to higher dimensions, i.e., we lift the constraint of having purely one-dimensional particles. In this case the wave-function is therefore a complex-valued function of the vector $\mathbf{r} = (x, y, z)$:

$$\langle x, y, z|\Psi\rangle \equiv \Psi(x, y, z), \tag{4.2.3}$$

where we have postulated that Ψ is an eigenstate of all coordinates. This hypothesis is verified experimentally. As a result of the discussion in the previous Chapter, this implies that position operators commute:

$$[\hat{x}, \hat{y}] = 0, \tag{4.2.4}$$
$$[\hat{x}, \hat{z}] = 0, \tag{4.2.5}$$
$$[\hat{y}, \hat{z}] = 0. \tag{4.2.6}$$

4.3 The Translation Operator

In addition to the concept of *position* for a quantum particle, the other major observable concerning particles in continuous space is the *momentum*. In order to derive a consistent form for the momentum operator, we first need to introduce the concept of translation operator, since this will be instrumental in defining the form that the momentum operator takes in quantum mechanics.

We start by considering an infinitesimal translation operator, $\hat{T}(\delta\mathbf{r})$ parameterized by a certain 3-dimensional infinitesimal translation $\delta\mathbf{r} = (\delta x, \delta y, \delta z)$, whose job is to translate a certain eigen-ket of the position operator:

$$\hat{T}(\delta\mathbf{r})|\mathbf{r}\rangle = |\mathbf{r} + \delta\mathbf{r}\rangle. \tag{4.3.1}$$

The action of this operator is quite simple, since it takes a certain eigen-ket of the position operator, $|\mathbf{r}\rangle$, and returns another eigen-ket of the position operator, $|\mathbf{r}' + \delta\mathbf{r}'\rangle$. From this expression we also see that $|\mathbf{r}'\rangle$ is not an eigen-ket of the translation operator, since it is transformed into another eigen-ket and not into itself.

Applied on an arbitrary state, $|\Psi\rangle$, the action of the infinitesimal translation operator is

$$\hat{T}(\delta\mathbf{r})|\Psi\rangle = \hat{T}(\delta\mathbf{r}) \int d\mathbf{r}|\mathbf{r}\rangle\Psi(\mathbf{r}) \tag{4.3.2}$$
$$= \int d\mathbf{r}\hat{T}(\delta\mathbf{r})|\mathbf{r}\rangle\Psi(\mathbf{r}) \tag{4.3.3}$$
$$= \int d\mathbf{r}|\mathbf{r} + \delta\mathbf{r}\rangle\Psi(\mathbf{r}) \tag{4.3.4}$$
$$= \int d\mathbf{r}|\mathbf{r}\rangle\Psi(\mathbf{r} - \delta\mathbf{r}), \tag{4.3.5}$$

where in the last line we have considered the change of variable $\mathbf{r} \to \mathbf{r} - \delta\mathbf{r}$, that does not affect the value of the integral, since we are already integrating over the full space.

This expression also shows that, in position space, the effect of the translation operator is effectively $\Psi(\mathbf{r}) \to \Psi(\mathbf{r} - \delta\mathbf{r})$.
We can already derive several interesting properties of the operator $\hat{T}$, just looking at how the state transforms under its action. Specifically, we should have that the translated state $|\Psi'\rangle = \hat{T}(\delta\mathbf{r})|\Psi\rangle$, is still correctly normalized, i.e.

$$\langle\Psi'|\Psi'\rangle = \langle\Psi|\hat{T}^\dagger(\delta\mathbf{r})\hat{T}(\delta\mathbf{r})|\Psi\rangle \tag{4.3.6}$$
$$= \langle\Psi|\Psi\rangle. \tag{4.3.7}$$

This condition is satisfied if the translation operator is unitary:

$$\hat{T}^\dagger(\delta\mathbf{r})\hat{T}(\delta\mathbf{r}) = \hat{\mathbb{1}}. \tag{4.3.8}$$

The second property we expect from this operator is that it can be arbitrarily composed, in the sense that subsequent translations of $\delta\mathbf{r}_1, \delta\mathbf{r}_2, \delta\mathbf{r}_3, \ldots$ must be equivalent to a single translation of the sum vector:

$$\hat{T}(\delta\mathbf{r}_1)\hat{T}(\delta\mathbf{r}_2)\hat{T}(\delta\mathbf{r}_3)\ldots = \hat{T}(\delta\mathbf{r}_1 + \delta\mathbf{r}_2 + \delta\mathbf{r}_3 + \ldots). \tag{4.3.9}$$

Furthermore, if we translate a certain system back to its original position, this operation should be equivalent to applying the inverse transformation:

$$\hat{T}(-\delta\mathbf{r}) = \hat{T}^{-1}(\delta\mathbf{r}), \tag{4.3.10}$$

where $\hat{T}^{-1}$ denotes the inverse of the operator.
The last property that we can intuitively expect is that in the limit of vanishing translations the operator $\hat{T}$ should strictly reduce to the identity

$$\lim_{|\delta\mathbf{r}|\to 0} \hat{T}(\delta\mathbf{r}) = \hat{\mathbb{1}}. \tag{4.3.11}$$

As we have already seen for the case of the time evolution operator, and as a consequence of Stone's theorem, all these conditions are satisfied if we take the infinitesimal translation operator to be described by the following unitary operator

$$\hat{T}(\delta\mathbf{r}) = e^{-i\hat{\mathbf{K}}\cdot\delta\mathbf{r}}, \tag{4.3.12}$$

where $\hat{\mathbf{K}}$ is a vector operator $\hat{\mathbf{K}} = (\hat{K}_x, \hat{K}_y, \hat{K}_z)$ where each of the individual components are Hermitian operators. Here, the exponential of the operator has exactly the same meaning it would have for finite vector spaces, and it is again understood in terms of its Taylor expansion:

$$e^{-i\hat{\mathbf{K}}\cdot\delta\mathbf{r}} = \hat{\mathbb{1}} - i\hat{\mathbf{K}}\cdot\delta\mathbf{r} - \frac{1}{2}(\hat{\mathbf{K}}\cdot\delta\mathbf{r})(\hat{\mathbf{K}}\cdot\delta\mathbf{r}) + \mathcal{O}\Big[(\delta\mathbf{r})^3\Big]. \tag{4.3.13}$$

From this expansion, we immediately see that Eq. (4.3.11) is verified. The unitarity assumption is also quick to verify, since it is an elementary property of the exponential of an operator that $e^{X^+} = (e^X)^\dagger$, thus

$$\hat{T}^\dagger(\delta\mathbf{r}) = e^{i(\hat{\mathbf{K}})^\dagger\cdot\delta\mathbf{r}} \tag{4.3.14}$$
$$= e^{i\hat{\mathbf{K}}\cdot\delta\mathbf{r}}, \tag{4.3.15}$$

where in the last line we have used the fact that $\hat{\mathbf{K}}$ is Hermitian. The composition property is also a consequence of the exponential structure

$$e^{-i\hat{\mathbf{K}}\cdot\delta_1} e^{-i\hat{\mathbf{K}}\cdot\delta_2} \cdots = e^{-i\hat{\mathbf{K}}\cdot(\delta_1+\delta_2+\cdots)}, \tag{4.3.16}$$

as well as the inversion property

$$\hat{T}(-\delta\mathbf{r}) = e^{i\hat{\mathbf{K}}\cdot\delta\mathbf{r}}, \tag{4.3.17}$$
$$e^{i\hat{\mathbf{K}}\cdot\delta\mathbf{r}} e^{-i\hat{\mathbf{K}}\cdot\delta\mathbf{r}} = \hat{\mathbb{I}}, \tag{4.3.18}$$
$$\hat{T}^{\dagger}(-\delta\mathbf{r})\hat{T}(\delta\mathbf{r}) = \hat{\mathbb{I}}, \tag{4.3.19}$$
$$\hat{T}(-\delta\mathbf{r}) = \hat{T}^{-1}(\delta\mathbf{r}). \tag{4.3.20}$$

Commutation relations of $\hat{\mathbf{K}}$

The operator $\hat{\mathbf{K}}$ introduced earlier is Hermitian and thus qualifies as a physical observable according to the fundamental axioms of quantum theory. An essential question is whether this observable is compatible with measurements of the position operator. To address this, we compute the commutator $[\hat{\mathbf{K}}, \hat{\mathbf{r}}]$ and check whether it vanishes.
First, consider the action of an infinitesimal translation followed by the position operator:

$$\hat{\mathbf{r}}'\hat{\mathbf{T}}(\delta\mathbf{r})|\mathbf{r}'\rangle = \hat{\mathbf{r}}'|\mathbf{r}' + \delta\mathbf{r}\rangle, \tag{4.3.21}$$
$$= (\mathbf{r}' + \delta\mathbf{r})|\mathbf{r}' + \delta\mathbf{r}\rangle. \tag{4.3.22}$$

Next, consider the action of the position operator followed by the translation:

$$\hat{\mathbf{T}}(\delta\mathbf{r})\hat{\mathbf{r}}'|\mathbf{r}'\rangle = \mathbf{r}'\hat{\mathbf{T}}(\delta\mathbf{r})|\mathbf{r}'\rangle, \tag{4.3.23}$$
$$= \mathbf{r}'|\mathbf{r}' + \delta\mathbf{r}\rangle. \tag{4.3.24}$$

Subtracting these two results yields:

$$[\hat{\mathbf{r}}, \hat{\mathbf{T}}(\delta\mathbf{r})]|\mathbf{r}'\rangle = \delta\mathbf{r}|\mathbf{r}' + \delta\mathbf{r}\rangle, \tag{4.3.25}$$
$$= \delta\mathbf{r}|\mathbf{r}'\rangle + \mathcal{O}((\delta\mathbf{r})^2). \tag{4.3.26}$$

Since this equation must hold for all kets $|\mathbf{r}'\rangle$, we conclude that the commutator identity is:

$$[\hat{\mathbf{r}}, \hat{\mathbf{T}}(\delta\mathbf{r})] = \delta\mathbf{r}\hat{\mathbb{I}}. \tag{4.3.27}$$

Remark: In many cases, we omit the identity operator $\hat{\mathbb{I}}$ from the right-hand side for simplicity. However, it should be noted that a commutator of two operators is always itself an operator.
From the definition of the translation operator in terms of $\hat{\mathbf{K}}$, we have:

$$[\hat{\mathbf{r}}, \hat{\mathbb{I}} - i\hat{\mathbf{K}}\cdot\delta\mathbf{r}] = -i[\hat{\mathbf{r}}, \hat{\mathbf{K}}\cdot\delta\mathbf{r}], \tag{4.3.28}$$
$$= \delta\mathbf{r}. \tag{4.3.29}$$

Component-wise relations: For the x-component:

$$[\hat{x}, \hat{K}_x] = i, \tag{4.3.30}$$

and, more generally:

$$[\hat{r}_\alpha, \hat{K}_\beta] = i\delta_{\alpha\beta}. \tag{4.3.31}$$

4.4 The Momentum Operator

Here, show deinition of momentum operator as well as the momentum operator representation. , and hte momentum operator in the position basis.

4.4.1 The Momentum Operator

Similarly to the time evolution case, where we identified the operator $\hat{\mathcal{O}}$ with the Hamiltonian $\hat{H}$ through a unit rescaling $\hat{H} = \hbar\hat{\mathcal{O}}$, we can perform a similar analysis for $\hat{\mathbf{K}}$. In analogy to classical mechanics, the generator of spatial translations is identified with the momentum operator $\hat{\mathbf{p}}$. From a dimensional perspective, this identification is achieved by setting:

$$\hat{\mathbf{p}} = \hbar\hat{\mathbf{K}}, \tag{4.4.1}$$

which implies the commutation relations:

$$[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}. \tag{4.4.2}$$

The factor $\hbar$ is essential not only for dimensional reasons but also for recovering classical mechanics in the appropriate limit and explaining experimental results from atomic physics.

4.4.2 Correspondence Principle

Dirac remarked that the commutation relations:

$$[\hat{r}_\alpha, \hat{r}_\beta] = 0, \tag{4.4.3}$$
$$[\hat{p}_\alpha, \hat{p}_\beta] = 0, \tag{4.4.4}$$
$$[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}, \tag{4.4.5}$$

are formally analogous to the classical Poisson bracket relations between position and momentum. These relations naturally arise in the Hamiltonian formalism of classical mechanics. The correspondence principle is expressed through the replacement:

$$[\cdot, \cdot]_{\text{classical}} \to \frac{1}{i\hbar}[\cdot, \cdot], \tag{4.4.6}$$

where the classical Poisson bracket of two functions $A(\mathbf{r}, \mathbf{p})$ and $B(\mathbf{r}, \mathbf{p})$ is defined as:

$$[A, B]_{\text{classical}} = \sum_\alpha \left(\frac{\partial A}{\partial r_\alpha}\frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial r_\alpha} \right). \tag{4.4.7}$$

For classical mechanics, the relation:

$$[r_\alpha, p_\beta]_{\text{classical}} = \delta_{\alpha\beta}, \tag{4.4.8}$$

when combined with Eq. (4.4.6), directly reduces to the canonical quantum commutation relations.
This analogy also extends to the dynamics of observables, where a classical observable $A(\mathbf{r}, \mathbf{p})$ satisfies:

$$\frac{d}{dt}A(\mathbf{r}, \mathbf{p}) = [A, H]_{\text{classical}}, \tag{4.4.9}$$

where H is the classical Hamiltonian. The Hamiltonian satisfies the canonical equations of motion:

$$\begin{aligned}\dot{\mathbf{r}} &= \frac{\partial H}{\partial \mathbf{p}} = [\mathbf{r}, H]_{\text{classical}},\\ \dot{\mathbf{p}} &= -\frac{\partial H}{\partial \mathbf{r}} = [\mathbf{p}, H]_{\text{classical}}.\end{aligned} \tag{4.4.10}$$

From this, we see that Eq. (4.4.9) corresponds formally to Heisenberg's equation of motion, provided the replacement in Eq. (4.4.6) is made.

4.4.3 Position Representation

We now discuss key properties of the position representation, specifically how quantum states are expanded in the basis of the position operator. To simplify, we first consider the one-dimensional case, avoiding unnecessary bold symbols and indices. As seen earlier in this chapter, an arbitrary state can be expanded in a continuous basis as:

$$|\Psi\rangle = \int dx|x\rangle\langle x|\Psi\rangle, \tag{4.4.11}$$

$$= \int dx|x\rangle\psi(x). \tag{4.4.12}$$

Overlaps between states in the position representation are given by integrating over space:

$$\langle\Phi|\Psi\rangle = \int dx\langle\Phi|x\rangle\langle x|\Psi\rangle, \tag{4.4.13}$$

$$= \int dx\Phi^*(x)\Psi(x). \tag{4.4.14}$$

Matrix elements of an operator $\hat{A}$ in this representation are:

$$\langle\Phi|\hat{A}|\Psi\rangle = \int dx\langle\Phi|x\rangle\langle x|\hat{A}|\Psi\rangle, \tag{4.4.15}$$

$$= \int dxdx'\langle\Phi|x\rangle\langle x|\hat{A}|x'\rangle\langle x'|\Psi\rangle, \tag{4.4.16}$$

$$= \int dxdx'\Phi^*(x)A(x, x')\Psi(x'). \tag{4.4.17}$$

These results follow directly from the completeness relation for kets defined on continuous variables. Eq. (4.4.17) demonstrates that, for an arbitrary operator, we must evaluate its matrix elements $\langle x|\hat{A}|x'\rangle = A(x, x')$ in the position representation.

A simplification occurs when the operator $\hat{A}$ is diagonal in this basis. This happens for operators of the form $\hat{A}_f = f(\hat{x})$, where f is an arbitrary analytic function of the coordinates (e.g., $f(\hat{x}) = a\hat{x}^2 - b\hat{x}$, etc.). By expanding f in a Taylor series, it is straightforward to verify that:

$$[\hat{A}_f, \hat{x}] = 0\,, \tag{4.4.18}$$

indicating that $\hat{A}_f$ is diagonal in the position basis. Consequently:

$$\hat{A}_f|x\rangle = f(x)|x\rangle\,, \tag{4.4.19}$$

and the matrix elements of the operator in this basis are:

$$\langle x|\hat{A}_f|x'\rangle = \delta(x - x')f(x)\,. \tag{4.4.20}$$

In this special case, the matrix elements of the operator between two general states simplify to:

$$\langle\Phi|\hat{A}_f|\Psi\rangle = \int dx\, \Phi(x)^* f(x)\Psi(x)\,. \tag{4.4.21}$$

4.4.4 Momentum Operator in the Position Basis

To compute the matrix elements of the momentum operator in the position basis, we focus on one spatial dimension and consider only the x-component of the momentum, $\hat{p}_x$. This computation is fundamental for determining expectation values of momentum, kinetic energy, etc.

Starting with the action of the translation operator on an arbitrary ket $|\Psi\rangle$ for a small displacement δ_x:

$$e^{-i\hat{K}_x\delta_x}|\Psi\rangle = \int dx'|x'\rangle\psi(x' - \delta_x)\,, \tag{4.4.22}$$

where $\psi(x) = \langle x|\Psi\rangle$. Expanding $\psi(x' - \delta_x)$ in a Taylor series gives:

$$\psi(x' - \delta_x) = \psi(x') - \delta_x \frac{\partial\psi(x')}{\partial x'} + \mathcal{O}(\delta_x^2)\,, \tag{4.4.23}$$

so that:

$$\langle x|e^{-i\hat{K}_x\delta_x}|\Psi\rangle = \psi(x) - \delta_x \frac{\partial\psi(x)}{\partial x} + \mathcal{O}(\delta_x^2)\,. \tag{4.4.24}$$

Using the definition of the translation operator, we also write:

$$e^{-i\hat{K}_x\delta_x}|\Psi\rangle = \left(\hat{I} - i\hat{K}_x\delta_x\right)|\Psi\rangle + \mathcal{O}(\delta_x^2)\,, \tag{4.4.25}$$

which implies:

$$\langle x|e^{-i\hat{K}_x\delta_x}|\Psi\rangle = \psi(x) - \frac{i}{\hbar}\delta_x\langle x|\hat{p}_x|\Psi\rangle + \mathcal{O}(\delta_x^2)\,. \tag{4.4.26}$$

Equating Eq. (4.4.24) and Eq. (4.4.26) to first order in δ_x, we find:

$$\langle x|\hat{p}_x|\Psi\rangle = -i\hbar\frac{\partial\psi(x)}{\partial x}\,. \tag{4.4.27}$$

This result shows that the effect of the momentum operator is to take the derivative of the wave function (up to a factor of $-i\hbar$). For the specific case where $|\Psi\rangle = |x'\rangle$, such that $\psi(x) = \langle x|x'\rangle = \delta(x - x')$, we obtain:

$$\langle x|\hat{p}_x|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x - x') \,. \tag{4.4.28}$$

Thus, the matrix elements of the momentum operator between arbitrary states $|\Phi\rangle$ and $|\Psi\rangle$ in the position basis are:

$$\langle\Phi|\hat{p}_x|\Psi\rangle = -i\hbar\int dxdx'\Phi^*(x)\frac{\partial}{\partial x}\delta(x - x')\Psi(x'), \tag{4.4.29}$$

$$= -i\hbar\int dx\Phi^*(x)\frac{\partial\Psi(x)}{\partial x} \,. \tag{4.4.30}$$

Arbitrary analytic functions of the momentum can also be obtained, using the corresponding Taylor series, and knowing that each power of the momentum performs a derivative with respect to the coordinates. An important higher order function is just the square of the momentum, giving rise to the kinetic energy $E_T = p^2/2m$, for a massive particle. In this case,

$$\begin{aligned}\langle x|\,\hat{p}_x^2\,|\Psi\rangle &= \int dx'\,\langle x|\,\hat{p}_x\,|x'\rangle\,\langle x'|\,\hat{p}_x\,|\Psi\rangle = \\ &= (-i\hbar)^2\int dx'\left(\frac{\partial}{\partial x}\delta(x - x')\right)\left(\frac{\partial}{\partial x'}\psi(x')\right) = \\ &= -\hbar^2\frac{\partial^2}{\partial x^2}\psi(x) \,. \end{aligned}\tag{4.4.31}$$

4.5 Momentum representation

Until now we have worked solely with eigenstates of the position operator, however it is interesting to look at the eigenstates of the momentum operator as well. These are defined by the usual eigenvalue relation:

$$\hat{p}\,|p\rangle = p\,|p\rangle \ , \tag{4.5.1}$$

and can be useful, for example, if we wanted to represent a certain wave function in this basis. In order to avoid cluttering the notation, in this section we will omit the lower index x to characterize the x component of the momentum, thus it is assumed, starting from the equation above, that $\hat{p} \equiv \hat{p}_x$. Since in the previous discussion we have already derived the action of the momentum operator on an arbitrary ket, we can rewrite the eigenvalue equation as

$$\langle x|\hat{p}|p\rangle = p\,\langle x|p\rangle = -i\hbar\frac{\partial}{\partial x}\,\langle x|p\rangle \ . \tag{4.5.2}$$

We therefore see that the eigenfunctions of the momentum satisfy this simple differential equation

$$\langle p|\hat{x}|p\rangle = -i\hbar\frac{\partial}{\partial x}\,\langle x|p\rangle \ . \tag{4.5.3}$$

It is easy to see that we are after an exponential form:

$$\langle x|p\rangle = N e^{i\frac{px}{\hbar}}\,, \tag{4.5.4}$$

where N is a normalization that should be fixed imposing the usual constraint:

$$\langle p|p'\rangle = \delta(p-p'), \tag{4.5.5}$$

$$\int dx\, \langle p|x\rangle \langle x|p'\rangle = \delta(p-p'). \tag{4.5.6}$$

We can explicitly write the l.h.s. of this equation and notice that it is just a representation of the delta function:

$$|N|^2 \int dx e^{i\frac{(p'-p)x}{\hbar}} = |N|^2 2\pi\hbar\delta(p-p'). \tag{4.5.7}$$

We therefore conclude that $N = \frac{1}{\sqrt{2\pi\hbar}}$ is a good normalization (there is an arbitrary phase to be picked in choosing N and the convention is just to take N to be real and positive). We thus have that the eigenstates of the momentum operators are plane waves:

$$\langle x|p\rangle = \frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}. \tag{4.5.8}$$

This also allows us to find the relationship between wave functions in different bases. For example, a wave-function in real space, $\psi(x)$, has a representation $\tilde{\psi}(p)$ in momentum space:

$$\langle p|\psi\rangle = \int dx\, \langle p|x\rangle \langle x|\psi\rangle\,, \tag{4.5.9}$$

$$\tilde{\psi}(p) = \int dx \frac{e^{-i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}\psi(x), \tag{4.5.10}$$

and vice-versa:

$$\langle x|\psi\rangle = \int dp\, \langle x|p\rangle \langle p|\psi\rangle\,, \tag{4.5.11}$$

$$\psi(x) = \int dp \frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}\tilde{\psi}(p). \tag{4.5.12}$$

The correspondence between real-space and momentum-space wave-function is now evident in its beauty: transforming a given quantum state between these two bases requires performing (inverse and direct) Fourier transforms of the corresponding wave functions. It should be stressed that all of these results have been obtained using the few postulates of completeness for quantum states, and the connection between translation operator and the momentum operator.

4.6 Quantum and classical particles

We are now already in position to make an intermediate summary of the results we have obtained so far, and clarify the fundamentally different description of particles arising from quantum mechanics. The summary is presented in Table 4.2.

	Classical	**Quantum**
State	Two vector quantities: $\mathbf{r} = (x, y, z)$ and $\mathbf{p} = (p_x, p_y, p_z)$	A ray in Hilbert space: the state vector $\|\Psi\rangle$
Quantities	The values of $\mathbf{r}$ and $\mathbf{p}$ can be measured directly	$\|\Psi(\mathbf{r})\|^2$ and $\|\tilde{\Psi}(\mathbf{p})\|^2$ are the probability densities of observing a certain $\mathbf{r}$ or $\mathbf{p}$
Uncertainty	No constraint	Heisenberg principle
Time Evolution	$\dot{\mathbf{r}} = [\mathbf{r}, H]_{\text{classical}}$, $\dot{\mathbf{p}} = [\mathbf{p}, H]_{\text{classical}}$	$\dot{\hat{\mathbf{r}}} = \frac{1}{i\hbar}[\hat{\mathbf{r}}, \hat{H}]$, $\dot{\hat{\mathbf{p}}} = \frac{1}{i\hbar}[\hat{\mathbf{p}}, \hat{H}]$

Table 4.2: Comparing the classical and quantum description of a particle.

4.7 Gaussian wave packet

In the following Chapter we will see how the wave functions can be obtained from first principles, solving the Schroedinger equation. For the moment however, it is already interesting to look at specific cases of wave functions that can help us familiarize with the basic concepts of the theory.
An important example is called the *gaussian wave packet* and allows us, in a certain limit, also to connect to the classical behavior we would expect from a point-like particle. The wave function in position space takes the form:

$$\Psi(x; k, d) = \frac{1}{\sqrt[4]{2\pi}\sqrt{d}} e^{ikx} e^{-\frac{x^2}{4d^2}} , \tag{4.7.1}$$

thus this state is parameterized by two constants k and d we can vary at will. We will drop the explicit parametric dependence on these two parameters in the following. First important observation is that the Born probability density in real space is:

$$|\Psi(x)|^2 = \frac{1}{d\sqrt{2\pi}} e^{-\frac{x^2}{2d^2}} , \tag{4.7.2}$$

thus it is a Gaussian centered at the origin and variance d^2. This is the reason why we referred to this before as a gaussian wave packet. The first consequence of this observation is that the parameter d controls how localized the particle is around the origin. The smaller d, the more localized the particle position will be, and a measurement of the position operator will result in small variations across different measurements. On the other hand, the larger d, the more delocalized it is, and an observation of the position operator will result in wildly different values for x at each measurement outcome. The expectation value of the position operator is 0 for symmetry reasons (it is also just the mean of the Gaussian):

$$\langle \hat{x} \rangle = \langle \Psi | \hat{x} | \Psi \rangle = \int dx\, x |\Psi(x)|^2 = 0 . \tag{4.7.3}$$

The spread of the measurement of x can be quantified by the expectation value of $\hat{x}^2$, which in turn coincides with the variance of the gaussian:

$$\left\langle \hat{x}^2 \right\rangle = \int dx\, x^2 |\Psi(x)|^2 = d^2 . \tag{4.7.4}$$

Thus the *intrinsic uncertainty* related to the probabilistic nature of the measurement process (quantum noise, if you wish) is given by

$$\left\langle \Delta\hat{x}^2 \right\rangle = \left\langle \hat{x}^2 \right\rangle - \langle \hat{x} \rangle^2 = d^2 \,. \tag{4.7.5}$$

Again this expression should be interpreted in terms of many repeated measurements on identical systems, imagining that each outcome for the measurement of x is recorded, and that in the limit of a large number of measurements the variance of the observed x approaches d^2. The expectation value of the momentum operator is conveniently computed recalling that $\langle x|\hat{p}|\Psi\rangle = -i\hbar\frac{\partial}{\partial x}\Psi(x)$ thus

$$\langle \hat{p} \rangle = \langle \Psi|\hat{p}|\Psi\rangle = -i\hbar \int dx\, \Psi(x)^* \frac{\partial}{\partial x}\Psi(x) = \hbar k \,. \tag{4.7.6}$$

The detailed derivation of the last line is left as an exercise. From this expression we see that the parameter k also has a transparent physical meaning: it is the "average" wave number The vector of the quantum particle described by this wave packet. One can also show that

$$\left\langle \hat{p}^2 \right\rangle = \frac{\hbar^2}{4d^2} + \hbar^2 k^2 \,, \tag{4.7.7}$$

and thus the dispersion in momentum is found

$$\left\langle \Delta\hat{p}^2 \right\rangle = \frac{\hbar^2}{4d^2} \,. \tag{4.7.8}$$

From Eqs. (4.7.5) and (4.7.7), we see that the Gaussian wave packet saturates the Heisenberg indetermination principle:

$$\left\langle \Delta\hat{x}^2 \right\rangle \left\langle \Delta\hat{p}^2 \right\rangle = \frac{\hbar^2}{4} \,. \tag{4.7.9}$$

That is why the gaussian wave packet is often called the minimum uncertainty wave function, in the sense that it is not possible to find other states with less uncertainty, as quantified by the Heisenberg bound. This also tells us that if we are in a limit in which $d \to 0$ there will be huge indeterminacy in the value of the momentum, and vice versa. To form some intuition of this behavior, we can think that the more we try to spatially squeeze the particle, the "hotter" it gets, with its kinetic energy increasing. While useful, as all analogies with the classical world (in this case with thermodynamics) this analogy too should be taken with a grain of salt. In the quantum case there is absolutely no dynamics (yet) involved, and these rapid oscillations are just a result of the intrinsic probabilistic nature of quantum mechanics.

This result also tells us that, as long as our classical observer has an experimental *resolution* (intrinsic precision of the instrument) on the momentum significantly worse than $\frac{\hbar^2}{4d^2}$ (i.e., they are not able to resolve features below that scale), and as long as the experimental resolution on the position is significantly worse than d^2, both position and momentum will *appear* to take constant values, every time their measurement is performed. This tells us that in order to see quantum mechanical effects, it is often the case that we need to go at scales (both in space and momentum) that have for long been not accessible to experimentalists before the beginning of the 20th century.

Exercise 4.1 Prove Eqs. (4.7.6) and (4.7.7).
Exercise 4.2 Find the momentum representation of the Gaussian wave-packet state.

4.8 References and Further Reading

The discussion done in this Chapter is adapted from Sakurai's "Modern Quantum Mechanics" (Chapter 1, sections 1.6 and 1.7). A detailed treatment of the position and momentum representations can be found also in Cohen-Tannoudji's book (Chapter 2 in general, and also complement DII).

Appendix 4.A: Dirac's Delta Function

The only more subtle point in this correspondence concerns the introduction of Dirac's delta $\delta(x)$, a generalized function that plays a very important role in the study of Hilbert spaces. Here we just recall that Dirac delta can be seen as the limit of an infinitely tight Gaussian:

$$\delta(x) = \lim_{\sigma\to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{4.8.1}$$

From this limiting expression, it follows directly that the delta function is an even function of the argument x, $\delta(x) = \delta(-x)$, and that it integrates to one

$$\int_{-\infty}^{\infty} dx\, \delta(x) = 1\,. \tag{4.8.2}$$

Another distinctive feature of the delta is that

$$\int_{-\infty}^{\infty} dx\, F(x)\delta(x) = F(0) \tag{4.8.3}$$

which is quite natural when thinking of the delta as a very sharp gaussian, that is zero almost everywhere but close to the origin. This property of course generalizes to arbitrary arguments of the delta, that correspond to shifting the mean value of the corresponding limiting gaussian:

$$\int_{-\infty}^{\infty} dx\, F(x)\delta(x - x_0) = F(x_0) \tag{4.8.4}$$

Other important properties of Dirac's delta can be found in math textbooks.

Exercise 4.3 Show that $\delta(ax) = \delta(x)/|a|$. Hint: Consider $\int d(ax)\, \delta(ax)$ and remember that $\delta(x) = \delta(-x)$.

Exercise 4.4 Consider the Heaviside function defined as

$$\Theta(x-x_0)=\begin{cases}1\,, & x>x_0\\ 0\,, & x<x_0\end{cases} \tag{4.8.5}$$

Show that $\delta(x-x')=\frac{\mathrm{d}}{\mathrm{d}x}\Theta(x-x')$.

Appendix 4.B: Fourier Transformation

In this Appendix we review some concepts of Fourier transformation.

The Fourier transform is a mathematical tool that expresses a function in terms of its frequency (wavenumber) components. In quantum mechanics, it's crucial for switching between position and momentum representations. From basic Fourier analysis, given a function $f(x)$, its transform is defined as

$$\tilde{f}(k)=\frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}dx\,f(x)e^{-ikx} \tag{4.8.6}$$

and its inverse is given by

$$f(x')=\frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}dk\,\tilde{f}(k)e^{ikx} \tag{4.8.7}$$

The more localized $f(x)$ is, the more spread out $\tilde{f}(k)$ becomes, and vice versa. We can feed Eq. (4.8.7) into Eq. (4.8.6) and get

$$f(x')=\int_{-\infty}^{\infty}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,e^{ik(x'-x)}\right)f(x)\,dx \tag{4.8.8}$$

Comparing this result with $\int dx\,\delta(x-x_0)f(x)=x_0$, we see that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,e^{ik(x'-x)}=\delta(x'-x). \tag{4.8.9}$$

This precisely demonstrates the spread in the $\tilde{f}(k)$ which is infinite since this is a constant, while the wavefunction in real space is entirely localized.