# Chapter 3

# Operator methods in quantum mechanics

While the wave mechanical formulation has proved successful in describing the quantum mechanics of bound and unbound particles, some properties can not be represented through a wave-like description. For example, the electron spin degree of freedom does not translate to the action of a gradient operator. It is therefore useful to reformulate quantum mechanics in a framework that involves only operators.

Before discussing properties of operators, it is helpful to introduce a further simplification of notation. One advantage of the operator algebra is that it does not rely upon a particular basis. For example, when one writes $\hat{H} = \frac{\hat{p}^2}{2m}$, where the hat denotes an operator, we can equally represent the momentum operator in the spatial coordinate basis, when it is described by the differential operator, $\hat{p} = -i\hbar\partial_x$, or in the momentum basis, when it is just a number $\hat{p} = p$. Similarly, it would be useful to work with a basis for the wavefunction which is coordinate independent. Such a representation was developed by Dirac early in the formulation of quantum mechanics.

In the parlons of mathematics, square integrable functions (such as wavefunctions) are said form a vector space, much like the familiar three-dimensional vector spaces. In the **Dirac notation**, a state vector or wavefunction, $\psi$, is represented as a "ket", $|\psi\rangle$. Just as we can express any three-dimensional vector in terms of the basis vectors, $\mathbf{r} = x\hat{\mathbf{e}}_1 + y\hat{\mathbf{e}}_2 + z\hat{\mathbf{e}}_3$, so we can expand any wavefunction as a superposition of basis state vectors,

$$|\psi\rangle = \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle + \cdots .$$

Alongside the ket, we can define the "bra", $\langle\psi|$. Together, the bra and ket define the **scalar product**

$$\langle\phi|\psi\rangle \equiv \int_{-\infty}^{\infty} dx\, \phi^*(x)\psi(x)\,,$$

from which follows the identity, $\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$. In this formulation, the real space representation of the wavefunction is recovered from the inner product $\psi(x) = \langle x|\psi\rangle$ while the momentum space wavefunction is obtained from $\psi(p) = \langle p|\psi\rangle$. As with a three-dimensional vector space where $\mathbf{a}\cdot\mathbf{b} \leq |a|\,|b|$, the magnitude of the scalar product is limited by the magnitude of the vectors,

$$\langle\psi|\phi\rangle \leq \sqrt{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}\,,$$

a relation known as the **Schwartz inequality**.

## 3.1 Operators

An operator $\hat{A}$ is a "mathematical object" that maps one state vector, $|\psi\rangle$, into another, $|\phi\rangle$, i.e. $\hat{A}|\psi\rangle = |\phi\rangle$. If

$$\boxed{\hat{A}|\psi\rangle = a|\psi\rangle\,,}$$

with $a$ real, then $|\psi\rangle$ is said to be an **eigenstate** (or **eigenfunction**) of $\hat{A}$ with eigenvalue $a$. For example, the plane wave state $\psi_p(x) = \langle x|\psi_p\rangle = A\,e^{ipx/\hbar}$ is an eigenstate of the **momentum operator**, $\hat{p} = -i\hbar\partial_x$, with eigenvalue $p$. For a free particle, the plane wave is also an eigenstate of the Hamiltonian, $\hat{H} = \frac{\hat{p}^2}{2m}$ with eigenvalue $\frac{p^2}{2m}$.

In quantum mechanics, for any observable $A$, there is an operator $\hat{A}$ which acts on the wavefunction so that, if a system is in a state described by $|\psi\rangle$, the expectation value of $A$ is

$$\boxed{\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} dx\,\psi^*(x)\hat{A}\psi(x)\,.} \tag{3.1}$$

Every operator corresponding to an observable is both linear and Hermitian: That is, for any two wavefunctions $|\psi\rangle$ and $|\phi\rangle$, and any two complex numbers $\alpha$ and $\beta$, **linearity** implies that

$$\hat{A}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha(\hat{A}|\psi\rangle) + \beta(\hat{A}|\phi\rangle)\,.$$

Moreover, for any linear operator $\hat{A}$, the **Hermitian conjugate** operator (also known as the adjoint) is defined by the relation

$$\boxed{\langle\phi|\hat{A}\psi\rangle = \int dx\,\phi^*(\hat{A}\psi) = \int dx\,\psi(\hat{A}^\dagger\phi)^* = \langle\hat{A}^\dagger\phi|\psi\rangle\,.} \tag{3.2}$$

From the definition, $\langle\hat{A}^\dagger\phi|\psi\rangle = \langle\phi|\hat{A}\psi\rangle$, we can prove some useful relations: Taking the complex conjugate, $\langle\hat{A}^\dagger\phi|\psi\rangle^* = \langle\psi|\hat{A}^\dagger\phi\rangle = \langle\hat{A}\psi|\phi\rangle$, and then finding the Hermitian conjugate of $\hat{A}^\dagger$, we have

$$\langle\psi|\hat{A}^\dagger\phi\rangle = \langle(\hat{A}^\dagger)^\dagger\psi|\phi\rangle = \langle\hat{A}\psi|\phi\rangle, \qquad \text{i.e. } (\hat{A}^\dagger)^\dagger = \hat{A}\,.$$

Therefore, if we take the Hermitian conjugate twice, we get back to the same operator. Its easy to show that $(\lambda\hat{A})^\dagger = \lambda^*\hat{A}^\dagger$ and $(\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger$ just from the properties of the dot product. We can also show that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$ from the identity, $\langle\phi|\hat{A}\hat{B}\psi\rangle = \langle\hat{A}^\dagger\phi|\hat{B}\psi\rangle = \langle\hat{B}^\dagger\hat{A}^\dagger\phi|\psi\rangle$. Note that operators are **associative** but not (in general) **commutative**,

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle) = (\hat{A}\hat{B})|\psi\rangle \neq \hat{B}\hat{A}|\psi\rangle\,.$$

A physical variable must have real expectation values (and eigenvalues). This implies that the operators representing physical variables have some special properties. By computing the complex conjugate of the expectation value of a physical variable, we can easily show that physical operators are their own Hermitian conjugate,

$$\langle\psi|\hat{H}|\psi\rangle^* = \left[\int_{-\infty}^{\infty}\psi^*(x)\hat{H}\psi(x)dx\right]^* = \int_{-\infty}^{\infty}\psi(x)(\hat{H}\psi(x))^*dx = \langle\hat{H}\psi|\psi\rangle\,.$$

i.e. $\langle\hat{H}\psi|\psi\rangle = \langle\psi|\hat{H}\psi\rangle = \langle\hat{H}^\dagger\psi|\psi\rangle$, and $\hat{H}^\dagger = \hat{H}$. Operators that are their own Hermitian conjugate are called **Hermitian** (or self-adjoint).

▷ EXERCISE. Prove that the momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla$ is Hermitian. Further show that the parity operator, defined by $\hat{P}\psi(x) = \psi(-x)$ is also Hermitian.

Eigenfunctions of Hermitian operators $\hat{H}|i\rangle = E_i|i\rangle$ form an orthonormal (i.e. $\langle i|j\rangle = \delta_{ij}$) complete basis: For a complete set of states $|i\rangle$, we can expand a state function $|\psi\rangle$ as $|\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle$. Equivalently, in a coordinate representation, we have $\psi(x) = \langle x|\psi\rangle = \sum_i \langle x|i\rangle\langle i|\psi\rangle = \sum_i \langle i|\psi\rangle\phi_i(x)$, where $\phi_i(x) = \langle x|i\rangle$.

▷ INFO. **Projection operators and completeness:** A 'ket' state vector followed by a 'bra' state vector is an example of an operator. The operator which projects a vector onto the $j$th eigenstate is given by $|j\rangle\langle j|$. First the bra vector dots into the state, giving the coefficient of $|j\rangle$ in the state, then its multiplied by the unit vector $|j\rangle$, turning it back into a vector, with the right length to be a projection. An operator maps one vector into another vector, so this is an operator. If we sum over a complete set of states, like the eigenstates of a Hermitian operator, we obtain the (useful) **resolution of identity**

$$\boxed{\sum_i |i\rangle\langle i| = \mathbb{I}\,.}$$

Again, in coordinate form, we can write $\sum_i \phi_i^*(x)\phi_i(x') = \delta(x - x')$. Indeed, we can form a projection operator into a subspace, $\hat{P} = \sum_{\text{subspace}} |i\rangle\langle i|$.

As in a three-dimensional vector space, the expansion of the vectors $|\phi\rangle$ and $|\psi\rangle$, as $|\phi\rangle = \sum_i b_i|i\rangle$ and $|\psi\rangle = \sum_i c_i|i\rangle$, allows the dot product to be taken by multiplying the components, $\langle\phi|\psi\rangle = \sum_i b_i^* c_i$.

▷ EXAMPLE: The basis states can be formed from any complete set of orthogonal states. In particular, they can be formed from the basis states of the position or the momentum operator, i.e. $\int_{-\infty}^{\infty} dx|x\rangle\langle x| = \int_{-\infty}^{\infty} dp|p\rangle\langle p| = \mathbb{I}$. If we apply these definitions, we can then recover the familiar Fourier representation,

$$\psi(x) \equiv \langle x|\psi\rangle = \int_{-\infty}^{\infty} dp \underbrace{\langle x|p\rangle}_{e^{ipx/\hbar}/\sqrt{2\pi\hbar}} \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\, \psi(p)\,,$$

where $\langle x|p\rangle$ denotes the plane wave state $|p\rangle$ expressed in the real space basis.

### 3.1.1 Time-evolution operator

The ability to develop an eigenfunction expansion provides the means to explore the time evolution of a general wave packet, $|\psi\rangle$ under the action of a Hamiltonian. Formally, we can evolve a wavefunction forward in time by applying the time-evolution operator. For a Hamiltonian which is time-indepenent, we have $|\psi(t)\rangle = \hat{U}|\psi(0)\rangle$, where

$$\boxed{\hat{U} = e^{-i\hat{H}t/\hbar}\,,}$$

denotes the time-evolution operator.[1] By inserting the resolution of identity, $\mathbb{I} = \sum_i |i\rangle\langle i|$, where the states $|i\rangle$ are eigenstates of the Hamiltonian with eigenvalue $E_i$, we find that

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} \sum_i |i\rangle\langle i|\psi(0)\rangle = \sum_i |i\rangle\langle i|\psi(0)\rangle e^{-iE_i t/\hbar}\,.$$

[1] This equation follows from integrating the time-dependent Schrödinger equation, $\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle$.

▷ EXAMPLE: Consider the harmonic oscillator Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2$. Later in this chapter, we will see that the eigenstates, $|n\rangle$, have equally-spaced eigenvalues, $E_n = \hbar\omega(n + 1/2)$, for $n = 0, 1, 2, \cdots$. Let us then consider the time-evolution of a general wavepacket, $|\psi(0)\rangle$, under the action of the Hamiltonian. From the equation above, we find that $|\psi(t)\rangle = \sum_n |n\rangle\langle n|\psi(0)\rangle e^{-iE_n t/\hbar}$. Since the eigenvalues are equally spaced, let us consider what happens when $t = t_r \equiv 2\pi r/\omega$, with $r$ integer. In this case, since $e^{2\pi i n r} = 1$, we have

$$|\psi(t_r)\rangle = \sum_n |n\rangle\langle n|\psi(0)\rangle e^{-i\omega t_r/2} = (-1)^r |\psi(0)\rangle\,.$$

From this result, we can see that, up to an overall phase, the wave packet is perfectly reconstructed at these times. This recurrence or "echo" is not generic, but is a manifestation of the equal separation of eigenvalues in the harmonic oscillator.

▷ EXERCISE. Using the symmetry of the harmonic oscillator wavefunctions under parity show that, at times $t_r = (2r + 1)\pi/\omega$, $\langle x|\psi(t_r)\rangle = e^{-i\omega t_r/2}\langle -x|\psi(0)\rangle$. Explain the origin of this recurrence.

The time-evolution operator is an example of a **unitary operator**. The latter are defined as transformations which preserve the scalar product, $\langle\phi|\psi\rangle = \langle\hat{U}\phi|\hat{U}\psi\rangle = \langle\phi|\hat{U}^\dagger\hat{U}\psi\rangle \stackrel{!}{=} \langle\phi|\psi\rangle$, i.e.

$$\boxed{\hat{U}^\dagger\hat{U} = \mathbb{I}\,.}$$

### 3.1.2 Uncertainty principle for non-commuting operators

For non-commuting Hermitian operators, $[\hat{A}, \hat{B}] \neq 0$, it is straightforward to establish a bound on the uncertainty in their expectation values. Given a state $|\psi\rangle$, the mean square uncertainty is defined as

$$(\Delta A)^2 = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2\psi\rangle = \langle\psi|\hat{U}^2\psi\rangle$$
$$(\Delta B)^2 = \langle\psi|(\hat{B} - \langle\hat{B}\rangle)^2\psi\rangle = \langle\psi|\hat{V}^2\psi\rangle\,,$$

where we have defined the operators $\hat{U} = \hat{A} - \langle\psi|\hat{A}\psi\rangle$ and $\hat{V} = \hat{B} - \langle\psi|\hat{B}\psi\rangle$. Since $\langle\hat{A}\rangle$ and $\langle\hat{B}\rangle$ are just constants, $[\hat{U}, \hat{V}] = [\hat{A}, \hat{B}]$. Now let us take the scalar product of $\hat{U}|\psi\rangle + i\lambda\hat{V}|\psi\rangle$ with itself to develop some information about the uncertainties. As a modulus, the scalar product must be greater than or equal to zero, i.e. expanding, we have $\langle\psi|\hat{U}^2\psi\rangle + \lambda^2\langle\psi|\hat{V}^2\psi\rangle + i\lambda\langle\hat{U}\psi|\hat{V}\psi\rangle - i\lambda\langle\hat{V}\psi|\hat{U}\psi\rangle \geq 0$. Reorganising this equation in terms of the uncertainties, we thus find

$$(\Delta A)^2 + \lambda^2(\Delta B)^2 + i\lambda\langle\psi|[\hat{U}, \hat{V}]|\psi\rangle \geq 0\,.$$

If we minimise this expression with respect to $\lambda$, we can determine when the inequality becomes strongest. In doing so, we find

$$2\lambda(\Delta B)^2 + i\langle\psi|[\hat{U}, \hat{V}]|\psi\rangle = 0, \qquad \lambda = -\frac{i}{2}\frac{\langle\psi|[\hat{U}, \hat{V}]|\psi\rangle}{(\Delta B)^2}\,.$$

Substiuting this value of $\lambda$ back into the inequality, we then find,

$$(\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}\langle\psi|[\hat{U}, \hat{V}]|\psi\rangle^2\,.$$

We therefore find that, for non-commuting operators, the uncertainties obey the following inequality,

$$\boxed{\Delta A\,\Delta B \geq \frac{i}{2}\langle[\hat{A},\hat{B}]\rangle\,.}$$

If the commutator is a constant, as in the case of the conjugate operators $[\hat{p},x] = -i\hbar$, the expectation values can be dropped, and we obtain the relation, $(\Delta A)(\Delta B) \geq \frac{i}{2}[\hat{A},\hat{B}]$. For momentum and position, this result recovers **Heisenberg's uncertainty principle**,

$$\boxed{\Delta p\,\Delta x \geq \frac{i}{2}\langle[\hat{p},x]\rangle = \frac{\hbar}{2}\,.}$$

Similarly, if we use the conjugate coordinates of time and energy, $[\hat{E},t] = i\hbar$, we have

$$\boxed{\Delta E\,\Delta t \geq \frac{\hbar}{2}\,.}$$

### 3.1.3 Time-evolution of expectation values

Finally, to close this section on operators, let us consider how their expectation values evolve. To do so, let us consider a general operator $\hat{A}$ which may itself involve time. The time derivative of a general expectation value has three terms.

$$\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \partial_t(\langle\psi|)\hat{A}|\psi\rangle + \langle\psi|\partial_t\hat{A}|\psi\rangle + \langle\psi|\hat{A}(\partial_t|\psi\rangle)\,.$$

If we then make use of the time-dependent Schrödinger equation, $i\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle$, and the Hermiticity of the Hamiltonian, we obtain

$$\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \underbrace{\frac{i}{\hbar}\Big(\langle\psi|\hat{H}\hat{A}|\psi\rangle - \langle\psi|\hat{A}\hat{H}|\psi\rangle\Big)}_{\frac{i}{\hbar}\langle\psi|[\hat{H},\hat{A}]|\psi\rangle} + \langle\psi|\partial_t\hat{A}|\psi\rangle\,.$$

This is an important and general result for the time derivative of expectation values which becomes simple if the operator itself does not explicitly depend on time,

$$\boxed{\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{A}]|\psi\rangle\,.}$$

From this result, which is known as **Ehrenfest's theorem**, we see that expectation values of operators that commute with the Hamiltonian are constants of the motion.

▷ Exercise. Applied to the non-relativistic Schrödinger operator for a single particle moving in a potential, $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, show that $\langle\dot{x}\rangle = \frac{\langle\hat{p}\rangle}{m}$, $\langle\dot{\hat{p}}\rangle = -\langle\partial_x V\rangle$. Show that these equations are consistent with the relations,

$$\frac{d}{dt}\langle x\rangle = \left\langle\frac{\partial H}{\partial p}\right\rangle, \qquad \frac{d}{dt}\langle\hat{p}\rangle = -\left\langle\frac{\partial H}{\partial x}\right\rangle,$$

the counterpart of Hamilton's classical equations of motion.

**Paul Ehrenfest 1880-1933**

An Austrian physicist and mathematician, who obtained Dutch citizenship in 1922. He made major contributions to the field of statistical mechanics and its relations with quantum mechanics, including the theory of phase transition and the Ehrenfest theorem.

## 3.2 Symmetry in quantum mechanics

Symmetry considerations are very important in quantum theory. The structure of eigenstates and the spectrum of energy levels of a quantum system reflect the symmetry of its Hamiltonian. As we will see later, the transition probabilities between different states under a perturbation, such as that imposed by an external electromagnetic field, depend in a crucial way on the transformation properties of the perturbation and lead to "selection rules". Symmetries can be classified into two types, discrete and continuous, according to the transformations that generate them. For example, a mirror symmetry is an example of a discrete symmetry while a rotation in three-dimensional space is continuous.

Formally, the symmetries of a quantum system can be represented by a group of unitary transformations (or operators), $\hat{U}$, that act in the Hilbert space.[2] Under the action of such a unitary transformation, operators corresponding to observables $\hat{A}$ of the quantum model will then transform as,

$$\hat{A} \to \hat{U}^\dagger \hat{A} \hat{U} \,.$$

For unitary transformations, we have seen that $\hat{U}^\dagger \hat{U} = \mathbb{I}$, i.e. $\hat{U}^\dagger = \hat{U}^{-1}$. Under what circumstances does such a group of transformations represent a **symmetry group**? Consider a Schrödinger particle in three dimensions:[3] The basic observables are the position and momentum vectors, $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$. We can always define a transformation of the coordinate system, or the observables, such that a vector $\hat{\mathbf{A}} = \hat{\mathbf{r}}$ or $\hat{\mathbf{p}}$ is mapped to $\mathbf{R}[\hat{\mathbf{A}}]$.[4] If $\mathbf{R}$ is an element of the group of transformations, then this transformation will be represented by a unitary operator $\hat{U}(\mathbf{R})$, such that

$$\hat{U}^\dagger \hat{\mathbf{A}} \hat{U} = \mathbf{R}[\hat{\mathbf{A}}] \,.$$

Such unitary transformations are said to be **symmetries of a general operator** $\hat{O}(\hat{\mathbf{p}}, \hat{\mathbf{r}})$ if

$$\boxed{\hat{U}^\dagger \hat{O} \hat{U} = \hat{O}, \qquad \text{i.e.} \quad [\hat{O}, \hat{U}] = 0 \,.}$$

If $\hat{O}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) \equiv \hat{H}$, the quantum Hamiltonian, such unitary transformations are said to be symmetries of the quantum system.

### 3.2.1 Observables as generators of transformations

The vector operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ for a Schrödinger particle are themselves generators of space-time transformations. From the standard commutation relations

[2] In quantum mechanics, the possible states of a system can be represented by unit vectors (called "state vectors") residing in "state space" known as the **Hilbert space**. The precise nature of the Hilbert space is dependent on the system; for example, the state space for position and momentum states is the space of square-integrable functions.

[3] In the following, we will focus our considerations on the realm of "low-energy" physics where the relevant space-time transformations belong to the **Galilei group**, leaving our discussion of **Lorentz invariance** to the chapter on relativistic quantum mechanics.

[4] e.g., for a clockwise spatial rotation by an angle $\theta$ around $\mathbf{e}_z$, we have,

$$\mathbf{R}[\mathbf{r}] = R_{ij} \hat{x}_j, \qquad \mathbf{R} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

Similarly, for a spatial translation by a vector $\mathbf{a}$, $\mathbf{R}[\mathbf{r}] = \mathbf{r} + \mathbf{a}$. (Exercise: construct representations for transformations corresponding to spatial reflections, and inversion.)

one can show that, for a constant vector $\mathbf{a}$, the unitary operator

$$\hat{U}(\mathbf{a}) = \exp\left[-\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{p}}\right],$$

acting in the Hilbert space of a Schrödinger particle performs a **spatial translation**, $\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) = f(\mathbf{r}+\mathbf{a})$, where $f(\mathbf{r})$ denotes a general algebraic function of $\mathbf{r}$.

▷ INFO. The **proof** runs as follows: With $\hat{\mathbf{p}} = -i\hbar\nabla$,

$$\hat{U}^\dagger(\mathbf{a}) = e^{\mathbf{a}\cdot\nabla} = \sum_{n=0}^{\infty}\frac{1}{n!}a_{i_1}\cdots a_{i_n}\nabla_{i_1}\cdots\nabla_{i_n},$$

where summation on the repeated indicies, $i_m$ is assumed. Then, making use of the **Baker-Hausdorff identity** (exercise)

$$\boxed{e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \cdots,} \tag{3.3}$$

it follows that

$$\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) = f(\mathbf{r}) + a_{i_1}(\nabla_{i_1}f(\mathbf{r})) + \frac{1}{2!}a_{i_1}a_{i_2}(\nabla_{i_1}\nabla_{i_2}f(\mathbf{r})) + \cdots = f(\mathbf{r}+\mathbf{a}),$$

where the last identity follows from the Taylor expansion.

▷ EXERCISE. Prove the Baker-Hausdorff identity (3.3).

Therefore, a quantum system has spatial translation as an invariance group if and only if the following condition holds,

$$\hat{U}(\mathbf{a})\hat{H} = \hat{H}\hat{U}(\mathbf{a}), \qquad \text{i.e.} \quad \hat{\mathbf{p}}\hat{H} = \hat{H}\hat{\mathbf{p}}.$$

This demands that the Hamiltonian is independent of position, $\hat{H} = \hat{H}(\hat{\mathbf{p}})$, as one might have expected! Similarly, the group of unitary transformations, $\hat{U}(\mathbf{b}) = \exp[-\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{r}}]$, performs **translations in momentum space**. Moreover, **spatial rotations** are generated by the transformation $\hat{U}(\mathbf{b}) = \exp[-\frac{i}{\hbar}\theta\mathbf{e}_n\cdot\hat{\mathbf{L}}]$, where $\hat{\mathbf{L}} = \hat{\mathbf{r}}\times\hat{\mathbf{p}}$ denotes the angular momentum operator.

▷ EXERCISE. For an infinitesimal rotation by an angle $\theta$ by a fixed axis, $\hat{\mathbf{e}}_n$, construct $\mathbf{R}[\mathbf{r}]$ and show that $\hat{U} = \mathbb{I} - \frac{i}{\hbar}\theta\hat{\mathbf{e}}_n\cdot\mathbf{L} + O(\theta^2)$. Making use of the identity $\lim_{N\to\infty}(1-\frac{a}{N})^N = e^{-a}$, show that "large" rotations are indeed generated by the unitary transformations $\hat{U} = \exp\left[-\frac{i}{\hbar}\theta\hat{\mathbf{e}}_n\cdot\mathbf{L}\right]$.

As we have seen, **time translations** are generated by the time evolution operator, $\hat{U}(t) = \exp[-\frac{i}{\hbar}\hat{H}t]$. Therefore, every observable which commutes with the Hamiltonian is a constant of the motion (invariant under time translations),

$$\hat{H}\hat{A} = \hat{A}\hat{H} \;\Rightarrow\; e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar} = \hat{A}, \qquad \forall t.$$

We now turn to consider some examples of discrete symmetries. Amongst these, perhaps the most important in low-energy physics are parity and time-reversal. The **parity** operation, denoted $\hat{P}$, involves a reversal of sign on all coordinates.

$$\boxed{\hat{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}).}$$

This is clearly a discrete transformation. Application of parity twice returns the initial state implying that $\hat{P}^2 = 1$. Therefore, the eigenvalues of the parity operation (if such exist) are $\pm 1$. A wavefunction will have a defined parity if and only if it is an even or odd function. For example, for $\psi(x) = \cos(x)$, $\hat{P}\psi = \cos(-x) = \cos(x) = \psi$; thus $\psi$ is even and $P = 1$. Similarly $\psi = \sin(x)$ is odd with $P = -1$. Later, in the next chapter, we will encounter the spherical harmonic functions which have the following important symmetry under parity, $\hat{P}Y_{\ell m} = (-1)^{\ell} Y_{lm}$. Parity will be conserved if the Hamiltonian is invariant under the parity operation, i.e. if the Hamiltonian is invariant under a reversal of sign of all the coordinates.[5]

In classical mechanics, the **time-reversal** operation involves simply "running the movie backwards". The time-reversed state of the phase space coordinates $(x(t), p(t))$ is defined by $(x_T(t), p_T(t))$ where $x_T(t) = x(t)$ and $p_T(t) = -p(t)$. Hence, if the system evolved from $(x(0), p(0))$ to $(x(t), p(t))$ in time $t$ and at $t$ we reverse the velocity, $p(t) \to -p(t)$ with $x(t) \to x(t)$, at time $2t$ the system would have returned to $x(2t) = x(0)$ while $p(2t) = -p(0)$. If this happens, we say that the system is time-reversal invariant. Of course, this is just the statement that Newton's laws are the same if $t \to -t$. A notable case where this is not true is that of a charged particle in a magnetic field.

As with classical mechanics, time-reversal in quantum mechanics involves the operation $t \to -t$. However, referring to the time-dependent Schrödinger equation, $i\hbar\partial_t\psi(x,t) = \hat{H}\psi(x,t)$, we can see that the operation $t \to -t$ is equivalent to complex conjugation of the wavefunction, $\psi \to \psi^*$ if $\hat{H}^* = \hat{H}$. Let us then consider the time-evolution of $\psi(x,t)$,

$$\psi(x,0) \to e^{-\frac{i}{\hbar}\hat{H}(x)t}\psi(x,0) \overset{\text{c.c.}}{\to} e^{+\frac{i}{\hbar}\hat{H}^*(x)t}\psi^*(x,0) \overset{\text{evolve}}{\to} e^{-\frac{i}{\hbar}\hat{H}(x)t}e^{+\frac{i}{\hbar}\hat{H}^*(x)t}\psi^*(x,0)\,.$$

If we require that $\psi(x,2t) = \psi^*(x,0)$, we must have $\hat{H}^*(x) = \hat{H}(x)$. Therefore, $\hat{H}$ is invariant under time-reversal if and only if $\hat{H}$ is real.

▷ INFO. Although the group of space-transformations covers the symmetries that pertain to "low-energy" quantum physics, such as atomic physics, quantum optics, and quantum chemistry, in nuclear physics and elementary particle physics new observables come into play (e.g. the isospin quantum numbers and the other quark charges in the standard model). They generate symmetry groups which lack a classical counterpart, and they do not have any obvious relation with space-time transformations. These symmetries are often called **internal symmetries** in order to underline this fact.

### 3.2.2 Consequences of symmetries: multiplets

Having established how to identify whether an operator belongs to a group of symmetry transformations, we now consider the consequences. Consider a single unitary transformation $\hat{U}$ in the Hilbert space, and an observable $\hat{A}$ which commutes with $\hat{U}$, $[\hat{U}, \hat{A}] = 0$. If $\hat{A}$ has an eigenvector $|a\rangle$, it follows that $\hat{U}|a\rangle$ will be an eigenvector with the same eigenvalue, i.e.

$$\hat{U}\hat{A}|a\rangle = \hat{A}U|a\rangle = aU|a\rangle\,.$$

This means that either:

[5] In high energy physics, parity is a symmetry of the strong and electromagnetic forces, but does not hold for the weak force. Therefore, parity is conserved in strong and electromagnetic interactions, but is violated in weak interactions.

1. $|a\rangle$ is an eigenvector of both $\hat{A}$ and $\hat{U}$, or
2. the eigenvalue $a$ is degenerate: the linear space spanned by the vectors $\hat{U}^n|a\rangle$ ($n$ integer) are eigenvectors with the same eigenvalue.

This mathematical argument leads to the conclusion that, given a group G of unitary operators $\hat{U}(x)$, $x \in \mathrm{G}$, for any observable which is invariant under these transformations, i.e.

$$[\hat{U}(x), \hat{A}] = 0 \quad \forall x \in \mathrm{G}\,,$$

its discrete eigenvalues and eigenvectors will show a characteristic multiplet structure: there will be a degeneracy due to the symmetry such that the eigenvectors belonging to each eigenvalue form an invariant subspace under the group of transformations.

▷ EXAMPLE: For example, if the Hamiltonian commutes with the angular momentum operators, $\hat{L}_i$, $i = x, y, z$, i.e. it is invariant under three-dimensional rotations, an energy level with a given orbital quantum number $\ell$ is at least $(2\ell + 1)$-fold degenerate. Such a degeneracy can be seen as the result of non-trivial actions of the operator $\hat{L}_x$ and $\hat{L}_y$ on an energy (and $\hat{L}_z$) eigenstate $|E, \ell, m\rangle$ (where $m$ is the magnetic quantum number asssociated with $\hat{L}_z$).

## 3.3 The Heisenberg Picture

Until now, the time dependence of an evolving quantum system has been placed within the wavefunction while the operators have remained constant – this is the **Schrödinger picture** or **representation**. However, it is sometimes useful to transfer the time-dependence to the operators. To see how, let us consider the expectation value of some operator $\hat{B}$,

$$\langle\psi(t)|\hat{B}|\psi(t)\rangle = \langle e^{-i\hat{H}t/\hbar}\psi(0)|\hat{B}|e^{-i\hat{H}t/\hbar}\psi(0)\rangle = \langle\psi(0)|e^{i\hat{H}t/\hbar}\hat{B}e^{-i\hat{H}t/\hbar}|\psi(0)\rangle\,.$$

According to rules of associativity, we can multiply operators together before using them. If we define the operator $\hat{B}(t) = e^{i\hat{H}t/\hbar}\hat{B}e^{-i\hat{H}t/\hbar}$, the time-dependence of the expectation values has been transferred from the wavefunction. This is called the **Heisenberg picture** or **representation** and in it, the operators evolve with time while the wavefunctions remain constant. In this representation, the time derivative of the operator itself is given by

$$\begin{aligned}\partial_t\hat{B}(t) &= \frac{i\hat{H}}{\hbar}e^{i\hat{H}t/\hbar}\hat{B}e^{-i\hat{H}t/\hbar} - e^{i\hat{H}t/\hbar}\hat{B}\frac{i\hat{H}}{\hbar}e^{-i\hat{H}t/\hbar}\\ &= \frac{i}{\hbar}e^{i\hat{H}t/\hbar}[\hat{H}, \hat{B}]e^{-i\hat{H}t/\hbar} = \frac{i}{\hbar}[\hat{H}, \hat{B}(t)]\,.\end{aligned}$$

▷ EXERCISE. For the general Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, show that the position and momentum operators obey Hamilton's classical equation of motion.

**Werner Heisenberg 1901-76**

A German physicist and one of the founders of the quantum theory, he is best known for his uncertainty principle which states that it is impossible to determine with arbitrarily high accuracy both the position and momentum of a particle. In 1926, Heisenberg developed a form of the quantum theory known as matrix mechanics, which was quickly shown to be fully equivalent to Erwin Schrödinger's wave mechanics. His 1932 Nobel Prize in Physics cited not only his work on quantum theory but also work in nuclear physics in which he predicted the subsequently verified existence of two allotropic forms of molecular hydrogen, differing in their values of nuclear spin.

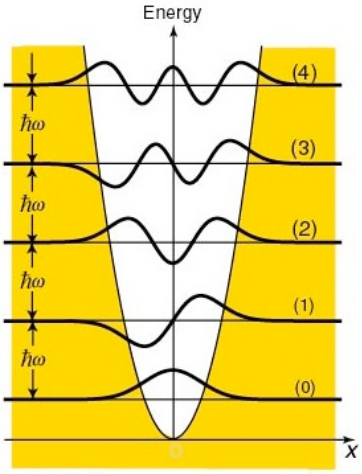
## 3.4 Quantum harmonic oscillator

As we will see time and again in this course, the harmonic oscillator assumes a priveledged position in quantum mechanics and quantum field theory finding

numerous and somtimes unexpected applications. It is useful to us now in that it provides a platform for us to implement some of the technology that has been developed in this chapter. In the one-dimensional case, the quantum harmonic oscillator Hamiltonian takes the form,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \,,$$

where $\hat{p} = -i\hbar\partial_x$. To find the eigenstates of the Hamiltonian, we could look for solutions of the linear second order differential equation corresponding to the time-independent Schrödinger equation, $\hat{H}\psi = E\psi$, where $\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2 x^2$. The integrability of the Schrödinger operator in this case allows the stationary states to be expressed in terms of a set of orthogonal functions known as Hermite polynomials. However, the complexity of the exact eigenstates obscure a number of special and useful features of the harmonic oscillator system. To identify these features, we will instead follow a method based on an operator formalism.



First few states of the quantum harmonic oscillator. Not that the parity of the state changes from even to odd through consecutive states.

The form of the Hamiltonian as the sum of the squares of momenta and position suggests that it can be recast as the "square of an operator". To this end, let us introduce the operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + i\frac{\hat{p}}{m\omega}\right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{\hat{p}}{m\omega}\right),$$

where, for notational convenience, we have not drawn hats on the operators $a$ and its Hermitian conjuate $a^\dagger$. Making use of the identity,

$$a^\dagger a = \frac{m\omega}{2\hbar}x^2 + \frac{\hat{p}}{2\hbar m\omega} + \frac{i}{2\hbar}[x,\hat{p}] = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$$

and the parallel relation, $aa^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2}$, we see that the operators fulfil the commutation relations

$$\boxed{[a, a^\dagger] \equiv aa^\dagger - a^\dagger a = 1\,.}$$

Then, setting $\hat{n} = a^\dagger a$, the Hamiltonian can be cast in the form

$$\boxed{\hat{H} = \hbar\omega(\hat{n} + 1/2)\,.}$$

Since the operator $\hat{n} = a^\dagger a$ must lead to a positive definite result, we see that the eigenstates of the harmonic oscillator must have energies of $\hbar\omega/2$ or higher. Moreover, the ground state $|0\rangle$ can be identified by finding the state for which $a|0\rangle = 0$. Expressed in the coordinate basis, this translates to the equation,[6]

$$\left(x + \frac{\hbar}{m\omega}\partial_x\right)\psi_0(x) = 0, \qquad \psi_0(x) = \langle x|0\rangle = \sqrt{\frac{m\omega}{\pi^{1/2}\hbar}}e^{-m\omega x^2/2\hbar}\,.$$

Since $\hat{n}|0\rangle = a^\dagger a|0\rangle = 0$, this state is an eigenstate with energy $\hbar\omega/2$. The higher lying states can be found by acting upon this state with the operator $a^\dagger$. The proof runs as follows: If $\hat{n}|n\rangle = n|n\rangle$, we have

$$\hat{n}(a^\dagger|n\rangle) = a^\dagger \underbrace{aa^\dagger}_{a^\dagger a+1}|n\rangle = (a^\dagger \underbrace{a^\dagger a}_{\hat{n}} + a^\dagger)|n\rangle = (n+1)a^\dagger|n\rangle$$

[6] Formally, in coordinate basis, we have $\langle x'|a|x\rangle = \delta(x'-x)(a + \frac{\hbar}{m\omega}\partial_x)$ and $\langle x|0\rangle = \psi_0(x)$. Then making use of the resolution of identity $\int dx|x\rangle\langle x| = \mathbb{I}$, we have

$$\langle x|a|0\rangle = 0 = \int dx\,\langle x|a|x'\rangle\langle x'|0\rangle = \left(x + \frac{\hbar}{m\omega}\partial_x\right)\psi_0(x)\,.$$

or, equivalently, $[\hat{n}, a^\dagger] = a^\dagger$. In other words, if $|n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $n$, then $a^\dagger|n\rangle$ is an eigenstate with eigenvalue $n+1$.

From this result, we can deduce that the eigenstates for a "tower" $|0\rangle$, $|1\rangle = C_1 a^\dagger|0\rangle$, $|2\rangle = C_2(a^\dagger)^2|0\rangle$, etc., where $C_n$ denotes the normalization. If $\langle n|n\rangle = 1$ we have

$$\langle n|aa^\dagger|n\rangle = \langle n|(\hat{n}+1)|n\rangle = (n+1)\,.$$

Therefore, with $|n+1\rangle = \frac{1}{\sqrt{n+1}}a^\dagger|n\rangle$ the state $|n+1\rangle$ is also normalized, $\langle n+1|n+1\rangle = 1$. By induction, we can deduce the general normalization,

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle\,,}$$

with $\langle n|n'\rangle = \delta_{nn'}$, $\hat{H}|n\rangle = \hbar\omega(n+1/2)|n\rangle$ and

$$\boxed{a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \qquad a|n\rangle = \sqrt{n}|n-1\rangle\,.}$$

The operators $a$ and $a^\dagger$ represent **ladder operators** and have the effect of lowering or raising the energy of the state.

In fact, the operator representation achieves something quite remarkable and, as we will see, unexpectedly profound. The quantum harmonic oscillator describes the motion of a *single* particle in a one-dimensional potential well. It's eigenvalues turn out to be equally spaced – a ladder of eigenvalues, separated by a constant energy $\hbar\omega$. If we are energetic, we can of course translate our results into a coordinate representation $\psi_n(x) = \langle x|n\rangle$.[7] However, the operator representation affords a second interpretation, one that lends itself to further generalization in quantum field theory. We can instead interpret the quantum harmonic oscillator as a simple system involving many fictitious particles, each of energy $\hbar\omega$. In this representation, known as the **Fock space**, the vacuum state $|0\rangle$ is one involving no particles, $|1\rangle$ involves a single particle, $|2\rangle$ has two and so on. These fictitious particles are created and annihilated by the action of the raising and lowering operators, $a^\dagger$ and $a$ with canonical commutation relations, $[a, a^\dagger] = 1$. Later in the course, we will find that these commutation relations are the hallmark of **bosonic** quantum particles and this representation, known as the **second quantization** underpins the quantum field theory of the electromagnetic field.

▷ INFO. There is evidently a huge difference between a stationary (Fock) state of the harmonic oscillator and its classical counterpart. For the classical system, the equations of motion are described by Hamilton's equations of motion,

$$\dot{X} = \partial_P H = \frac{P}{m}, \qquad \dot{P} = -\partial_X H = -\partial_x U = -m\omega^2 X\,,$$

where we have used capital letters to distinguish them from the arguments used to describe the quantum system. In the phase space, $\{X(t), P(t)\}$, these equations describe a clockwise rotation along an elliptic trajectory specified by the initial conditions $\{X(0), P(0)\}$. (Normalization of momentum by $m\omega$ makes the trajectory circular.)

[7] Expressed in real space, the harmonic oscillator wavefunctions are in fact described by the Hermite polynomials,

$$\psi_n(x) = \langle x|n\rangle = \sqrt{\frac{1}{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left[-\frac{m\omega x^2}{2\hbar}\right]\,,$$

where $H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$.

On the other hand, the time dependence of the Fock space state, as of any stationary state, is exponential,

$$\psi_n(x,t) = \langle x|n\rangle e^{-iE_n t/\hbar}\,,$$

and, as a result, gives time-independent expectation values of $x$, $p$, or any function thereof. The best classical image for such a state on the phase plane is a circle of radius $r = x_0(2n+1)^{1/2}$, where $x_0 = (\hbar/m\omega)^{1/2}$, along which the wavefunction is uniformly spread as a standing wave.

It is natural to ask how to form a wavepacket whose properties would be closer to the classical trajectories. Such states, with the centre in the classical point $\{X(t), P(t)\}$, and the smallest possible product of quantum uncertainties of coordinate and momentum, are called **Glauber states**.[8] Conceptually the simplest way to present the Glauber state $|\alpha\rangle$ is as the Fock ground state $|0\rangle$ with the centre shifted from the origin to the classical point $\{X(t), P(t)\}$. (After such a shift, the state automatically rotates, following the classical motion.) Let us study how this shift may be implemented in quantum mechanics. The mechanism for such shifts are called the translation operators.

Previously, we have seen that the space and momentum translation operators are given by

$$\hat{\mathcal{F}}_X = \exp\left[-\frac{i}{\hbar}\hat{p}X\right], \qquad \hat{\mathcal{F}}_P = \exp\left[-\frac{i}{\hbar}P\hat{x}\right].$$

A shift by both $X$ and $P$ is then given by

$$\hat{\mathcal{F}}_\alpha = \exp\left[\frac{i}{\hbar}(P\hat{x} - \hat{p}X)\right] = e^{\alpha a^\dagger - \alpha^* a}, \qquad \hat{\mathcal{F}}_\alpha^\dagger = e^{\alpha^* a - \alpha a^\dagger}\,,$$

where $\alpha$ is the (normalised) complex amplitude of the classical oscillations we are trying to approximate, i.e. $\alpha = \frac{1}{\sqrt{2}x_0}(X + i\frac{P}{m\omega})$. The Glauber state is then defined by $|\alpha\rangle = \hat{\mathcal{F}}_\alpha|0\rangle$.

Working directly with the shift operator is not too convenient because of its exponential form. However, it turns out that a much simpler representation for the Glauber state is possible. To see this, let us start with the following general property of exponential operators: if $[\hat{A}, \hat{B}] = \mu$ (where $\hat{A}$ and $\hat{B}$ are operators, and $\mu$ is a c-number), then (exercise – cf. Eq. (3.3)),

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \mu\,. \tag{3.4}$$

If we define $\hat{A} = \alpha^* a - \alpha a^\dagger$, then $\hat{\mathcal{F}}_\alpha = e^{-\hat{A}}$ and $\hat{\mathcal{F}}_\alpha^\dagger = e^{\hat{A}}$. If we then take $\hat{B} = \mathbb{I}$, we have $\mu = 0$, and $\hat{\mathcal{F}}_\alpha^\dagger\hat{\mathcal{F}}_\alpha = \mathbb{I}$. This merely means that the shift operator is unitary - not a big surprise, because if we shift the phase point by $(+\alpha)$ and then by $(-\alpha)$, we certainly come back to the initial position.

If we take $\hat{B} = a$, using the commutation relations,

$$[\hat{A}, \hat{B}] = [\alpha^* a - \alpha a^\dagger, a] = -\alpha[a^\dagger, a] = \alpha\,,$$

so that $\mu = \alpha$, and $\hat{\mathcal{F}}_\alpha^\dagger a\hat{\mathcal{F}}_\alpha = a + \alpha$. Now let us consider the operator $\hat{\mathcal{F}}_\alpha\hat{\mathcal{F}}_\alpha^\dagger a\hat{\mathcal{F}}_\alpha$. From the unitarity condition, this must equal $a\hat{\mathcal{F}}_\alpha$, while application of Eq. (3.4) yields $\hat{\mathcal{F}}_\alpha a + \alpha\hat{\mathcal{F}}_\alpha$, i.e.

$$a\hat{\mathcal{F}}_\alpha = \hat{\mathcal{F}}_\alpha a + \alpha\hat{\mathcal{F}}_\alpha\,.$$

Applying this equality to the ground state $|0\rangle$ and using the following identities, $a|0\rangle = 0$ and $\hat{\mathcal{F}}_\alpha|0\rangle = |\alpha\rangle$, we finally get a very simple and elegant result:

$$\boxed{a|\alpha\rangle = \alpha|\alpha\rangle\,.}$$

[8] After R. J. Glauber who studied these states in detail in the mid-1960s, though they were known to E. Schrödinger as early as in 1928. Another popular name, **coherent states**, does not make much sense, because all the quantum states we have studied so far (including the Fock states) may be presented as coherent superpositions.

Thus the Glauber state is an eigenstate of the annihilation operator, corresponding to the eigenvalue $\alpha$, i.e. to the (normalized) complex amplitude of the classical process approximated by the state. This fact makes the calculations of the Glauber state properties much simpler.

Presented as a superposition of Fock states, the Glauber state takes the form (exercise – try making use of the BCH identity (3.3).)

$$|\alpha\rangle = \sum_{n=0}^{\infty} \alpha_n |n\rangle, \qquad \alpha_n = e^{-|\alpha|^2/2} \frac{\alpha^n}{(n!)^{1/2}} .$$

This means that the probability of finding the system in level $n$ is given by the Poisson distribution, $P_n = |\alpha_n|^2 = \langle n\rangle^n e^{-\langle n\rangle}/n!$ where $\langle n\rangle = |\alpha|^2$. More importantly, $\delta n = \langle n\rangle^{1/2} \ll \langle n\rangle$ when $\langle n\rangle \gg 1$ – the Poisson distribution approaches the Gaussian distribution when $\langle n\rangle$ is large.

The time-evolution of Glauber states may be described most easily in the Schrödinger representation when the time-dependence is transferred to the wavefunction. In this case, $\alpha(t) \equiv \frac{1}{\sqrt{2}x_0}(X(t) + i\frac{P(t)}{m\omega})$, where $\{X(t), P(t)\}$ is the solution to the classical equations of motion, $\dot{\alpha}(t) = -i\omega\alpha(t)$. From the solution, $\alpha(t) = \alpha(0)e^{-i\omega t}$, one may show that the average position and momentum evolve classically while their fluctuations remain stationary,

$$\Delta x = \frac{x_0}{\sqrt{2}} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}, \qquad \Delta p = \frac{m\omega x_0}{\sqrt{2}} = \left(\frac{\hbar m\omega}{2m}\right)^{1/2} .$$

In the quantum theory of measurements these expressions are known as the "standard quantum limit". Notice that their product $\Delta x\, \Delta p = \hbar/2$ corresponds to the lower bound of the Heisenberg's uncertainty relation.

▷ Exercise. Show that, in position space, the Glauber state takes the form

$$\langle x|\alpha\rangle = \psi_\alpha(x) = C \exp\left[-\frac{m\omega}{2\hbar}(x - X)^2 + i\frac{Px}{\hbar}\right] .$$

This completes our abridged survey of operator methods in quantum mechanics. With this background, we are now in a position to summarize the basic postulates of quantum mechanics.

## 3.5 Postulates of quantum theory

Since there remains no "first principles" derivation of the quantum mechanical equations of motion, the theory is underpinned by a set of "postulates" whose validity rest on experimental verification. Needless to say, quantum mechanics remains perhaps the most successful theory in physics.

▷ **Postulate 1.** The state of a quantum mechanical system is completely specified by a function $\Psi(\mathbf{r}, t)$ that depends upon the coordinates of the particle(s) and on time. This function, called the wavefunction or state function, has the important property that $|\Psi(\mathbf{r}, t)|^2\, d\mathbf{r}$ represents the probability that the particle lies in the volume element $d\mathbf{r} \equiv d^d r$ located at position $\mathbf{r}$ at time $t$.

The wavefunction must satisfy certain mathematical conditions because of this probabilistic interpretation. For the case of a single particle, the net probability of finding it at some point in space must be unity leading to the normalization condition, $\int_{-\infty}^{\infty} |\Psi(\mathbf{r}, t)|^2\, d\mathbf{r} = 1$. It is customary to also normalize many-particle wavefunctions to unity. The wavefunction must also be single-valued, continuous, and finite.

▷ **Postulate 2.** To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics.

If we require that the expectation value of an operator $\hat{A}$ is real, then it follows that $\hat{A}$ must be a Hermitian operator. If the result of a measurement of an operator $\hat{A}$ is the number $a$, then $a$ must be one of the eigenvalues, $\hat{A}\Psi = a\Psi$, where $\Psi$ is the corresponding eigenfunction. This postulate captures a central point of quantum mechanics – the values of dynamical variables can be quantized (although it is still possible to have a continuum of eigenvalues in the case of unbound states).

▷ **Postulate 3.** If a system is in a state described by a normalized wavefunction $\Psi$, then the average value of the observable corresponding to $\hat{A}$ is given by

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi d\mathbf{r} \,.$$

If the system is in an eigenstate of $\hat{A}$ with eigenvalue $a$, then any measurement of the quantity $A$ will yield $a$. Although measurements must always yield an eigenvalue, the state does not have to be an eigenstate of $\hat{A}$ initially. An arbitrary state can be expanded in the complete set of eigenvectors of $\hat{A}$ ( $\hat{A}\Psi_i = a_i\Psi_i$) as $\Psi = \sum_i^n c_i \Psi_i$, where $n$ may go to infinity. In this case, the probability of obtaining the result $a_i$ from the measurement of $\hat{A}$ is given by $P(a_i) = |\langle \Psi_i | \Psi \rangle|^2 = |c_i|^2$. The expectation value of $\hat{A}$ for the state $\Psi$ is the sum over all possible values of the measurement and given by

$$\langle A \rangle = \sum_i a_i |\langle \Psi_i | \Psi \rangle|^2 = \sum_i a_i |c_i|^2 \,.$$

Finally, a measurement of $\Psi$ which leads to the eigenvalue $a_i$, causes the wavefunction to "collapses" into the corresponding eigenstate $\Psi_i$. (In the case that $a_i$ is degenerate, then $\Psi$ becomes the projection of $\Psi$ onto the degenerate subspace). Thus, measurement affects the state of the system.

▷ **Postulate 4.** The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi(\mathbf{r}, t) \,,$$

where $\hat{H}$ is the Hamiltonian of the system. If $\Psi$ is an eigenstate of $\hat{H}$, it follows that $\Psi(\mathbf{r}, t) = \Psi(\mathbf{r}, 0)e^{-iEt/\hbar}$.