1 Fundamentals of Quantum Mechanics

In this chapter we summarize the main elements of non-relativistic quantum mechanics. We will do so through a list of postulates and principles that can be followed for the application of the quantum mechanical formalism to specific problems. Although some of the postulates could be "derived" from more fundamental principles (e.g., the Schrödinger equation), we will not proceed along that path, which is covered in more elementary textbooks on quantum mechanics. We will also derive some important results, dealing with aspects of quantum mechanics that either physical or mathematical in nature.

Most of the material presented in this chapter is taken from Auletta, Fortunato and Parisi, Chaps. 1-3, and Cohen-Tannoudji, Diu and Laloë, Vol. I, Chap. 3.

1.1 The Postulates of Quantum Mechanics

1.1.1 First Postulate

At a given time t, the physical state of a system is described by a ***ket*** *$|\psi(t)\rangle$ (using Dirac's notation). From this ket a wave function dependent on position and time can be defined by the projection onto a basis defined by the* ***bra*** *$\langle\mathbf{r}|$. That is, the wave function is given by*

$$\psi(\mathbf{r},t) \equiv \langle\mathbf{r}\,|\,\psi(t)\rangle\,. \tag{1.1}$$

The symbol $\langle\,|\,\rangle$ is usually called a ***bracket****.*

Equation (1.1) is the result of the following two definitions. First, the bracket is by definition a scalar product

$$\langle\varphi\,|\,\chi\rangle \equiv \int_{-\infty}^{\infty} d^3x\,\varphi^*(\mathbf{x})\,\chi(\mathbf{x})\,, \tag{1.2}$$

where * stands for complex conjugation. Second, to the ket $|\mathbf{r}\rangle$ is associated a Dirac distribution

$$|\mathbf{r}\rangle \Longleftrightarrow \delta(\mathbf{x}-\mathbf{r})\,, \tag{1.3}$$

such that

$$\begin{aligned}\langle\mathbf{r}\,|\,\psi(t)\rangle &= \int_{-\infty}^{\infty} d^3x\,\delta(\mathbf{x}-\mathbf{r})\,\psi(\mathbf{x},t)\\ &\equiv \psi(\mathbf{r},t)\end{aligned} \tag{1.4}$$

since $\delta^*(\mathbf{x}) = \delta(\mathbf{x})$. Note that the "orthogonality" of the $|\mathbf{r}\rangle$ kets is apparent from

$$\begin{aligned}\langle \mathbf{r}' \,|\, \mathbf{r}\rangle &= \int_{-\infty}^{\infty} d^3x\, \delta\left(\mathbf{x}-\mathbf{r}'\right)\delta\left(\mathbf{x}-\mathbf{r}\right)\\ &= \delta\left(\mathbf{r}-\mathbf{r}'\right)\int_{-\infty}^{\infty} d^3x\, \delta\left(\mathbf{x}-\mathbf{r}\right)\\ &= \delta\left(\mathbf{r}-\mathbf{r}'\right).\end{aligned} \tag{1.5}$$

1.1.2 Second Postulate

*For every measurable physical quantity $\mathcal{A}$ corresponds an operator $\hat{A}$, and this operator is an **observable**.*

It is often the case that a representation of kets and operators is done through vectors and matrices, respectively. The action of the operator on the ket, in general, produces a new ket

$$|\varphi\rangle = \hat{A}\,|\psi\rangle\,, \tag{1.6}$$

and this action is the mathematical equivalent of the multiplication of a matrix and a vector. It follows that a bra can be represented by a row vector such that, for example

$$\begin{aligned}\langle\varphi| &= \left(\hat{A}\,|\psi\rangle\right)^{\dagger}\\ &= \langle\psi|\,\hat{A}^{\dagger},\end{aligned} \tag{1.7}$$

with $\hat{A}^{\dagger}$ the adjoint of $\hat{A}$ and, by definition, $(|\psi\rangle)^{\dagger} = \langle\psi|$.

1.1.3 Third Postulate

The outcome of the measurement of a physical quantity $\mathcal{A}$ must be an eigenvalue of the corresponding observable $\hat{A}$.

Since observables are related to physical quantities, then the matrix associated with them must be Hermitian. This is because the eigenvalues of Hermitian matrices are real quantities (in a mathematical sense). Recall that a matrix is Hermitian when

$$\hat{A}_{ij} = \hat{A}^*_{ji}, \tag{1.8}$$

Alternatively, a Hermitian operator is one that is self-adjoint. That is,

$$\hat{A}^{\dagger} = \hat{A}. \tag{1.9}$$

When the matrix is of finite dimension the eigenvalues are quantized (a "matrix" of infinite dimension would correspond to a continuum; for example, a matrix acting on $|\mathbf{r}\rangle$ would have to be of infinite dimension as $|\mathbf{r}\rangle$ encompasses the continuum made of all possible positions).

1.1.4 Fourth Postulate

The ket, say $|\psi(t)\rangle$, specifying the state of a system is assumed normalized to unity. That is,

$$\langle\psi(t)\,|\,\psi(t)\rangle = 1. \tag{1.10}$$

Alternatively, the associated wave function is also normalized, since

$$\begin{aligned}\langle\psi(t)\,|\,\psi(t)\rangle &= \int_{-\infty}^{\infty} d^3x\,\psi^*(\mathbf{x},t)\,\psi(\mathbf{x},t)\\ &= \int_{-\infty}^{\infty} d^3x\,|\psi(\mathbf{x},t)|^2\\ &= 1.\end{aligned} \tag{1.11}$$

This ket can also be expanded using any suitable (complete) basis of kets. For example, using the $\{|\mathbf{r}\rangle\}$ basis we have

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} d^3r\,c(\mathbf{r},t)\,|\mathbf{r}\rangle\,, \tag{1.12}$$

where $c(\mathbf{r},t)$ is a complex coefficient (for this particular case it is actually the wave function itself, see equations (1.1) and (1.4)) resulting from the projection of $|\psi(t)\rangle$ on $\langle\mathbf{r}|$. Equation (1.12) can therefore be written as

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} d^3r\,[\langle\mathbf{r}\,|\,\psi(t)\rangle]\,|\mathbf{r}\rangle\,. \tag{1.13}$$

Rearranging this last equation we have

$$|\psi(t)\rangle = \left[\int_{-\infty}^{\infty} d^3r\,|\mathbf{r}\rangle\langle\mathbf{r}|\right]|\psi(t)\rangle\,, \tag{1.14}$$

which implies that

$$\int_{-\infty}^{\infty} d^3r\,|\mathbf{r}\rangle\langle\mathbf{r}| = \hat{1}, \tag{1.15}$$

where $\hat{1}$ is the unit operator (or matrix). Similarly any other normalized ket $|\varphi\rangle$ that can be expanded with a (complete) discrete and orthonormal basis $|u_i\rangle$ (i.e., $\langle u_i\,|\,u_j\rangle = \delta_{ij}$) with

$$\begin{aligned}|\varphi\rangle &= \sum_i [\langle u_i\,|\,\varphi\rangle]\,|u_i\rangle\\ &= \sum_i c_i\,|u_i\rangle\,,\end{aligned} \tag{1.16}$$

is also normalized to unity, and we have the following relation for the basis

$$\sum_i |u_i\rangle\langle u_i| = \hat{1}. \tag{1.17}$$

Equation (1.17) (as well as equation (1.15)) is a completeness relation that must be satisfied for the corresponding basis to be complete. In consideration of these facts and definitions, we can state the fourth postulate of quantum mechanics as follows:

In measuring the physical quantity $\mathcal{A}$ on a system in the state $|\psi\rangle$, the probability of obtaining the (possibly degenerate) eigenvalue "a" of the corresponding observable is

$$\mathcal{P}(a) = \sum_i^{g_n} \left|\left\langle u_n^i \,\middle|\, \psi\right\rangle\right|^2, \tag{1.18}$$

for discrete states, with g_n the degree of degeneracy of "a", and $\left\{\left|u_n^i\right\rangle\right\}$ the set of degenerate eigenvectors. For continuum states the corresponding probability is given by

$$d\mathcal{P}(a) = \left|\langle v_a \,|\, \psi\rangle\right|^2 da, \tag{1.19}$$

where $|v_a\rangle$ is the eigenvector associated with the eigenvalue "a".

We can apply this postulate to the case of a discrete degenerate state by starting with a generalization of equation (1.16)

$$|\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i \left|u_n^i\right\rangle. \tag{1.20}$$

Projecting this state on the set of states $\left|u_m^j\right\rangle$ of degeneracy g_m (i.e., $j = 1, 2, \ldots, g_m$), and taking the sum of the square of the norm we get

$$\begin{aligned} \sum_{j=1}^{g_m} \left|\left\langle u_m^j \,\middle|\, \psi\right\rangle\right|^2 &= \sum_{j=1}^{g_m} \left| \sum_n \sum_{i=1}^{g_n} c_n^i \left\langle u_m^j \,\middle|\, u_n^i\right\rangle \right|^2 \\ &= \sum_{j=1}^{g_m} \left| \sum_n \sum_{i=1}^{g_n} c_n^i \delta_{ij}\delta_{mn} \right|^2 \\ &= \sum_{j=1}^{g_m} \left|c_m^j\right|^2. \end{aligned} \tag{1.21}$$

We therefore see that the probability of finding the system in a state (or group of states) possessing a given eigenvalue is proportional to the square of the coefficients c_m^j that appear in the expansion defining the state in term of the basis under consideration (as is evident from equation (1.20)).

Alternatively, we define the **projector** $\hat{P}_n$

$$\hat{P}_n \equiv \sum_{i=1}^{g_n} \left|u_n^i\right\rangle\left\langle u_n^i\right| \tag{1.22}$$

as the operator that projects a given state, say $|\psi\rangle$, on the subspace containing the set of eigenvectors $\left\{\left|u_n^i\right\rangle\right\}$ that share the same eigenvalue. For example, using equation (1.22) on $|\psi\rangle$ we find

$$\begin{aligned} \hat{P}_n \left|\psi\right\rangle &= \sum_{i=1}^{g_n} \left|u_n^i\right\rangle \left\langle u_n^i \mid \psi\right\rangle \\ &= \sum_{i=1}^{g_n} c_n^i \left|u_n^i\right\rangle, \end{aligned} \tag{1.23}$$

and it is clear from a comparison with equation (1.20) that the only part of $|\psi\rangle$ that is left is that corresponding to the subspace containing the eigenvectors $\left\{\left|u_n^i\right\rangle\right\}$. It should be clear that there are as many projectors $\hat{P}_n$, similarly defined through equation (1.22) for all possible g_n, as there are independent subspaces. We then have a generalization of equation (1.17) with

$$\begin{aligned} \hat{P}_\mathrm{d} &= \sum_n \hat{P}_n \\ &= \sum_n \sum_{i=1}^{g_n} \left|u_n^i\right\rangle\left\langle u_n^i\right| \\ &= \hat{1}, \end{aligned} \tag{1.24}$$

where the unit operator $\hat{1}$ covers the full space. For a continuum of states, the projector on the subspace $\{|v_a\rangle\}$ corresponding to the domain of eigenvalues specified by $a_1 \leq a \leq a_2$ is

$$\hat{P}_{\Delta a} = \int_{a_1}^{a_2} |v_a\rangle\langle v_a|\, da, \tag{1.25}$$

and for the full space we have

$$\begin{aligned} \hat{P}_\mathrm{c} &= \int_{-\infty}^{\infty} |v_a\rangle\langle v_a|\, da \\ &= \hat{1}. \end{aligned} \tag{1.26}$$

It is important to note that projectors can always be used to define quantum observables as follows (for the discrete case)

$$\hat{A} = \sum_n a_n \hat{P}_n. \tag{1.27}$$

When applied to an eigenvector $\left|u_m^j\right\rangle$ the operator yields

$$\begin{aligned}
\hat{A}\left|u_m^j\right\rangle &= \sum_n a_n \hat{P}_n \left|u_m^j\right\rangle \\
&= \sum_n a_n \sum_{i=1}^{g_n} \left|u_n^i\right\rangle \left\langle u_n^i \mid u_m^j\right\rangle \\
&= \sum_n a_n \sum_{i=1}^{g_n} \left|u_n^i\right\rangle \delta_{ij}\delta_{mn} \\
&= a_m \left|u_m^j\right\rangle . \qquad (1.28)
\end{aligned}$$

That is, when operating on an eigenvector the observable yields a measurement of the associated eigenvalue. For continuous states the counterpart to equation (1.27) is

$$\hat{A} = \int da\, a\hat{P}\left(a\right), \qquad (1.29)$$

with $\hat{P}\left(a\right) = |v_a\rangle\langle v_a|$. It is, however, important to note that the action of an observable on a generic state vector does not always yield a measurement (i.e., the result is not the same state vector multiplied by its eigenvalue). For example, let us consider the state

$$|\varphi\rangle = \frac{1}{\sqrt{2}}\left(|u_1\rangle + |u_2\rangle\right), \qquad (1.30)$$

then with $\hat{A}$ defined with equation (1.27)

$$\hat{A}\left|\varphi\right\rangle = \frac{1}{\sqrt{2}}\left(a_1\left|u_1\right\rangle + a_2\left|u_2\right\rangle\right). \qquad (1.31)$$

Rather than resulting in a measurement this process yields a transformation of the initial state vector.

Finally, it can happen that the spectrum (i.e., the set of all possible eigenvalues) of an observable contains both discrete and continuum subspaces. For example, if the eigenvalues $a \geq a_m$ are part of the continuum then

$$\begin{aligned}
\hat{P} &= \hat{P}_{\mathrm{d}} + \hat{P}_{\mathrm{c}} \\
&= \sum_{n<m}\sum_{i=1}^{g_n} \left|u_n^i\right\rangle\left\langle u_n^i\right| + \int_{a_m}^{\infty} |v_a\rangle\langle v_a|\, da \\
&= \hat{1}. \qquad (1.32)
\end{aligned}$$

Exercise 1.1. Let us consider a three-dimensional discrete space where an observable $\hat{A}$ has the following eigenkets, represented as column vectors,

$$|u_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{1.33}$$

$$\left|u_2^1\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix} \tag{1.34}$$

$$\left|u_2^2\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix}. \tag{1.35}$$

The ket $|u_1\rangle$ has the eigenvalue a_1, while $\left|u_2^1\right\rangle$ and $\left|u_2^2\right\rangle$ are degenerate and share the eigenvalue a_2. Determine *i)* the matrices for the projectors $\hat{P}_1$ and $\hat{P}_2$ for the two subspaces that span the whole three-dimensional space, *ii)* the matrix for the overall projector of that three-dimensional space, *iii)* the matrix for the observable $\hat{A}$, and *iv)* verify that in general $\hat{P}_j^n = \hat{P}_j$.

Solution.

First, we can verify that all the eigenvectors are normalized. That is,

$$\begin{aligned} \langle u_1 \,|\, u_1\rangle &= \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \\ &= 1 \end{aligned} \tag{1.36}$$

$$\begin{aligned} \left\langle u_2^1 \,\middle|\, u_2^1\right\rangle &= \frac{1}{2} \begin{pmatrix} 0 & 1 & -i \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix} \\ &= 1 \end{aligned} \tag{1.37}$$

$$\begin{aligned} \left\langle u_2^2 \,\middle|\, u_2^2\right\rangle &= \frac{1}{2} \begin{pmatrix} 0 & 1 & i \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix} \\ &= 1. \end{aligned} \tag{1.38}$$

It is also straightforward to verify that they are mutually orthogonal. That is, $\left\langle u_1 \,\middle|\, u_2^i\right\rangle = \left\langle u_2^i \,\middle|\, u_2^j\right\rangle = 0$, with $i \neq j$.

i) For the projectors we have

$$\begin{aligned}\hat{P}_1 &= |u_1\rangle\langle u_1| \\ &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\end{aligned} \tag{1.39}$$

and

$$\begin{aligned}\hat{P}_2 &= \left|u_2^1\right\rangle\left\langle u_2^1\right| + \left|u_2^2\right\rangle\left\langle u_2^2\right| \\ &= \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix} \begin{pmatrix} 0 & 1 & -i \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix} \begin{pmatrix} 0 & 1 & i \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.\end{aligned} \tag{1.40}$$

ii) The projector for the three-dimensional space is therefore

$$\begin{aligned}\hat{P} &= \hat{P}_1 + \hat{P}_2 \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \hat{1}.\end{aligned} \tag{1.41}$$

iii) Using the $\left\{|u_1\rangle, \left|u_2^1\right\rangle, \left|u_2^2\right\rangle\right\}$ basis we can determine the matrix representation for the observable as

$$\begin{aligned}\hat{A} &= a_1\hat{P}_1 + a_2\hat{P}_2 \\ &= \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_2 \end{pmatrix}.\end{aligned} \tag{1.42}$$

And it is easy to verify that $\hat{A}\,|u_1\rangle = a_1\,|u_1\rangle$ and $\hat{A}\,\left|u_2^i\right\rangle = a_2\,\left|u_2^i\right\rangle$, with $i = 1, 2$.

iv) For any projector, either in a subspace or the full space, we have

$$\begin{aligned}
\hat{P}_j^n &= \hat{P}_j^{n-2}\hat{P}_j^2 \\
&= \hat{P}_j^{n-2}\sum_l \left|u_j^l\right\rangle\left\langle u_j^l\right| \cdot \sum_m \left|u_j^m\right\rangle\left\langle u_j^m\right| \\
&= \hat{P}_j^{n-2}\sum_{l,m} \left|u_j^l\right\rangle \left\langle u_j^l \,\middle|\, u_j^m\right\rangle \left\langle u_j^m\right| \\
&= \hat{P}_j^{n-2}\sum_{l,m} \left|u_j^l\right\rangle \delta_{lm} \left\langle u_j^m\right| \\
&= \hat{P}_j^{n-2}\sum_m \left|u_j^m\right\rangle\left\langle u_j^m\right| \\
&= \hat{P}_j^{n-1},
\end{aligned} \tag{1.43}$$

and through repeating the same steps another $n-2$ times we can easily find that

$$\hat{P}_j^n = \hat{P}_j. \tag{1.44}$$

1.1.5 Fifth Postulate

If the measurement of the physical quantity $\mathcal{A}$ on a system in the state $|\psi\rangle$ gave the value "a" as a result, then state of the system immediately following the measurement is given by the new state $|\psi'\rangle$ such that (for discrete states)

$$\left|\psi'\right\rangle = \frac{\hat{P}_n\,|\psi\rangle}{\sqrt{\left\langle \psi \,\middle|\, \hat{P}_n \,\middle|\, \psi\right\rangle}}, \tag{1.45}$$

where $\hat{P}_n$ is the projector corresponding to the subspace of eigenvalue a. This postulate simply ensures that the new ket (or wave function) describing the system after a measurement is suitably normalized to unity. Indeed, we can verify from equations (1.20) and (1.22) that

$$\begin{aligned}
\left|\psi'\right\rangle &= \frac{\sum_{i=1}^{g_n} \left|u_n^i\right\rangle \left\langle u_n^i \,\middle|\, \psi\right\rangle}{\sqrt{\sum_{i=1}^{g_n} \left\langle \psi \,\middle|\, u_n^i\right\rangle \left\langle u_n^i \,\middle|\, \psi\right\rangle}} \\
&= \frac{\sum_{i=1}^{g_n} c_n^i \left|u_n^i\right\rangle}{\sqrt{\sum_{i=1}^{g_n} \left|c_n^i\right|^2}}
\end{aligned} \tag{1.46}$$

and therefore

$$\begin{aligned}
\langle \psi' \,|\, \psi' \rangle &= \frac{\sum_{j=1}^{g_n} \left\langle u_n^j \right| \left(c_n^j\right)^* \cdot \sum_{i=1}^{g_n} c_n^i \left| u_n^i \right\rangle}{\sum_{i=1}^{g_n} \left|c_n^i\right|^2} \\
&= \frac{\sum_{j=1}^{g_n} \sum_{i=1}^{g_n} \left(c_n^j\right)^* c_n^i \delta_{ij}}{\sum_{i=1}^{g_n} \left|c_n^i\right|^2} \\
&= \frac{\sum_{i=1}^{g_n} \left|c_n^i\right|^2}{\sum_{i=1}^{g_n} \left|c_n^i\right|^2} \\
&= 1.
\end{aligned} \tag{1.47}$$

It is important to note that some wave functions, related to observables possessing a continuous spectrum, are not normalizable. For example, let us consider the one-dimensional case where an eigenvector $|\psi\rangle$ is expanded using the basis $\{|\xi\rangle\}$ associated to some observable $\hat{\xi}$ as follows

$$|\psi\rangle = \int_{-\infty}^{\infty} d\xi \, c(\xi) \, |\xi\rangle \, , \tag{1.48}$$

with ξ a variable possessing a continuous spectrum and $c(\xi) = \langle \xi \,|\, \psi \rangle$. Resorting to the (one-dimensional) position representation we can also write

$$\begin{aligned}
c(\xi) &= \left\langle \xi \left| \int_{-\infty}^{\infty} dx \, |x\rangle\langle x| \right| \psi \right\rangle \\
&= \int_{-\infty}^{\infty} dx \, \langle \xi \,|\, x \rangle \, \langle x \,|\, \psi \rangle \\
&= \int_{-\infty}^{\infty} dx \, \varphi_\xi^*(x) \, \psi(x) \, ,
\end{aligned} \tag{1.49}$$

with $\varphi_\xi(x) = \langle x \,|\, \xi \rangle$ and, as usual, $\psi(x) = \langle x \,|\, \psi \rangle$. Projecting equation (1.48) on $\langle x|$ gives

$$\begin{aligned}
\psi(x) &= \langle x \,|\, \psi \rangle \\
&= \int_{-\infty}^{\infty} d\xi \, c(\xi) \, \langle x \,|\, \xi \rangle \\
&= \int_{-\infty}^{\infty} d\xi \, c(\xi) \, \varphi_\xi(x) \, ,
\end{aligned}$$

which upon insertion in equation (1.49) yields

$$c(\xi) = \int_{-\infty}^{\infty} d\xi' \, c(\xi') \left[\int_{-\infty}^{\infty} dx \, \varphi_\xi^*(x) \, \varphi_{\xi'}(x) \right] \tag{1.50}$$

and we must therefore have

$$\int_{-\infty}^{\infty} dx\, \varphi_{\xi}^{*}(x)\, \varphi_{\xi'}(x) = \delta\left(\xi - \xi'\right). \tag{1.51}$$

It is clear that setting $\xi' = \xi$ in this equation shows that the wave function $\varphi_{\xi}(x)$ associated to the observable $\hat{\xi}$, which possesses a continuous spectrum, is not normalized since the probability $|c(\xi)|^2 d\xi$ that it is found between ξ and $\xi + d\xi$ is infinite. Nonetheless, such representations are still useful as ratios of probabilities at, say, two values ξ_1 and ξ_2 can still be evaluated. That is, $|c(\xi_1)|^2 / |c(\xi_2)|^2$ is a well defined and meaningful quantity.

1.1.6 Sixth Postulate

The dynamical evolution of a quantum mechanical system can be calculated using different approaches. Originally, Heisenberg and Schrödinger independently came up with different but equivalent pictures, but other points of view also exist (e.g., Feynman's sum over histories or path integral approach). For the present chapter we will concentrate on the Schrödinger picture (and the corresponding equation), while other approaches will be investigated later on.

Although it is possible to give a "derivation" of the Schrödinger equation, it is sufficient for our purposes to introduce it as the sixth, and last, postulate of quantum mechanics:

The time evolution of the state vector of a system is dictated by the ***Schrödinger equation***

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle, \tag{1.52}$$

where $\hat{H}(t)$ is the Hamiltonian of the system, i.e., the observable associated with the energy of the system.

In most cases, we will be dealing with a time-independent Hamiltonian that has so-called **stationary states** whose norms do not change as a function of time (see below). It is also easy to see that in this case a formal solution to equation (1.52) is

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle. \tag{1.53}$$

In cases where $|\psi(0)\rangle = |\varphi\rangle$, with $|\varphi\rangle$ is an eigenvector of $\hat{H}$ (i.e., one of the aforementioned stationary states), equation (1.53) becomes

$$|\psi(t)\rangle = e^{-iEt/\hbar} |\varphi\rangle \tag{1.54}$$

for E the energy eigenvalue associated with the state $|\varphi\rangle$. It is clear that

$$\langle \psi(t) \,|\, \psi(t) \rangle = \langle \varphi \,|\, \varphi \rangle, \tag{1.55}$$

and if we insert equation (1.54) into the Schrödinger equation (i.e., (1.52)), then we find that

$$\hat{H}\,|\varphi\rangle = E\,|\varphi\rangle\,. \tag{1.56}$$

Equation (1.56) is often referred to as the **time-independent Schrödinger equation**.

Finally, we note that in the more general case $|\psi\,(0)\rangle$ can always be expanded with the basis $\{|\varphi_n\rangle\}$ containing the eigenvectors of $\hat{H}$ of energy eigenvalues E_n with

$$|\psi\,(0)\rangle = \sum_n c_n\,(0)\,|\varphi_n\rangle\,. \tag{1.57}$$

It follows from equation (1.53) that the time evolution of a given state $|\psi\,(t)\rangle$ is expressed as

$$|\psi\,(t)\rangle = \sum_n e^{-iE_n t/\hbar} c_n\,(0)\,|\varphi_n\rangle \tag{1.58}$$

It is important to note that since the observables $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ associated with the position and the momentum, respectively, do not commute (i.e., $\hat{\mathbf{r}}\cdot\hat{\mathbf{p}} \neq \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}$; see Section 1.3) and that they usually appear in expressions for the Hamiltonian, rules of symmetry must be used when dealing with their products. For example, the following transformation would be applied for the simple product $\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}$

$$\hat{\mathbf{r}}\cdot\hat{\mathbf{p}} \Longrightarrow \frac{1}{2}\left(\hat{\mathbf{r}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\right). \tag{1.59}$$

1.2 The Principles of Quantum Mechanics

A few principles need to be added to the previous postulates in order to use the formalism of quantum mechanics to make predictions on experiments, and to ensure that it is consistent with the results of classical mechanics on the large scale.

1.2.1 The Principle of Superposition

We already know that the state of a quantum mechanical system is entirely contained within a ket, say, φ_1, which can be a function of time. It may be the case, however, that several different states φ_j, with $j = 1, 2, \ldots, n$, are available for the system. **The Principle of Superposition** then states that

If several states are available for a quantum mechanical system, then it can also be in any possible linear combinations of them.

In mathematical terms this means that the most general form for the state ψ of the system is given by

$$\psi = \sum_{j=1}^{n} c_j\,|\varphi_j\rangle \tag{1.60}$$

where $c_j = \langle\varphi_j\,|\,\psi\rangle$ are complex coefficients. As we shall see later, the superposition of states is essential to explain the coherence observed in quantum mechanical systems.

1.2.2 The Principle of Complementarity

The superposition of states is responsible for the presence of interference (and coherence) in quantum mechanical systems. This experimental fact can be understood if one accepts that a system evolves as a "wave" (i.e., according to the Schrödinger equation) while measurements always yield the detection of particles (e.g., photons, electrons, etc.). This was first made explicit by Bohr when he enunciated his **Principle of Complementarity**, which can be stated as follows[1]

It is not possible to describe physical observables simultaneously and completely in terms of particles and waves.

What this principle implies is that attempts to acquire knowledge on the state of a system (e.g., the path a particle takes) cannot be accomplished without disturbing it and changing its state. In other word, the interference that would be detected for the undisturbed system (i.e., the wave-like behaviour) will be affected by the act of acquiring information on its state. It is important to emphasize that this complementarity does not imply that the wave character of the system has to be completely suppressed in the process (although it can be).

1.2.3 The Correspondence Principle

Although the picture of the microscopic world provided by quantum mechanics is often completely at odds with what we would expect on large scales with classical mechanics, it must be that the two realms are consistent with one another and come to an agreement at some intermediate scale. Importantly, predictions made with quantum mechanics must agree with those of classical mechanics in conditions where the applicability of the latter is warranted. This requirement is formulated through Bohr's **Correspondence Principle**

Quantum mechanical physical quantities should tend to the classical mechanical counterparts in the macroscopic limit.

Mathematically, the macroscopic limit is reached when the Planck constant h is negligible compared to the action of the system[2]. In such cases, quantum mechanical effects and phenomena have no consequence on the behaviour of the system.

[1] There are many different ways with which the Principle of Complementarity can be stated. Alternatively, Auletta, Fortunato and Parisi define it with "*Complete knowledge of the path is not compatible with the presence of interference.*"

[2] The action is defined by $S = \int L(q_i, \dot{q}_i, t)\, dt$, where the Lagrangian $L(q_i, \dot{q}_i, t)$ is a function of the generalized coordinates q_i and velocities $\dot{q}_i$, and potentially time ($i = 1, \ldots, n$, with n the number of degrees of freedom of the system under consideration).

1.3 The Position and Momentum Operators and their Commutators

Two measurable physical quantities that are included in the expression for the classical Hamiltonian are the position $\mathbf{r}$ and the momentum $\mathbf{p}$ vectors. Correspondingly, it is necessary to introduce these operators $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ when setting up the quantum mechanical Hamiltonian. These two operators can be broken down into the usual three components

$$\hat{\mathbf{r}} = \hat{x}\mathbf{e}_x + \hat{y}\mathbf{e}_y + \hat{z}\mathbf{e}_z \tag{1.61}$$
$$\hat{\mathbf{p}} = \hat{p}_x\mathbf{e}_x + \hat{p}_y\mathbf{e}_y + \hat{p}_z\mathbf{e}_z. \tag{1.62}$$

The complete basis $\{|\mathbf{r}\rangle\}$ contains the eigenvectors for $\hat{\mathbf{r}}$. More precisely, we can write

$$|\mathbf{r}\rangle = |x\rangle\,|y\rangle\,|z\rangle\,, \tag{1.63}$$

and

$$\hat{x}\,|x\rangle = x\,|x\rangle \tag{1.64}$$

or

$$\hat{x}\,|\mathbf{r}\rangle = x\,|\mathbf{r}\rangle\,. \tag{1.65}$$

Similar relations hold for $\hat{y}$ and $\hat{z}$. We can also define a complete basis $\{|\mathbf{p}\rangle\}$ of eigenvectors for the momentum operator such that

$$|\mathbf{p}\rangle = |p_x\rangle\,|p_y\rangle\,|p_z\rangle \tag{1.66}$$
$$\hat{p}_x\,|p_x\rangle = p_x\,|p_x\rangle \tag{1.67}$$
$$\hat{p}_x\,|\mathbf{p}\rangle = p_x\,|\mathbf{p}\rangle\,, \tag{1.68}$$

and so on. The question is: what is the representation for $\hat{\mathbf{p}}$ when acting on the basis $|\mathbf{r}\rangle$ (or that of $\hat{\mathbf{r}}$ on $\{|\mathbf{p}\rangle\}$)? To answer this question we first note that the momentum basis satisfies relations that are similar to that satisfied by the position basis. That is,

$$|\mathbf{p}_0\rangle \Longleftrightarrow \delta\left(\mathbf{p}-\mathbf{p}_0\right) \tag{1.69}$$
$$\langle\mathbf{p}\,|\,\mathbf{p}'\rangle = \delta\left(\mathbf{p}-\mathbf{p}'\right) \tag{1.70}$$
$$\int_{-\infty}^{\infty} d^3p\,|\mathbf{p}\rangle\langle\mathbf{p}| = \hat{1} \tag{1.71}$$
$$\langle\mathbf{p}\,|\,\psi\rangle = \overline{\psi}\left(\mathbf{p}\right). \tag{1.72}$$

We now combine equation (1.70) with equation (1.15) for the completeness of the $|\mathbf{r}\rangle$ basis

$$\begin{aligned}
\langle \mathbf{p} \,|\, \mathbf{p}' \rangle &= \int_{-\infty}^{\infty} d^3x \, \langle \mathbf{p} \,|\, \mathbf{r} \rangle \langle \mathbf{r} \,|\, \mathbf{p}' \rangle \\
&= \int_{-\infty}^{\infty} d^3x \, v^* (\mathbf{r}; \mathbf{p}) \, v (\mathbf{r}; \mathbf{p}') \\
&= \delta (\mathbf{p} - \mathbf{p}'), \qquad (1.73)
\end{aligned}$$

where $v(\mathbf{r};\mathbf{p}) \equiv \langle \mathbf{r} \,|\, \mathbf{p} \rangle$ and is to be determined. Alternatively, we can combine equation (1.5) and equation (1.71) and get

$$\begin{aligned}
\langle \mathbf{r} \,|\, \mathbf{r}' \rangle &= \int_{-\infty}^{\infty} d^3p \, \langle \mathbf{r} \,|\, \mathbf{p} \rangle \langle \mathbf{p} \,|\, \mathbf{r}' \rangle \\
&= \int_{-\infty}^{\infty} d^3p \, v (\mathbf{r}; \mathbf{p}) \, v^* (\mathbf{r}'; \mathbf{p}) \\
&= \delta (\mathbf{r} - \mathbf{r}'). \qquad (1.74)
\end{aligned}$$

We can consider equations (1.73) and (1.74) as the relations that define $v(\mathbf{r};\mathbf{p})$. One form that satisfy these conditions is

$$v(\mathbf{r};\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \qquad (1.75)$$

with $\hbar$ Planck's constant (divided by 2π).

[**Note:** The fact that equation (1.75) satisfies both equations (1.73) and (1.74) can be verified by considering the Fourier transform pair between a function $f(\mathbf{r})$ and its transform $\overline{f}(\mathbf{p})$

$$\begin{aligned}
f(\mathbf{r}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3p \, \overline{f}(\mathbf{p}) \, e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \qquad (1.76) \\
\overline{f}(\mathbf{p}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3r \, f(\mathbf{r}) \, e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}. \qquad (1.77)
\end{aligned}$$

These equations imply the following duality between the Fourier transform and its inverse

$$\begin{aligned}
f(\mathbf{r}) &\iff \overline{f}(\mathbf{p}) \qquad (1.78) \\
\overline{f}(-\mathbf{r}) &\iff f(\mathbf{p}). \qquad (1.79)
\end{aligned}$$

For example, if we set $f(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')$, it is then easy to show from equation (1.77) that

$$\begin{aligned}\overline{f}(\mathbf{p}) &= \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3r\,\delta\left(\mathbf{r}-\mathbf{r}'\right)e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \\ &= \frac{1}{(2\pi\hbar)^{3/2}}e^{-i\mathbf{p}\cdot\mathbf{r}'/\hbar}.\end{aligned}$$

Therefore, from equations (1.76) and (1.79) we have

$$\delta\left(\mathbf{p}-\mathbf{p}'\right) = \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3r\left[\frac{1}{(2\pi\hbar)^{3/2}}e^{i\mathbf{r}\cdot\mathbf{p}'/\hbar}\right]e^{-i\mathbf{r}\cdot\mathbf{p}/\hbar}, \tag{1.80}$$

which is the same as equation (1.73) when $v(\mathbf{r};\mathbf{p})$ is given by equation (1.75). Similarly, we can first set $\overline{f}(\mathbf{p}) = \delta(\mathbf{p}+\mathbf{p}')$ in equation (1.76) to get

$$\begin{aligned}f(\mathbf{r}) &= \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3p\,\delta\left(\mathbf{p}+\mathbf{p}'\right)e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \\ &= \frac{1}{(2\pi\hbar)^{3/2}}e^{-i\mathbf{p}'\cdot\mathbf{r}/\hbar},\end{aligned}$$

and again from equations (1.77) and (1.79)

$$\begin{aligned}\delta\left(-\mathbf{r}+\mathbf{r}'\right) &= \delta\left(\mathbf{r}-\mathbf{r}'\right) \\ &= \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3p\left[\frac{1}{(2\pi\hbar)^{3/2}}e^{-i\mathbf{r}'\cdot\mathbf{p}/\hbar}\right]e^{i\mathbf{r}\cdot\mathbf{p}/\hbar},\end{aligned}$$

which is the same as equation (1.74) with $v(\mathbf{r};\mathbf{p})$ defined by equation (1.75).**]**

Having established that

$$\langle\mathbf{r}\,|\,\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\mathbf{r}\cdot\mathbf{p}/\hbar}, \tag{1.81}$$

consider equation (1.1) while using the completeness relation for $\{|\mathbf{p}\rangle\}$ (i.e., equation (1.71))

$$\begin{aligned}\psi(\mathbf{r},t) &= \langle\mathbf{r}\,|\,\psi(t)\rangle \\ &= \int_{-\infty}^{\infty} d^3p\,\langle\mathbf{r}\,|\,\mathbf{p}\rangle\,\langle\mathbf{p}\,|\,\psi(t)\rangle \\ &= \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3p\,e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\overline{\psi}(\mathbf{p},t),\end{aligned} \tag{1.82}$$

with $\overline{\psi}(\mathbf{p},t) \equiv \langle\mathbf{p}\,|\,\psi(t)\rangle$. It is therefore apparent from this last equation that the two different forms of the wave function are related through the Fourier transform pair

$$\psi(\mathbf{r},t) \Longleftrightarrow \overline{\psi}(\mathbf{p},t). \tag{1.83}$$

Finally, consider the action of the momentum operator on the ket $|\psi(t)\rangle$ with

$$\begin{aligned}
\langle \mathbf{r} \,|\, \hat{\mathbf{p}} \,|\, \psi(t) \rangle &= \int_{-\infty}^{\infty} d^3p \, \langle \mathbf{r} \,|\, \hat{\mathbf{p}} \,|\, \mathbf{p} \rangle \langle \mathbf{p} \,|\, \psi(t) \rangle \\
&= \int_{-\infty}^{\infty} d^3p \, \mathbf{p} \, \langle \mathbf{r} \,|\, \mathbf{p} \rangle \, \overline{\psi}(\mathbf{p},t) \\
&= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3p \, \mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \overline{\psi}(\mathbf{p},t) \\
&= -i\hbar\nabla \left[\frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} d^3p \, e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \overline{\psi}(\mathbf{p},t) \right] \\
&= -i\hbar\nabla \langle \mathbf{r} \,|\, \psi(t) \rangle.
\end{aligned} \tag{1.84}$$

We therefore find the fundamental result that the action of the momentum operator *in the position basis* $\{|\mathbf{r}\rangle\}$ is represented by

$$\hat{\mathbf{p}} \Rightarrow -i\hbar\nabla. \tag{1.85}$$

In quantum mechanics the order with which measurements are made (or we apply operators) can be important. For example, the act of measuring the momentum of a system can affect its position, and vice-versa. It is therefore interesting to calculate the difference between two sets of operations. Consider the following

$$|\Delta\rangle = (\hat{\mathbf{r}}\hat{\mathbf{p}} - \hat{\mathbf{p}}\hat{\mathbf{r}}) |\psi\rangle, \tag{1.86}$$

the ket resulting from the difference between operating with the momentum before the position on a system $|\psi\rangle$ and the opposite sequence. To proceed further, we project both sides of equation (1.86) on $\langle\mathbf{r}|$, and use equation (1.85) to get

$$\begin{aligned}
\langle \mathbf{r} \,|\, \Delta \rangle &= \langle \mathbf{r} \,|\, (\hat{\mathbf{r}}\hat{\mathbf{p}} - \hat{\mathbf{p}}\hat{\mathbf{r}}) \,|\, \psi \rangle \\
&= \mathbf{r} \langle \mathbf{r} \,|\, \hat{\mathbf{p}} \,|\, \psi \rangle - \langle \mathbf{r} | \, \hat{\mathbf{p}} \, (\hat{\mathbf{r}} \, |\psi\rangle) \\
&= -i\hbar \left[\mathbf{r}\nabla \langle \mathbf{r} \,|\, \psi \rangle - \nabla \langle \mathbf{r} \,|\, \hat{\mathbf{r}} \,|\, \psi \rangle \right] \\
&= -i\hbar \left[\mathbf{r}\nabla \langle \mathbf{r} \,|\, \psi \rangle - \nabla \left(\mathbf{r} \langle \mathbf{r} \,|\, \psi \rangle \right) \right] \\
&= -i\hbar \left[\mathbf{r}\nabla \langle \mathbf{r} \,|\, \psi \rangle - \hat{\mathbf{1}} \langle \mathbf{r} \,|\, \psi \rangle - \mathbf{r}\nabla \langle \mathbf{r} \,|\, \psi \rangle \right] \\
&= i\hbar\hat{\mathbf{1}} \langle \mathbf{r} \,|\, \psi \rangle.
\end{aligned}$$

We, therefore, find the following important result

$$\begin{aligned}
[\hat{\mathbf{r}}, \hat{\mathbf{p}}] &\equiv \hat{\mathbf{r}}\hat{\mathbf{p}} - \hat{\mathbf{p}}\hat{\mathbf{r}} \\
&= i\hbar\hat{\mathbf{1}}
\end{aligned} \tag{1.87}$$

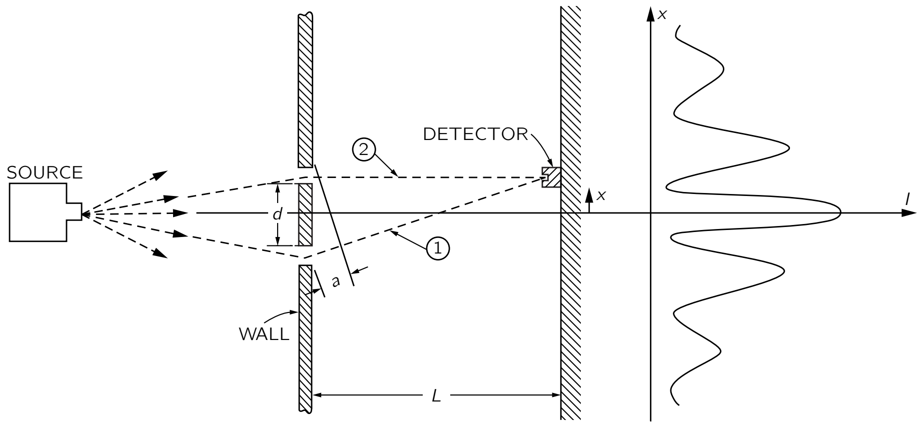

Figure 1.1: The Young double slit experiment where electrons are diffracted by two narrow slits separated by a distance d to a screen some distance L away. From *The Feynman Lectures on Physics - Vol. II.*

or alternatively

$$[\hat{r}_j, \hat{p}_k] = i\hbar\delta_{jk}, \tag{1.88}$$

where $[\hat{\mathbf{r}}, \hat{\mathbf{p}}]$ is the **commutator** of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$. It should also be obvious that

$$[\hat{r}_j, \hat{r}_k] = [\hat{p}_j, \hat{p}_k] = 0. \tag{1.89}$$

Exercise 1.2. The Young Double Slit Experiment and the Principle of Complementarity

Let us consider the double slit experiment shown in Figure 1.1, where electrons are emitted from a source and diffracted by two narrow slits separated by a distance d to a screen some distance $L \gg d$ away. *i)* Find the probability density $\mathcal{P}(x)$ of detecting an electron at position x on the detector, assuming that the transmissivity through the two slits are A^2 and B^2 (with $A^2 + B^2 = 1$), and *ii)* vary A (and therefore also B) to discuss the system's behaviour from the point of view of the Principle of Complementarity.

Solution.

i) As we have seen with the Sixth Postulate, a quantum mechanical system in a stationary state $\psi(\mathbf{r}, t_0)$ of (constant) energy E at time t_0 will evolve according to the Schrödinger equation such that at a later time t the wave function becomes (see equation (1.54))

$$\psi(\mathbf{r}, t) = e^{-iE(t-t_0)/\hbar}\psi(\mathbf{r}, t_0). \tag{1.90}$$

For simplicity, let us set $\varphi(\mathbf{r}) = \psi(\mathbf{r}, t_0)$ from now on. For a free particle, such an the electron in this set-up, the time-independent Schrödinger equation is

$$\begin{aligned} \hat{H}\varphi(\mathbf{r}) &= \frac{\hat{p}^2}{2m}\varphi(\mathbf{r}) \\ &= -\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) \\ &= E\varphi(\mathbf{r}). \end{aligned} \tag{1.91}$$

and is easily solved to yield

$$\varphi(\mathbf{r}) = Ae^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \tag{1.92}$$

with A some constant we choose to be real and greater than 0 (note that this wave function is not normalizable over all space). These equations also imply that $E = p^2/(2m)$. Referring to the figure, as an electron diffracts it will acquire a different phase depending which path (i.e., paths 1 and 2 in Figure 1.1) or slit it goes through as it reaches the detector at point x. Allowing for the possibility that an electron goes through either or both slits, we use the Principle of Superposition and write for the wave function of the system at x and time t (we set $t_0 = 0$ for simplicity)

$$\psi(\mathbf{r}, t) = Ae^{i(\mathbf{p}\cdot\mathbf{r}_1 - Et)/\hbar} + Be^{i(\mathbf{p}\cdot\mathbf{r}_2 - Et)/\hbar}. \tag{1.93}$$

The probabilities (or the corresponding transmissivities) that an electron goes through paths $\mathbf{r}_1$ and $\mathbf{r}_2$ are proportional to, respectively, A^2 and B^2, with $A^2 + B^2 = 1$. The probability density $\mathcal{P}(x)$ of detecting an electron at x on the detector is given by

$$\begin{aligned} \mathcal{P}(x) &\propto |\psi(\mathbf{r}, t)|^2 \\ &\propto A^2 + B^2 + 2AB\cos(\delta_0) \end{aligned} \tag{1.94}$$

with (using $\mathbf{p} = \hbar\mathbf{k}$)

$$\begin{aligned} \delta_0 &= \frac{1}{\hbar}\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_2) \\ &= 2\pi\frac{xd}{L\lambda}. \end{aligned} \tag{1.95}$$

The set consisting of equations (1.94)-(1.95) is a good solution for the problem as long as $x \ll L$, and its oscillatory behaviour is a typical example of quantum mechanical interference or coherence. Notably, we have that $\mathcal{P}_{\min} \propto A^2 + B^2 - 2AB$, at $x = nL\lambda/(2d)$ (with $|n| = 1, 3, \ldots$), and $\mathcal{P}_{\max} \propto A^2 + B^2 + 2AB$, at $x = mL\lambda/(2d)$ (with $|m| = 0, 2, \ldots$).

ii) Let us now quantify the wave characteristics of (or level of interference in) the system with the **visibility** (remember that $A^2 + B^2 = 1$)

$$\begin{aligned}\mathcal{V} &= \frac{\mathcal{P}_{\max} - \mathcal{P}_{\min}}{\mathcal{P}_{\max} + \mathcal{P}_{\min}} \\ &= 2AB.\end{aligned} \tag{1.96}$$

We further introduce the **predictability** (with $1/\sqrt{2} \leq A \leq 1$, such that $0 \leq Pr \leq 1$)

$$Pr = A^2 - B^2. \tag{1.97}$$

We see that for $A = B = 1/\sqrt{2}$ the visibility is maximum at $\mathcal{V} = 1$, while the predictability is minimum with $Pr = 0$. The converse is true when $A = 1$ (and $B = 0$) where $\mathcal{V} = 0$ and $Pr = 1$. The predictability is then tied to the precision with which we can assert through what slit the electrons are likely to go through. That is, when $A = B = 1/\sqrt{2}$ an electron is as likely to go through either slits (i.e., we have complete unpredictability with $Pr = 0$) and the systems exhibits the maximum amount of wavelike behaviour ($\mathcal{V} = 1$), while if $A = 1$ and $B = 0$ we are certain of the provenance of the electrons (i.e., we have total predictability with $Pr = 1$) and the systems loses its wavelike characteristics ($\mathcal{V} = 0$). We thus find that visibility and predictability are in opposition. In fact, it is easy to verify from equations (1.96)-(1.97) that

$$\mathcal{V}^2 + Pr^2 = 1. \tag{1.98}$$

We can associate this last equation to the Principle of Complementarity. That is, by increasing the degree of knowledge we have on the path taken by the electrons (the predictability) we suppress the amount of interference exhibited by the system (the visibility decreases), and vice-versa. We see that the complementarity between the particle and wave behaviours varies smoothly with the value assigned to A, i.e., complementarity is not limited to all of one of the other.

1.4 Matrix Elements, Expectation Values, and Unitary Operators

1.4.1 Matrix Elements

In case of an arbitrary observable $\hat{O}$ for which a basis $\{|u_i\rangle\}$ does not consists of its eigenvectors, we can always write

$$\begin{aligned}\hat{O} &= \sum_i |u_i\rangle\langle u_i|\,\hat{O} \\ &= \sum_{i,j} |u_i\rangle\langle u_i|\,\hat{O}\,|u_j\rangle\langle u_j| \\ &= \sum_{i,j} O_{ij}\,|u_i\rangle\langle u_j|\,,\end{aligned} \tag{1.99}$$

where $O_{ij} = \left\langle u_i \middle| \hat{O} \middle| u_j \right\rangle$. It can easily be shown that O_{ij} are the matrix elements of the observable $\hat{O}$ when represented using the basis $\{|u_i\rangle\}$.

Exercise 1.3. *i)* Consider the following two-dimensional basis

$$|u_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1.100}$$

$$|u_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.101}$$

and the observable

$$\hat{O} = \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix}. \tag{1.102}$$

Calculate the matrix elements $O_{ij} = \left\langle u_i \middle| \hat{O} \middle| u_j \right\rangle$, and verify that $\hat{O}$ is recovered with equation (1.99).

ii) Now consider the new basis

$$\begin{aligned} |v_1\rangle &= \frac{1}{\sqrt{2}} \left(|u_1\rangle + i\, |u_2\rangle \right) \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \end{aligned} \tag{1.103}$$

$$\begin{aligned} |v_2\rangle &= \frac{1}{\sqrt{2}} \left(|u_1\rangle - i\, |u_2\rangle \right) \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \end{aligned} \tag{1.104}$$

and the matrix representation of the observable for this basis

$$\hat{O}' = \begin{pmatrix} O'_{11} & O'_{12} \\ O'_{21} & O'_{22} \end{pmatrix}. \tag{1.105}$$

Calculate $O_{ij} = \left\langle v_i \middle| \hat{O}' \middle| v_j \right\rangle$. What do you conclude from these calculations?

Solution.

i) We can easily determine the matrix elements with

$$\begin{aligned} O_{11} &= \left\langle u_1 \middle| \hat{O} \middle| u_1 \right\rangle \\ &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= O_{11}, \end{aligned} \tag{1.106}$$

as expected, and similarly for O_{ij} using the other possible combinations of i and j. It is also easy to show that since, in this case,

$$\begin{aligned}
|u_1\rangle\langle u_1| &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\
|u_1\rangle\langle u_2| &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\
|u_2\rangle\langle u_1| &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\
|u_2\rangle\langle u_2| &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},
\end{aligned}$$

then we have from equation (1.99)

$$\hat{O} = \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix}. \tag{1.107}$$

ii) Things are different with the $\{|v_i\rangle\}$ basis. Although it would be possible to calculate O_{ij} using matrix and vector multiplication as was done for equation (1.106), it is perhaps easier to proceed as follows. We first note that we can write

$$|v_i\rangle = \sum_{m=1}^{2} c_{im}\,|u_m\rangle \tag{1.108}$$

and therefore

$$\begin{aligned}
O_{ij} &= \left\langle v_i \middle| \hat{O}' \middle| v_j \right\rangle \\
&= \sum_{m,n=1}^{2} c_{im}^* c_{jn} \left\langle u_m \middle| \hat{O}' \middle| u_n \right\rangle \\
&= \sum_{m,n=1}^{2} c_{im}^* c_{jn} O'_{mn},
\end{aligned} \tag{1.109}$$

where we used our result from part *i)* for the last step (see equation (1.106)). The coefficients are easily determined from equations (1.103) and (1.104) (i.e., $c_{11} = c_{21} = 1/\sqrt{2}$ and $c_{12} = -c_{22} = i/\sqrt{2}$). It follows that

$$O_{11} = \frac{1}{2}\left[\left(O'_{11} + O'_{22}\right) + i\left(O'_{12} - O'_{21}\right)\right] \tag{1.110}$$

$$O_{12} = \frac{1}{2}\left[\left(O'_{11} - O'_{22}\right) - i\left(O'_{12} + O'_{21}\right)\right] \tag{1.111}$$

$$O_{21} = \frac{1}{2}\left[\left(O'_{11} - O'_{22}\right) + i\left(O'_{12} + O'_{21}\right)\right] \tag{1.112}$$

$$O_{22} = \frac{1}{2}\left[\left(O'_{11} + O'_{22}\right) - i\left(O'_{12} - O'_{21}\right)\right]. \tag{1.113}$$

It is apparent that the form of the matrix elements O_{ij} is more complicated when the basis used is not the simplest (Cartesian) basis as that given by equations (1.100)-(1.101). That is, it should not in general be assumed that the elements obtained with $\left\langle v_i \middle| \hat{O}' \middle| v_j \right\rangle$ will yield those of the matrix in the corresponding representation (i.e., in this case $O_{ij} \neq O'_{ij}$).

1.4.2 Expectation Values

Let us now generalize the notation we used to define the matrix element $\left\langle u_i \middle| \hat{O} \middle| u_j \right\rangle$ to $\left\langle \psi \middle| \hat{O} \middle| \psi \right\rangle$, where $|\psi\rangle$ is the state of the system, and inquire as to the meaning of this quantity. We now assume that the basis $\{|u_i\rangle\}$ is composed of eigenvectors of the observable $\hat{O}$, and expand state ket

$$|\psi\rangle = \sum_i c_i |u_i\rangle . \tag{1.114}$$

We now write

$$\begin{aligned}
\left\langle \hat{O} \right\rangle_\psi &\equiv \left\langle \psi \middle| \hat{O} \middle| \psi \right\rangle \\
&= \sum_{i,j} c_i^* c_j \left\langle u_i \middle| \hat{O} \middle| u_j \right\rangle \\
&= \sum_{i,j} c_i^* c_j o_j \langle u_i \,|\, u_j \rangle \\
&= \sum_{i,j} c_i^* c_j o_j \delta_{ij} \\
&= \sum_j |c_j|^2 o_j.
\end{aligned} \tag{1.115}$$

Since the probability of finding the eigenvalue o_j (or, equivalently, to find the system in state $|u_j\rangle$) is given by $\mathcal{P}(o_j) = |c_j|^2$ (see equation (1.21)), we find that

$$\left\langle \hat{O} \right\rangle_\psi = \sum_j \mathcal{P}(o_j)\, o_j. \tag{1.116}$$

It should be clear that $\left\langle \hat{O} \right\rangle_\psi$ is simply the average of the eigenvalues of $\hat{O}$. Since the ket $|\psi\rangle$ can be expanded using any complete basis, not only the basis $\{|u_i\rangle\}$ composed of its eigenvectors, it follows that the relation $\left\langle \psi \middle| \hat{O} \middle| \psi \right\rangle$ is basis independent. That is, we can extend this definition for the expectation value $\left\langle \hat{A} \right\rangle_\psi$ to any observable $\hat{A}$ for any (normalized) state $|\psi\rangle$ of a quantum mechanical system whether or not it is expanded with the observables eigenvectors

$$\left\langle \hat{A} \right\rangle_{\psi} = \left\langle \psi \middle| \hat{A} \middle| \psi \right\rangle . \tag{1.117}$$

Finally, we note that equation (1.117) can be expressed using the wave function $\psi(\mathbf{r})$ through

$$\begin{aligned} \left\langle \hat{A} \right\rangle_{\psi} &= \int_{-\infty}^{\infty} d^3r \left\langle \psi \,|\, \mathbf{r} \right\rangle \left\langle \mathbf{r} \middle| \hat{A} \middle| \psi \right\rangle \\ &= \int_{-\infty}^{\infty} d^3r \, \psi^* (\mathbf{r}) \, \hat{A} \psi (\mathbf{r}) , \end{aligned} \tag{1.118}$$

where we defined $\hat{A}\psi(\mathbf{r}) \equiv \left\langle \mathbf{r} \middle| \hat{A} \middle| \psi \right\rangle$ (e.g., if $\hat{A} = \hat{p}_x$, then $\hat{p}_x \psi(\mathbf{r}) = -i\hbar \, \partial \psi(\mathbf{r}) / \partial x$).

1.4.3 Unitary Operators and Change of Basis

Given a state vector $|\psi\rangle$, we are, as we already know, free to expand it using any complete basis existing for the corresponding space. For example, if $\{|u_i\rangle\}$ and $\{|v_i\rangle\}$ are two such bases, then we can write

$$|\psi\rangle = \sum_i c_i |u_i\rangle \tag{1.119}$$

$$= \sum_i d_i |v_i\rangle \tag{1.120}$$

where $c_i = \langle u_i \,|\, \psi \rangle$ and $d_i = \langle v_i \,|\, \psi \rangle$. The two bases are related to each other through a transformation such that, for example,

$$\begin{aligned} |v_i\rangle &= \left[\sum_j |u_j\rangle\langle u_j| \right] |v_i\rangle \\ &= \sum_j \langle u_j \,|\, v_i \rangle \, |u_j\rangle \\ &= \sum_j U_{ji} \, |u_j\rangle , \end{aligned} \tag{1.121}$$

where $U_{ji} = \langle u_j \,|\, v_i \rangle$. Inserting equation (1.121) into equation (1.120) we find

$$\begin{aligned} |\psi\rangle &= \sum_i d_i \sum_j U_{ji} \, |u_j\rangle \\ &= \sum_j \left[\sum_i U_{ji} d_i \right] |u_j\rangle , \end{aligned} \tag{1.122}$$

which implies, from equation (1.119) that

$$c_j = \sum_i U_{ji} d_i. \tag{1.123}$$

We therefore see that U_{ji} are the elements of the transformation matrix $\hat{U}$ between the two bases. Interestingly, if we consider the adjoint of $\hat{U}$ and calculate $\hat{U}^\dagger \hat{U}$

$$\begin{aligned}
\sum_j \left(\hat{U}^\dagger\right)_{kj} U_{ji} &= \sum_j U_{jk}^* U_{ji} \\
&= \sum_j \left(\langle u_j \,|\, v_k\rangle\right)^* \langle u_j \,|\, v_i\rangle \\
&= \sum_j \langle v_k \,|\, u_j\rangle \langle u_j \,|\, v_i\rangle \\
&= \langle v_k| \left[\sum_j |u_j\rangle\langle u_j|\right] |v_i\rangle \\
&= \langle v_k \,|\, v_i\rangle \\
&= \delta_{ki},
\end{aligned} \tag{1.124}$$

or

$$\hat{U}^\dagger \hat{U} = \hat{1}. \tag{1.125}$$

Similarly, we can show that $\hat{U}\hat{U}^\dagger = \hat{1}$. Matrices that verify $\hat{U}^\dagger = \hat{U}^{-1}$ are called *unitary matrices.*

We saw in the previous section that matrix elements are of the form $O_{ij} = \left\langle v_i \middle| \hat{O} \middle| v_j \right\rangle$ in the basis $\{|v_i\rangle\}$. Let us now consider the trace of the matrix, while introducing a change to the basis $\{|u_i\rangle\}$

$$\begin{aligned}
\mathrm{Tr}\left(\hat{\mathrm{O}}\right) &= \sum_i \hat{O}_{ii} \\
&= \sum_i \left\langle v_i \middle| \hat{O} \middle| v_i \right\rangle \\
&= \sum_{i,j,k} \left[\langle u_j| \, U_{ji}^*\right] \hat{O} \left[U_{ki} \, |u_k\rangle\right] \\
&= \sum_{i,j,k} \langle u_j| \left(U_{ji}^* \hat{O} U_{ki}\right) |u_k\rangle\,,
\end{aligned} \tag{1.126}$$

which we are free to rearrange as

$$\begin{aligned}\mathrm{Tr}\left(\hat{\mathrm{O}}\right) &= \sum_{j,k}\langle u_j|\left[\hat{O}\left(\sum_i U_{ki}U_{ji}^*\right)\right]|u_k\rangle \\ &= \sum_{j,k}\delta_{jk}\left\langle u_j\left|\hat{O}\right|u_k\right\rangle \\ &= \sum_j\left\langle u_j\left|\hat{O}\right|u_j\right\rangle, \end{aligned} \tag{1.127}$$

with the result that the trace of an operator is independent of the basis used.

We can also verify that a unitary transformation preserves the scalar product between two arbitrary kets (vectors). For example, let us consider the kets $|\varphi_1\rangle$ and $|\varphi_2\rangle$ that can be expressed with two bases $\{|u_i\rangle\}$ and $\{|v_i\rangle\}$ related by a unitary transformation U through (see equations (1.121))

$$|v_i\rangle = \sum_j U_{ji}|u_j\rangle. \tag{1.128}$$

As was previously done, we also write ($\alpha = 1, 2$)

$$|\varphi_\alpha\rangle = \sum_i c_{\alpha i}|u_i\rangle \tag{1.129}$$

$$= \sum_i d_{\alpha i}|v_i\rangle, \tag{1.130}$$

while we know from equation (1.123) that

$$c_{\alpha i} = \sum_k U_{ik}d_{\alpha k}. \tag{1.131}$$

When calculating the scalar product, first using in turn equations (1.129), (1.131) and (1.124),

$$\begin{aligned}\langle\varphi_1\,|\,\varphi_2\rangle &= \sum_{i,j}c_{1i}^*c_{2j}\langle u_i\,|\,u_j\rangle \\ &= \sum_i c_{1i}^*c_{2i} \\ &= \sum_{i,k,m}d_{1k}^*d_{2m}U_{ik}^*U_{im} \\ &= \sum_{k,m}d_{1k}^*d_{2m}\delta_{km} \end{aligned} \tag{1.132}$$

and now with equation (1.130)

$$\begin{aligned}\langle \varphi_1 \,|\, \varphi_2 \rangle &= \sum_k d_{1k}^* d_{2k} \\ &= \sum_{j,k} d_{1j}^* d_{2k} \langle v_j \,|\, v_k \rangle \,, \end{aligned} \tag{1.133}$$

and we therefore see that the unitary transformation $\hat{U}$ does not affect the scalar product. That is, any of the two bases can be used for the expansion of the kets resulting in the same outcome for the scalar product.

Finally, it is straightforward to verify that unitary transformations preserve the form of the commutator for two operators. Since for a ket transformation $|\psi'\rangle = \hat{U}\,|\psi\rangle$ we have $\left\langle \psi' \,\middle|\, \hat{A}' \,\middle|\, \psi' \right\rangle = \left\langle \psi \,\middle|\, \hat{U}^\dagger \hat{A}' \hat{U} \,\middle|\, \psi \right\rangle$, then it must be that

$$\hat{A} = \hat{U}^\dagger \hat{A}' \hat{U}, \tag{1.134}$$

and therefore

$$\begin{aligned}\left[\hat{A}, \hat{B}\right] &= \left[\hat{U}^\dagger \hat{A}' \hat{U}, \hat{U}^\dagger \hat{B}' \hat{U}\right] \\ &= \hat{U}^\dagger \hat{A}' \hat{U} \hat{U}^\dagger \hat{B}' \hat{U} - \hat{U}^\dagger \hat{B}' \hat{U} \hat{U}^\dagger \hat{A}' \hat{U} \\ &= \hat{U}^\dagger \left[\hat{A}', \hat{B}'\right] \hat{U}. \end{aligned} \tag{1.135}$$

Importantly, for two canonical operators $\hat{Q}$ and $\hat{P}$, where $\left[\hat{Q}, \hat{P}\right] = i\hbar\hat{1}$, we have

$$\begin{aligned}\left[\hat{Q}', \hat{P}'\right] &= \hat{U} \left[\hat{Q}, \hat{P}\right] \hat{U}^\dagger \\ &= \hat{U} i\hbar \hat{1} \hat{U}^\dagger \\ &= i\hbar\hat{1}. \end{aligned} \tag{1.136}$$

Exercise 1.4. It should be apparent by now that the coefficients c_{ij} in equation (1.108) are those of a unitary matrix. Write down that matrix, verify that it is unitary and the trace of the operator $\hat{O}$ is invariant under the change of basis.

Solution.

Referring to equations (1.103)-(1.104) we can readily write the matrix containing the c_{ij} coefficients of equation (1.108) as

$$\hat{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \tag{1.137}$$

We therefore have

$$\begin{aligned}
\hat{U}\hat{U}^{\dagger} &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \\
&= \hat{1},
\end{aligned} \tag{1.138}$$

which verifies that the transformation is unitary. Using equations (1.110) and (1.113) we can calculate the trace of $\hat{O}$ in the $\{|u_i\rangle\}$ basis with

$$\begin{aligned}
O_{11} + O_{22} &= \frac{1}{2}\left[\left(O'_{11} + O'_{22}\right) + i\left(O'_{12} - O'_{21}\right)\right] + \frac{1}{2}\left[\left(O'_{11} + O'_{22}\right) - i\left(O'_{12} - O'_{21}\right)\right] \\
&= O'_{11} + O'_{22},
\end{aligned} \tag{1.139}$$

and the trace is invariant under the change of basis.

1.5 The Heisenberg Inequality

Whenever two observables $\hat{Q}$ and $\hat{P}$ satisfy the same commutation relation as the position and momentum operators, i.e.,

$$\left[\hat{Q}, \hat{P}\right] = i\hbar, \tag{1.140}$$

they are said to be **conjugate operators**. Let us assume that the mean value of both operators is zero, i.e.,

$$\begin{aligned}
\overline{Q} &= \left\langle \psi \middle| \hat{Q} \middle| \psi \right\rangle \\
&= 0
\end{aligned} \tag{1.141}$$

$$\begin{aligned}
\overline{P} &= \left\langle \psi \middle| \hat{P} \middle| \psi \right\rangle \\
&= 0
\end{aligned} \tag{1.142}$$

This is not a restriction, since we could always define new operators by subtracting $\overline{Q}$ and $\overline{P}$ from $\hat{Q}$ and $\hat{P}$, respectively, in the event that they were not null. Now consider the following quantity

$$I = \left\langle \psi \middle| \hat{Q}^2 \middle| \psi \right\rangle \left\langle \psi \middle| \hat{P}^2 \middle| \psi \right\rangle. \tag{1.143}$$

If we define new states such that

$$
\begin{aligned}
|1\rangle &\equiv \hat{Q}\,|\psi\rangle && (1.144)\\
|2\rangle &\equiv \hat{P}\,|\psi\rangle\,, && (1.145)
\end{aligned}
$$

then using the *Schwarz Inequality* we can write

$$
\begin{aligned}
I &= \langle 1\,|\,1\rangle\,\langle 2\,|\,2\rangle \\
&\geq \langle 1\,|\,2\rangle\,\langle 2\,|\,1\rangle\,, && (1.146)
\end{aligned}
$$

since $\langle 1\,|\,2\rangle$ is a scalar product. We can rewrite the last part of this inequality as follows

$$
\begin{aligned}
\langle 1\,|\,2\rangle\,\langle 2\,|\,1\rangle &= \frac{1}{4}\left[(\langle 1\,|\,2\rangle + \langle 2\,|\,1\rangle)^2 - (\langle 1\,|\,2\rangle - \langle 2\,|\,1\rangle)^2\right] \\
&= \frac{1}{4}\left[\left(\left\langle\psi\left|\hat{Q}\hat{P}\right|\psi\right\rangle + \left\langle\psi\left|\hat{P}\hat{Q}\right|\psi\right\rangle\right)^2 - \left(\left\langle\psi\left|\hat{Q}\hat{P}\right|\psi\right\rangle - \left\langle\psi\left|\hat{P}\hat{Q}\right|\psi\right\rangle\right)^2\right] \\
&= \frac{1}{4}\left[\left(\left\langle\psi\left|\hat{Q}\hat{P} + \hat{P}\hat{Q}\right|\psi\right\rangle\right)^2 - \left(\left\langle\psi\left|\hat{Q}\hat{P} - \hat{P}\hat{Q}\right|\psi\right\rangle\right)^2\right] \\
&= \frac{1}{4}\left[\left(\left\langle\psi\left|\left\{\hat{Q},\hat{P}\right\}\right|\psi\right\rangle\right)^2 - \left(\left\langle\psi\left|\left[\hat{Q},\hat{P}\right]\right|\psi\right\rangle\right)^2\right]. && (1.147)
\end{aligned}
$$

The quantity $\left\{\hat{Q},\hat{P}\right\} \equiv \hat{Q}\hat{P}+\hat{P}\hat{Q}$ is commonly called the **anti-commutator**, for obvious reasons. We should note that

$$
\begin{aligned}
\left(\left\langle\psi\left|\left\{\hat{Q},\hat{P}\right\}\right|\psi\right\rangle\right)^2 &= \left|\left\langle\psi\left|\left\{\hat{Q},\hat{P}\right\}\right|\psi\right\rangle\right|^2 \\
&\geq 0, && (1.148)
\end{aligned}
$$

since $\left\langle\psi\left|\left\{\hat{Q},\hat{P}\right\}\right|\psi\right\rangle = \left\langle\psi\left|\left\{\hat{Q},\hat{P}\right\}\right|\psi\right\rangle^*$ because $\hat{Q}$ and $\hat{P}$ are observables (i.e., Hermitian operators). Taking this result into account, we can now insert equation (1.140) into equation (1.147) and find

$$
\left\langle\psi\left|\hat{Q}^2\right|\psi\right\rangle\left\langle\psi\left|\hat{P}^2\right|\psi\right\rangle \geq \frac{\hbar^2}{4}. \tag{1.149}
$$

This last equation is a generalization of the so-called **Heisenberg inequality**, which is usually written as follows

$$
\Delta Q \cdot \Delta P \geq \frac{\hbar}{2}, \tag{1.150}
$$

with

$$
\begin{aligned}
\Delta Q &= \sqrt{\left\langle\psi\left|\hat{Q}^2\right|\psi\right\rangle} && (1.151)\\
\Delta P &= \sqrt{\left\langle\psi\left|\hat{P}^2\right|\psi\right\rangle}. && (1.152)
\end{aligned}
$$

1.6 Diagonalization of Operators

It is often the case that given an operator $\hat{A}$ we require to find its set of eigenvalues $\{a_i\}$ and corresponding eigenvectors $\{|v_i\rangle\}$, such that

$$\hat{A}\,|v_i\rangle = a_i\,|v_i\rangle\,. \tag{1.153}$$

We start with a basis $\{|u_i\rangle\}$, which is not that containing its eigenvectors, and write (see equation (1.121))

$$|v_j\rangle = \sum_k U_{kj}\,|u_k\rangle\,. \tag{1.154}$$

Let us now consider the following

$$\begin{aligned}
\left\langle u_i \middle| \hat{A} \middle| v_j \right\rangle &= \sum_k U_{kj} \left\langle u_i \middle| \hat{A} \middle| u_k \right\rangle \\
&= \sum_k U_{kj} A_{ik} \\
&= a_j \left\langle u_i \,|\, v_j \right\rangle \\
&= a_j \sum_k U_{kj}\delta_{ik},
\end{aligned} \tag{1.155}$$

where $A_{ik} = \left\langle u_i \middle| \hat{A} \middle| u_k \right\rangle$. The second and fourth equations imply that

$$\sum_k \left(A_{ik} - a_j\delta_{ik}\right) U_{kj} = 0. \tag{1.156}$$

A non-trivial solution to the system of equations specified by (1.156) will be obtained by setting the following determinant to zero

$$\left|A_{ik} - a\delta_{ik}\right| = 0, \tag{1.157}$$

when the eigenvalue $a = a_j$. In other words, this is just a typical eigenvalue problem where all eigenvalues can be evaluated with equation (1.157). Once the eigenvalues a_j have been found, the elements U_{kj} of the unitary matrix $\hat{U}$ can be determined with equation (1.156). Multiplying equation (1.156) from the left with $\hat{U}^\dagger$ we write

$$\begin{aligned}
\sum_{i,k} \left(\hat{U}^\dagger\right)_{mi} A_{ik} U_{kj} &= \sum_{i,k} \left(\hat{U}^\dagger\right)_{mi} a_j \delta_{ik} U_{kj} \\
&= a_j \sum_k \left(\hat{U}^\dagger\right)_{mk} U_{kj} \\
&= a_j \delta_{mj},
\end{aligned} \tag{1.158}$$

or in matrix form

$$\hat{U}^{\dagger}\hat{A}\hat{U} = \hat{\Lambda} \tag{1.159}$$

with $\hat{\Lambda}$ a diagonal matrix whose elements are the eigenvalues a_j (i.e., $\Lambda_{mj} = a_j \delta_{mj}$).

Exercise 1.5. Since the diagonalization procedure will often be applied to observables (i.e., Hermitian operators), we consider the case of a two-level system with the corresponding two-dimensional Hamiltonian matrix

$$\hat{H} = \begin{pmatrix} E_1^0 & H_{12} \\ H_{12}^* & E_2^0 \end{pmatrix}, \tag{1.160}$$

where E_1^0 and E_2^0 are the energy eigenvalues of a quantum mechanical system when unperturbed (i.e., when $H_{12} = 0$) by some interaction with the external world. The off-diagonal elements H_{12} and H_{12}^* are thus representative of that perturbation. In the unperturbed state the quantum mechanical system can be in the corresponding states $\left|u_1^0\right\rangle$ and $\left|u_2^0\right\rangle$. Diagonalize the perturbed Hamiltonian (i.e., equation (1.160)) find the perturbed eigenvalues E_1 and E_2 and the corresponding kets $|u_1\rangle$ and $|u_2\rangle$.

Solution.

A straightforward application of equation (1.157), after substituting $a \to E$ and $A_{ik} \to H_{ik}$, for the determination of the eigenvalues of the Hamiltonian yields

$$\begin{aligned} \left(E_1^0 - E\right)\left(E_2^0 - E\right) - \left|H_{12}\right|^2 &= E^2 - \left(E_1^0 + E_2^0\right)E - \left(\left|H_{12}\right|^2 - E_1^0 E_2^0\right) \\ &= 0, \end{aligned} \tag{1.161}$$

with the following roots

$$\begin{aligned} E_{1,2} &= \frac{1}{2}\left[\left(E_1^0 + E_2^0\right) \pm \sqrt{\left(E_1^0 + E_2^0\right)^2 + 4\left(\left|H_{12}\right|^2 - E_1^0 E_2^0\right)}\right] \\ &= \frac{1}{2}\left[\left(E_1^0 + E_2^0\right) \pm \sqrt{\left(E_2^0 - E_1^0\right)^2 + 4\left|H_{12}\right|^2}\right]. \end{aligned} \tag{1.162}$$

If we set for convenience $E_1^0 \leq E_2^0$, then we can write (with $E_1 \leq E_2$)

$$E_1 = E_1^0 - S \tag{1.163}$$

$$E_2 = E_2^0 + S, \tag{1.164}$$

where

$$\begin{aligned} S &= \frac{1}{2}\left[\sqrt{\Delta^2 + 4\left|H_{12}\right|^2} - \Delta\right] \\ &\geq 0 \end{aligned} \tag{1.165}$$

and $\Delta = E_2^0 - E_1^0$.

To find the corresponding eigenvectors, we insert these energy levels, one at a time, in equation (1.156), and then use $U^\dagger U = \hat{1}$. For example, in the case of E_1 equation (1.156) yields

$$\begin{aligned} \left(E_1^0 - E_1\right) U_{11} + H_{12} U_{21} &= 0 && (1.166) \\ H_{12}^* U_{11} + \left(E_2^0 - E_1\right) U_{21} &= 0, && (1.167) \end{aligned}$$

of from the second of these equations

$$U_{21} = -\frac{H_{12}^*}{S+\Delta} U_{11}, \qquad (1.168)$$

while the unitary condition ($\sum_j U_{ji}^* U_{jk} = \delta_{ik}$) adds the constraint

$$\begin{aligned} 1 &= U_{11}^* U_{11} + U_{21}^* U_{21} \\ &= |U_{11}|^2 \left[1 + \frac{|H_{12}|^2}{(S+\Delta)^2}\right] \\ &= |U_{11}|^2 \left[\frac{\left[\sqrt{\Delta^2 + 4|H_{12}|^2} + \Delta\right]^2 + 4|H_{12}|^2}{\left[\sqrt{\Delta^2 + 4|H_{12}|^2} + \Delta\right]^2}\right] \\ &= |U_{11}|^2 \, 2 \left[\frac{\sqrt{\Delta^2 + 4|H_{12}|^2}}{\sqrt{\Delta^2 + 4|H_{12}|^2} + \Delta}\right]. \qquad (1.169) \end{aligned}$$

We are certainly at liberty to write $H_{12} = |H_{12}| e^{i\phi}$, and we find that (choosing U_{11} to be real)

$$\begin{aligned} C_+ &\equiv U_{11} \\ &= \frac{1}{\sqrt{2}} \left[1 + \frac{\Delta}{\sqrt{\Delta^2 + 4|H_{12}|^2}}\right]^{1/2} \qquad (1.170) \\ C_- &\equiv -U_{21}^* \\ &= e^{i\phi} \sqrt{1 - U_{11}^2} \\ &= \frac{e^{i\phi}}{\sqrt{2}} \left[1 - \frac{\Delta}{\sqrt{\Delta^2 + 4|H_{12}|^2}}\right]^{1/2} \qquad (1.171) \end{aligned}$$

where the sign and phase of C_- (and U_{21}) are dictated by that of H_{12} through equation (1.168). A similar exercise for E_2 can be shown to yield $U_{22} = U_{11} = C_+$ and $U_{12} = -U_{21}^* = C_-$. The eigenvectors are thus given by (see equation (1.154))

$$\begin{aligned} |u_1\rangle &= U_{11}\left|u_1^0\right\rangle + U_{21}\left|u_2^0\right\rangle \\ &= C_+\left|u_1^0\right\rangle - C_-^*\left|u_2^0\right\rangle \qquad (1.172) \\ |u_2\rangle &= U_{12}\left|u_1^0\right\rangle + U_{22}\left|u_2^0\right\rangle \\ &= C_-\left|u_1^0\right\rangle + C_+\left|u_2^0\right\rangle . \qquad (1.173) \end{aligned}$$

Let's now concentrate on cases where H_{12} is real and small, i.e., $H_{12}^* = H_{12} \ll \Delta$. We can then calculate the following approximations

$$\begin{aligned} S &= \frac{1}{2}\left[\sqrt{\Delta^2 + 4\left|H_{12}\right|^2} - \Delta\right] \\ &\simeq \frac{1}{2}\left[\Delta\left(1 + \frac{2H_{12}^2}{\Delta^2}\right) - \Delta\right] \\ &\simeq \frac{H_{12}^2}{\Delta} \qquad (1.174) \\ C_+ &= \frac{1}{\sqrt{2}}\left[1 + \frac{\Delta}{\sqrt{\Delta^2 + 4\left|H_{12}\right|^2}}\right]^{1/2} \\ &\simeq \frac{1}{\sqrt{2}}\left[1 + \left(1 - \frac{2H_{12}^2}{\Delta^2}\right)\right]^{1/2} \\ &\simeq 1 - \frac{H_{12}^2}{2\Delta^2} \qquad (1.175) \end{aligned}$$

and

$$\begin{aligned} C_- &= \frac{1}{\sqrt{2}}\left[1 - \frac{\Delta}{\sqrt{\Delta^2 + 4\left|H_{12}\right|^2}}\right]^{1/2} \\ &\simeq \frac{1}{\sqrt{2}}\left[1 - \left(1 - \frac{2H_{12}^2}{\Delta^2}\right)\right]^{1/2} \\ &\simeq \frac{H_{12}}{\Delta}. \qquad (1.176) \end{aligned}$$

We see that the amount by which the states $\left|u_1^0\right\rangle$ and $\left|u_2^0\right\rangle$ mix to form the new eigenvectors is a function of both H_{12} and Δ. The smaller their ratio (i.e., H_{12}/Δ) the more the states and energies of the true Hamiltonian resemble that of the unperturbed two-level system. It is also apparent that the perturbation has for effect to increase the energy difference between the two levels (from equations (1.163)-(1.164) and (1.174)). Note that when the unperturbed system is degenerate (i.e., $\Delta = 0$), then $C_+ = C_- = 1$ and $S = |H_{12}|$.

1.7 The Heisenberg Representation

Everything we have covered so far was done in the so-called *Schrödinger representation*, where quantum mechanical calculations are done using the Schrödinger equation. With this formalism, we saw that the time evolution of a quantum mechanical system is contained in the state (or wave function) characterizing the system. We now introduce the *Heisenberg representation* where the time dependency is transferred to the observables.

Let us start with $|\psi_S(t)\rangle$ the time-dependent ket representing a quantum mechanical system and some observable $\hat{O}_S$, both in the Schrödinger representation. We already know from equation (1.53) that we can express the time evolution of the system using the unitary operator

$$\hat{U}_t = e^{-i\hat{H}t/\hbar} \tag{1.177}$$

such that

$$|\psi_S(t)\rangle = \hat{U}_t |\psi_S(0)\rangle . \tag{1.178}$$

Evidently, the ket $|\psi_S(0)\rangle$ evaluated at $t = 0$ is independent of time and we will from now on make this explicit by defining

$$|\psi_H\rangle \equiv |\psi_S(0)\rangle . \tag{1.179}$$

We now consider the expectation value

$$\begin{aligned}\left\langle \psi_S(t) \middle| \hat{O}_S \middle| \psi_S(t) \right\rangle &= \left\langle \psi_H \middle| \hat{U}_t^\dagger \hat{O}_S \hat{U}_t \middle| \psi_H \right\rangle \\ &= \left\langle \psi_H \middle| \hat{O}_H(t) \middle| \psi_H \right\rangle ,\end{aligned} \tag{1.180}$$

where we have introduced the time-dependent operator

$$\hat{O}_H(t) \equiv \hat{U}_t^\dagger \hat{O}_S \hat{U}_t . \tag{1.181}$$

The time derivative of the left-hand side of equation (1.180) yields

$$\begin{aligned}\frac{d}{dt}\left\langle \psi_S(t) \middle| \hat{O}_S \middle| \psi_S(t) \right\rangle &= \left[\frac{d}{dt}\langle \psi_S(t)|\right] \hat{O}_S |\psi_S(t)\rangle + \langle \psi_S(t)| \hat{O}_S \left[\frac{d}{dt}|\psi_S(t)\rangle\right] \\ &\quad + \left\langle \psi_S(t) \middle| \frac{\partial}{\partial t}\hat{O}_S \middle| \psi_S(t) \right\rangle ,\end{aligned} \tag{1.182}$$

while upon using the Schrödinger equation (1.52),

$$\begin{aligned}\frac{d}{dt}\left\langle \psi_{\mathrm{S}}(t)\middle|\hat{O}_{\mathrm{S}}\middle|\psi_{\mathrm{S}}(t)\right\rangle &= \left[-\frac{1}{i\hbar}\langle\psi_{\mathrm{S}}(t)|\hat{H}\right]\hat{O}_{\mathrm{S}}|\psi_{\mathrm{S}}(t)\rangle + \langle\psi_{\mathrm{S}}(t)|\hat{O}_{\mathrm{S}}\left[\frac{1}{i\hbar}\hat{H}|\psi_{\mathrm{S}}(t)\rangle\right]\\ &\quad+\left\langle\psi_{\mathrm{S}}(t)\middle|\frac{\partial}{\partial t}\hat{O}_{\mathrm{S}}\middle|\psi_{\mathrm{S}}(t)\right\rangle\\ &= -\frac{1}{i\hbar}\left\langle\psi_{\mathrm{H}}\middle|\hat{U}_t^{\dagger}\hat{H}\hat{O}_{\mathrm{S}}\hat{U}_t\middle|\psi_{\mathrm{H}}\right\rangle+\frac{1}{i\hbar}\left\langle\psi_{\mathrm{H}}\middle|\hat{U}_t^{\dagger}\hat{O}_{\mathrm{S}}\hat{H}\hat{U}_t\middle|\psi_{\mathrm{H}}\right\rangle\\ &\quad+\left\langle\psi_{\mathrm{H}}\middle|\hat{U}_t^{\dagger}\frac{\partial}{\partial t}\hat{O}_{\mathrm{S}}\hat{U}_t\middle|\psi_{\mathrm{H}}\right\rangle. \end{aligned}\tag{1.183}$$

But since $\left[\hat{U}_t, \hat{H}\right] = 0$ we can write

$$\frac{d}{dt}\left\langle \psi_{\mathrm{S}}(t)\middle|\hat{O}_{\mathrm{S}}\middle|\psi_{\mathrm{S}}(t)\right\rangle = \left\langle\psi_{\mathrm{H}}\middle|\left\{\frac{1}{i\hbar}\left[\hat{O}_{\mathrm{H}}(t),\hat{H}\right]+\frac{\partial}{\partial t}\hat{O}_{\mathrm{H}}\right\}\middle|\psi_{\mathrm{H}}\right\rangle, \tag{1.184}$$

where

$$\frac{\partial}{\partial t}\hat{O}_{\mathrm{H}} \equiv \hat{U}_t^{\dagger}\frac{\partial}{\partial t}\hat{O}_{\mathrm{S}}\hat{U}_t. \tag{1.185}$$

Referring once again to equation (1.180), it is clear that we also have

$$\begin{aligned}\frac{d}{dt}\left\langle \psi_{\mathrm{S}}(t)\middle|\hat{O}_{\mathrm{S}}\middle|\psi_{\mathrm{S}}(t)\right\rangle &= \frac{d}{dt}\left\langle\psi_{\mathrm{H}}\middle|\hat{O}_{\mathrm{H}}(t)\middle|\psi_{\mathrm{H}}\right\rangle\\ &= \left\langle\psi_{\mathrm{H}}\middle|\frac{d}{dt}\hat{O}_{\mathrm{H}}(t)\middle|\psi_{\mathrm{H}}\right\rangle,\end{aligned}\tag{1.186}$$

and, comparing with equation (1.184),

$$\frac{d}{dt}\hat{O}_{\mathrm{H}}(t) = \frac{1}{i\hbar}\left[\hat{O}_{\mathrm{H}}(t),\hat{H}\right]+\frac{\partial}{\partial t}\hat{O}_{\mathrm{H}}. \tag{1.187}$$

In cases where $\hat{O}_{\mathrm{S}}$ does not explicitly depend on time $\partial\hat{O}_{\mathrm{S}}/\partial t = \partial\hat{O}_{\mathrm{H}}/\partial t = 0$, and we obtain the so-called ***Heisenberg equation***

$$\frac{d}{dt}\hat{O}_{\mathrm{H}}(t) = \frac{1}{i\hbar}\left[\hat{O}_{\mathrm{H}}(t),\hat{H}\right]. \tag{1.188}$$

It is important to stress, as was made clear from the previous derivation, that the Schrödinger and Heisenberg representations are equivalent formulations of quantum mechanics and yield the same expectation values for observables and time evolution for a quantum mechanical system. The main difference being that the time dependence was transferred from the state vector (for Schrödinger) to the observables (for Heisenberg). Finally, the Heisenberg equation makes it obvious that an observable that commutes with Hamiltonian is a conserved quantity, since its time derivative then equals zero.

Exercise 1.6. Let us consider the one-dimensional quantum mechanical harmonic oscillator, which has the following Hamiltonian

$$\hat{H} = \frac{1}{2}m\omega^2\hat{x}^2 + \frac{\hat{p}_x^2}{2m}, \tag{1.189}$$

where m and ω are, respectively, the mass of the particle and its frequency of oscillation. Derive the relevant dynamical equations using the Heisenberg representation.

Solution.

Although it would possible to solve the Heisenberg equations corresponding to this problem using $\hat{x}$ and $\hat{p}_x$, we will approach it from a different point of view. More precisely, we introduce new generalized conjugate canonical variables

$$\hat{Q} = \sqrt{m\omega}\hat{x} \tag{1.190}$$

$$\hat{P} = \frac{\hat{p}_x}{\sqrt{m\omega}} \tag{1.191}$$

and the so-called *annihilation* (or *lowering*) and *creation* (or *raising*) operators

$$\hat{a} = \sqrt{\frac{1}{2\hbar}}\left(\hat{Q} + i\hat{P}\right) \tag{1.192}$$

$$\hat{a}^\dagger = \sqrt{\frac{1}{2\hbar}}\left(\hat{Q} - i\hat{P}\right), \tag{1.193}$$

respectively. We can now verify the following relations

$$\begin{aligned}\left[\hat{Q}, \hat{P}\right] &= [\hat{x}, \hat{p}_x] \\ &= i\hbar\hat{1} \qquad (1.194)\\ \left[\hat{a}, \hat{a}^\dagger\right] &= \frac{1}{2\hbar}\left(-i\left[\hat{Q}, \hat{P}\right] + i\left[\hat{P}, \hat{Q}\right]\right) \qquad (1.195)\\ &= \hat{1}, \qquad (1.196)\end{aligned}$$

and

$$\begin{aligned}\hat{a}^\dagger\hat{a} &= \frac{1}{2\hbar}\left(\hat{Q} - i\hat{P}\right)\left(\hat{Q} + i\hat{P}\right) \\ &= \frac{1}{2\hbar}\left(\hat{Q}^2 + \hat{P}^2 + i\left[\hat{Q}, \hat{P}\right]\right) \\ &= \frac{1}{2\hbar}\left(m\omega\hat{x}^2 + \frac{\hat{p}_x^2}{m\omega} - \hbar\hat{1}\right) \qquad (1.197)\end{aligned}$$

or equivalently

$$\begin{aligned}\hat{H} &= \frac{\hbar\omega}{2}\left(\hat{a}^{\dagger}\hat{a}+\hat{a}\hat{a}^{\dagger}\right) \\ &= \hbar\omega\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right). \end{aligned} \tag{1.198}$$

We see from equation (1.198) that although $\hat{a}$ and $\hat{a}^{\dagger}$ are not Hermitian, $\hat{a}^{\dagger}\hat{a}$ is (and so is $\hat{a}\hat{a}^{\dagger}$).

Choosing a basis $\{|n\rangle\}$ where the Hamiltonian is diagonal, i.e.,

$$\hat{H}|n\rangle = E_n|n\rangle \tag{1.199}$$

and

$$\left\langle m\left|\hat{H}\right|n\right\rangle = E_n\delta_{mn}, \tag{1.200}$$

we then verify that $\hat{a}^{\dagger}\hat{a}$ is also diagonal with

$$\left\langle m\left|\hat{a}^{\dagger}\hat{a}\right|n\right\rangle = \left(\frac{E_n}{\hbar\omega}-\frac{1}{2}\right)\delta_{mn} \tag{1.201}$$

From equation (1.198) we can further calculate the following commutators

$$\begin{aligned}\left[\hat{H},\hat{a}^{\dagger}\right] &= \hbar\omega\left[\hat{a}^{\dagger}\hat{a},\hat{a}^{\dagger}\right] \\ &= \hbar\omega\hat{a}^{\dagger}\left[\hat{a},\hat{a}^{\dagger}\right] \\ &= \hbar\omega\hat{a}^{\dagger} \end{aligned} \tag{1.202}$$

and

$$\left[\hat{H},\hat{a}\right] = -\hbar\omega\hat{a}. \tag{1.203}$$

These equations can be transformed and applied to a state $|m\rangle$ with the following results

$$\begin{aligned}\hat{H}\left(\hat{a}^{\dagger}|m\rangle\right) &= \left(\hat{a}^{\dagger}\hat{H}+\hbar\omega\hat{a}^{\dagger}\right)|m\rangle \\ &= \left(E_m+\hbar\omega\right)\left(\hat{a}^{\dagger}|m\rangle\right) \end{aligned} \tag{1.204}$$

$$\begin{aligned}\hat{H}\left(\hat{a}|m\rangle\right) &= \left(\hat{a}\hat{H}-\hbar\omega\hat{a}\right)|m\rangle \\ &= \left(E_m-\hbar\omega\right)\left(\hat{a}|m\rangle\right), \end{aligned} \tag{1.205}$$

which imply that both $\hat{a}^{\dagger}|m\rangle$ and $\hat{a}|m\rangle$ are eigenkets of $\hat{H}$ with associated eigenvalues, respectively, increased and decreased by $\hbar\omega$ from that of $|m\rangle$. Since the difference in energy between two adjacent eigenstates is $\hbar\omega$ and that, from the form of the Hamiltonian in equation (1.189), the energy of the oscillator cannot be negative, the minimum energy in equation (1.198) will be found to be $E_m = \hbar\omega/2$ when $\hat{a}^\dagger\hat{a}\,|m\rangle = 0$. If we ascribe $|0\rangle$ to that minimum energy state, then we can introduce the *number operator*

$$\hat{N} \equiv \hat{a}^\dagger\hat{a} \tag{1.206}$$

such that

$$\begin{aligned}\hat{N}\,|n\rangle &= \hat{a}^\dagger\hat{a}\,|n\rangle \\ &= n\,|n\rangle\,.\end{aligned} \tag{1.207}$$

It is then easy to verify that

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{1.208}$$

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \tag{1.209}$$

since

$$\begin{aligned}\hat{N}\,|n\rangle &= \hat{a}^\dagger\left(\hat{a}\,|n\rangle\right) \\ &= \sqrt{n}\left(\hat{a}^\dagger\,|n-1\rangle\right) \\ &= n\,|n\rangle\,,\end{aligned} \tag{1.210}$$

hence the previous definition of $\hat{N}$ as the number operator.

We are now in a position to calculate the dynamical equations that characterize the evolution of the quantum mechanical harmonic oscillator from the application of equation (1.188) (since $\hat{a}$ and $\hat{a}^\dagger$ have no implicit dependence on time). We therefore have

$$\begin{aligned}\frac{d\hat{a}}{dt} &= \frac{1}{i\hbar}\left[\hat{a},\hat{H}\right] \\ &= -i\omega\left[\hat{a},\hat{a}^\dagger\hat{a}\right] \\ &= -i\omega\left[\hat{a},\hat{a}^\dagger\right]\hat{a} \\ &= -i\omega\hat{a},\end{aligned} \tag{1.211}$$

and

$$\begin{aligned}\frac{d\hat{a}^\dagger}{dt} &= \left(\frac{d\hat{a}}{dt}\right)^\dagger \\ &= i\omega\hat{a}^\dagger.\end{aligned} \tag{1.212}$$

It follows from equations (1.190)-(1.193) that

$$\begin{aligned}\frac{d\hat{x}}{dt} &= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{d\hat{a}}{dt}+\frac{d\hat{a}^\dagger}{dt}\right)\\ &= i\sqrt{\frac{\hbar\omega}{2m}}\left(\hat{a}^\dagger-\hat{a}\right)\\ &= \frac{\hat{p}_x}{m}\end{aligned} \tag{1.213}$$

and

$$\begin{aligned}\frac{d\hat{p}_x}{dt} &= -i\sqrt{\frac{\hbar m\omega}{2}}\left(\frac{d\hat{a}}{dt}-\frac{d\hat{a}^\dagger}{dt}\right)\\ &= -\sqrt{\frac{\hbar m\omega^3}{2}}\left(\hat{a}+\hat{a}^\dagger\right)\\ &= -m\omega^2\hat{x}.\end{aligned} \tag{1.214}$$

Incidentally, we should note that equations (1.213) and (1.214) are in agreement with the general result (which you should try to prove) stating that

$$\frac{d\hat{x}}{dt} = \frac{\partial\hat{H}}{\partial\hat{p}_x} \tag{1.215}$$

$$\frac{d\hat{p}_x}{dt} = -\frac{\partial\hat{H}}{\partial\hat{x}}. \tag{1.216}$$

We can further verify that

$$\begin{aligned}\frac{d^2\hat{x}}{dt^2} &= \frac{1}{i\hbar}\left[\frac{d\hat{x}}{dt},\hat{H}\right]\\ &= \frac{1}{i\hbar m}\left[\hat{p}_x,\hat{H}\right]\\ &= \frac{1}{m}\frac{d\hat{p}_x}{dt}\\ &= -\omega^2\hat{x},\end{aligned} \tag{1.217}$$

which when combined with equation (1.213) yields

$$\ddot{\hat{x}}+\omega^2\hat{x}=0. \tag{1.218}$$

This equation is similar to the one found for the classical harmonic oscillator. It is interesting to calculate the following matrix elements

$$\left\langle m \left| \left(\ddot{\hat{x}} + \omega^2 \hat{x} \right) \right| n \right\rangle = \ddot{x}_{mn} + \omega^2 x_{mn}, \tag{1.219}$$

which requires us to determine $\ddot{\hat{x}}_{mn}$. This is accomplished using the Heisenberg equation for a given operator $\hat{O}_{\mathrm{H}}$

$$\begin{aligned} \dot{O}_{mn} &= \left\langle m \left| \left(\frac{1}{i\hbar} \left[\hat{O}_{\mathrm{H}}, \hat{H} \right] \right) \right| n \right\rangle \\ &= \left\langle m \left| \left[\frac{1}{i\hbar} \left(\hat{O}_{\mathrm{H}} \hat{H} - \hat{H} \hat{O}_{\mathrm{H}} \right) \right] \right| n \right\rangle \\ &= i \frac{(E_m - E_n)}{\hbar} O_{mn} \\ &= i\omega_{mn} O_{mn}, \end{aligned} \tag{1.220}$$

where

$$\omega_{mn} \equiv \frac{(E_m - E_n)}{\hbar}. \tag{1.221}$$

Differentiating one more time we find

$$\begin{aligned} \ddot{O}_{mn} &= \left\langle m \left| \left(\frac{1}{i\hbar} \left[\dot{\hat{O}}_{\mathrm{H}}, \hat{H} \right] \right) \right| n \right\rangle \\ &= i\omega_{mn} \dot{O}_{mn} \\ &= -\omega_{mn}^2 O_{mn}, \end{aligned} \tag{1.222}$$

and therefore

$$\ddot{x}_{mn} = -\omega_{mn}^2 x_{mn}. \tag{1.223}$$

Combining equations (1.219) and (1.223) yields

$$\left(\omega^2 - \omega_{mn}^2 \right) x_{mn} = 0, \tag{1.224}$$

which implies that $\omega = \pm\omega_{mn}$ or through equation (1.221)

$$E_m - E_n = \pm\hbar\omega. \tag{1.225}$$

This result is consistent with what was found earlier with equations (1.207) and (1.208), namely that the energy of the oscillator is quantized and changes by steps of energy $\hbar\omega$ between adjacent levels.