A. Simple Aspects of the Structure of Quantum Mechanics

In Chapters 2 to 16 we have used the formulation of quantum mechanics in terms of wave functions and differential operators. This is but one of many equivalent representations of quantum mechanics. In this appendix we shall briefly review that representation and develop an alternative representation in which state vectors correspond to the wave functions and matrices to the operators. To keep things simple we shall restrict ourselves to systems with discrete energy spectra exemplified on the one-dimensional harmonic oscillator.

A.1 Wave Mechanics

In Section 6.3 the stationary Schrödinger equation

\[
\left(-\frac{\hbar}{2m}\frac{d^2}{dx^2} + \frac{m}{2}\omega^2 x^2\right)\varphi_n = E_n \varphi_n(x)
\]

of the harmonic oscillator has been solved. The eigenvalues \(E_n\) were found to be

\[
E_n = (n + \frac{1}{2})\hbar\omega
\]

together with the corresponding eigenfunctions

\[
\varphi_n(x) = \frac{1}{(\sqrt{\pi}\sigma_0 2^n \sqrt{n})^{1/2}} H_n\left(\frac{x}{\sigma_0}\right) \exp\left\{-\frac{x^2}{2\sigma_0^2}\right\}, \quad \sigma_0 = \sqrt{\frac{\hbar}{m\omega}}.
\]

Quite generally, we can write the stationary Schrödinger equation as an eigenvalue equation

\[
H \varphi_n = E_n \varphi_n,
\]

where the Hamiltonian \(H\) – as in classical mechanics – is the sum

\[
H = T + V
\]

of the kinetic energy.
\[ T = \frac{\hat{p}^2}{2m} \]

and the potential energy
\[ V = \frac{m}{2} \omega^2 x^2. \]

The difference to classical mechanics consists in the momentum being given in one-dimensional quantum mechanics by the \textit{differential operator}
\[ \hat{p} = i \hbar \frac{d}{dx} \]

so that the kinetic energy takes the form
\[ T = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}. \]

Two eigenfunctions \( \varphi_n(x) \), \( \varphi_m(x) \), \( m \neq n \) belonging to different eigenvalues \( E_m \neq E_n \) are \textit{orthogonal}, i.e.,
\[ \int_{-\infty}^{+\infty} \varphi_m^*(x) \varphi_n(x) \, dx = 0. \]

Conventionally, for \( m = n \) the eigenfunctions are \textit{normalized} to one, i.e.,
\[ \int_{-\infty}^{+\infty} \varphi_n^*(x) \varphi_n(x) \, dx = 1, \]

so that we may summarize
\[ \int_{-\infty}^{+\infty} \varphi_m^*(x) \varphi_n(x) \, dx = \delta_{mn}, \]

where we have used the \textit{Kronecker symbol}
\[ \delta_{mn} = \begin{cases} 1, & m = n \\ 0, & m \neq n \end{cases}. \]

The infinite set of mutually orthogonal and normalized eigenfunctions \( \varphi_n(x) \), \( n = 0, 1, 2, \ldots \), forms a \textit{complete orthonormal basis} of all complex-valued functions \( f(x) \) which are square integrable, i.e.,
\[ \int_{-\infty}^{+\infty} f^*(x) f(x) \, dx = N^2, \quad N < \infty. \]

\( N \) is called the \textit{norm} of the function \( f(x) \). Functions with norm \( N \) can be normalized to one,

\footnote{The functions \( \varphi_m(x) \) are real functions. We add an asterisk (indicating the complex conjugate) to the function \( \varphi_m(x) \) in the integral, since in other cases one often has to deal with complex functions.}
A.2 Matrix Mechanics in an Infinite Vector Space

\[ \int_{-\infty}^{+\infty} \varphi^*(x)\varphi(x)\,dx = 1, \]

by dividing them by the normalization factor \( N \),

\[ \varphi(x) = \frac{1}{N} f(x). \]

The completeness of the set \( \varphi_n(x), n = 0, 1, 2, \ldots \), allows the expansion

\[ f(x) = \sum_{n=0}^{\infty} f_n \varphi_n(x). \]

Because of the orthonormality of the eigenfunctions the complex coefficients \( f_n \) are simply

\[ f_n = \int_{-\infty}^{+\infty} \varphi_n^*(x) f(x)\,dx. \]

We also get

\[ N^2 = \int_{-\infty}^{+\infty} f^*(x) f(x)\,dx = \sum_{n=0}^{\infty} |f_n|^2. \]

The superposition of two normalizable functions

\[ f(x) = \sum_{n=0}^{\infty} f_n \varphi_n(x), \quad g(x) = \sum_{n=0}^{\infty} g_n \varphi_n(x) \]

with complex coefficients \( \alpha, \beta \) may be expressed by

\[ \alpha f(x) + \beta g(x) = \sum_{n=0}^{\infty} (\alpha f_n + \beta g_n) \varphi_n(x). \]

Their scalar product is defined as

\[ \int_{-\infty}^{+\infty} g^*(x) f(x)\,dx = \sum_{n=0}^{\infty} g_n^* f_n. \]

A.2 Matrix Mechanics in an Infinite Vector Space

The normalizable functions \( f(x) \) form a linear vector space of infinite dimensionality, i.e., each function \( f(x) \) can be represented by a vector \( f \) in that space,

\[ f(x) \rightarrow f. \]
With the base vectors

\[\varphi_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \varphi_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad \varphi_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \quad \ldots\]

a general vector \( f \) takes the form

\[f = \sum_{n=0}^{\infty} f_n \varphi_n = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}.

The axioms of the infinite space of complex column vectors are the natural extension of the ones for finite complex vectors:

(i) **Linear superposition** (\( \alpha, \beta \) complex numbers):

\[\alpha f + \beta g = \begin{pmatrix} \alpha f_0 + \beta g_0 \\ \alpha f_1 + \beta g_1 \\ \alpha f_2 + \beta g_2 \\ \vdots \end{pmatrix}.

(ii) **Scalar product**:

\[g^+ \cdot f = (g_0^*, g_1^*, g_2^*, \ldots) \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix} = \sum_{n=0}^{\infty} g_n^* f_n.

Here the adjoint \( g^+ \) of the vector \( g \) has been introduced, \( g^+ = (g_0^*, g_1^*, g_2^*, \ldots) \), as the line vector of the complex conjugates \( g_0^*, g_1^*, g_2^*, \ldots \) of the components of the column vector

\[g = \begin{pmatrix} g_0 \\ g_1 \\ g_2 \\ \vdots \end{pmatrix}.

Because of the infinity of the set of natural numbers an additional axiom has to be added:
(iii) The norm $|f|$ of the vectors $f$ is finite,
\[ |f|^2 = f^+ \cdot f = \sum_{n=0}^{\infty} f^*_n f_n = N^2, \quad N < \infty, \]
i.e., the infinite sum has to converge. Because of Schwartz’s inequality
\[ |g^+ \cdot f| \leq |g||f| \]
all scalar products of vectors $f, g$ of the space are finite.

As in the ordinary finite-dimensional vector spaces we call a linear transformation $A$ of a function $f(x)$ into a function $g(x),$
\[ g(x) = Af(x), \]
the linear operator $A.$ Examples of linear transformations are
- the momentum operator $\hat{p} = -i\hbar \frac{d}{dx},$
  \[ \hat{p} f = \frac{\hbar}{i} \frac{df}{dx}(x), \]
- the Hamiltonian $H = -(\hbar^2/2m) \frac{d^2}{dx^2} + V(x),$
  \[ H f = -\frac{\hbar^2}{2m} \frac{d^2 f(x)}{dx^2} + V(x) f(x), \]
- the position operator $\hat{x} = x,$
  \[ \hat{x} f = xf(x). \]

Linear operators can be represented by matrices. We show this by the following argument. The function $g$ is represented by the coefficients $g_m,$
\[ g(x) = \sum_{m=0}^{\infty} g_m \varphi_m(x), \quad g_m = \int_{-\infty}^{+\infty} \varphi_m^*(x) g(x) dx. \]
The image function $g$ of $f$ is given by
\[ g(x) = Af(x) = A \left( \sum_{n=0}^{\infty} f_n \varphi_n(x) \right) = \sum_{n=0}^{\infty} A\varphi_n(x) f_n, \]
i.e., by a linear combination of the images $A\varphi_n$ of the elements $\varphi_n$ of the orthonormal basis. The $A\varphi_n$ themselves can be represented by a linear combination of the basis vectors.
\[ A\varphi_n = \sum_{m=0}^{\infty} \varphi_m(x)A_{mn} \ , \quad n = 0, 1, 2, \ldots \ , \]

with the coefficients

\[ A_{mn} = \int_{-\infty}^{+\infty} \varphi_m^*(x)A\varphi_n(x)\,dx \ . \]

Inserting this into the expression for \( g(x) \) we obtain

\[ g(x) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \varphi_m(x)A_{mn}f_n \ . \]

Comparing with the representation for \( g(x) \) we find for the coefficients \( g_n \) the expression

\[ g_m = \sum_{n=0}^{\infty} A_{mn}f_n \ . \]

We arrange the coefficients \( A_{mn} \) like matrix elements in an infinite matrix scheme

\[
A = \begin{pmatrix}
A_{00} & A_{01} & A_{02} & \cdots \\
A_{10} & A_{11} & A_{12} & \cdots \\
A_{20} & A_{21} & A_{22} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]

and recover an infinite dimensional extension of the matrix multiplication

\[ g = Af \]

in the form

\[
\begin{pmatrix}
g_0 \\
g_1 \\
g_2 \\
\vdots
\end{pmatrix} = \begin{pmatrix}
A_{00} & A_{01} & A_{02} & \cdots \\
A_{10} & A_{11} & A_{12} & \cdots \\
A_{20} & A_{21} & A_{22} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix} \begin{pmatrix}
f_0 \\
f_1 \\
f_2 \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\sum_{n=0}^{\infty} A_{0n}f_n \\
\sum_{n=0}^{\infty} A_{1n}f_n \\
\sum_{n=0}^{\infty} A_{2n}f_n \\
\vdots
\end{pmatrix} .
\]

It should be noted that the two descriptions by wave functions and operators or by vectors and matrices are equivalent. The correspondence relations

\[ \varphi(x) = \sum_{n=0}^{\infty} a_n\varphi_n(x) \leftrightarrow \varphi = \begin{pmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots
\end{pmatrix} \]

with

\[ a_n = \int_{-\infty}^{+\infty} \varphi_n^*(x)\varphi(x)\,dx \]
for wave functions and vectors work in both directions. For a given wave function \( \varphi(x) \) we can uniquely determine the vector \( \varphi \) relative to the basis \( \varphi_n(x) \), \( n = 0, 1, 2, \ldots \). Conversely, for a given vector \( \varphi \) relative to the basis \( \varphi_n(x) \) we can reconstruct the wave function \( \varphi(x) \) as the above superposition of the \( \varphi_n(x) \). The descriptions in terms of \( \varphi(x) \) and \( \varphi \) contain the same information about the state the system is in.

Thus, generally one does not distinguish the two descriptions and says the system is in the state \( \varphi \), often denoted by the ket \( |\varphi\rangle \) as introduced by Paul A. M. Dirac.

The wave function \( \varphi(x) \) or the vector \( \varphi \) are considered merely as two representations out of which many can be invented. The same statements hold true for the representation of operators in terms of differential operators or matrices. Also these are only representations of one and the same linear transformation called linear operator. The states \( \varphi \) like the wave functions or vectors \( \varphi \) form a linear vector space with scalar product. This general space is called \textit{Hilbert space}. The linear operators transform a state of the Hilbert space into another state.

### A.3 Matrix Representation of the Harmonic Oscillator

Since the \( \varphi_n(x) \) are normalized eigenfunctions of the Hamiltonian, we find for its matrix elements

\[
H_{mn} = \int_{-\infty}^{+\infty} \varphi_m^*(x)H\varphi_n(x) \, dx
= (n + \frac{1}{2})\hbar\omega \int_{-\infty}^{+\infty} \varphi_m^*(x)\varphi_n(x) \, dx
= (n + \frac{1}{2})\hbar\omega \delta_{mn}.
\]

Thus, the matrix representation of the Hamiltonian of the harmonic oscillator in its eigenfunction basis is diagonal:

\[
H = \hbar\omega \begin{pmatrix}
\frac{1}{2} & 0 & 0 & \cdots \\
0 & \frac{3}{2} & 0 & \cdots \\
0 & 0 & \frac{5}{2} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

The representation of the eigenfunctions \( \varphi_n(x) \) in their own basis are given by the standard columns

\[
\varphi_0 = \begin{pmatrix}
1 \\
0 \\
0 \\
\vdots
\end{pmatrix}, \quad \varphi_1 = \begin{pmatrix}
0 \\
1 \\
0 \\
\vdots
\end{pmatrix}, \quad \varphi_2 = \begin{pmatrix}
0 \\
0 \\
1 \\
\vdots
\end{pmatrix}, \quad \cdots
\]

Of course, the eigenvector equation is recovered also in matrix representation,

\[ H \psi_n = (n + \frac{1}{2}) \hbar \omega \psi_n \]

With the help of the recurrence relations for Hermite polynomials,

\[
\begin{align*}
\frac{d H_n(x)}{dx} &= 2n H_{n-1}(x), \\
H_{n+1}(x) &= 2x H_n(x) - 2n H_{n-1}(x),
\end{align*}
\]

we find the matrix representations for the position operator \( \hat{x} \) and the momentum operator \( \hat{p} \) in harmonic-oscillator representation,

\[
\hat{x} \psi_n = x \psi_n(x) = \frac{\sigma_0}{(\sqrt{\pi} \sigma_0^2 n!)^{1/2}} \left(n H_{n-1}(x) + \frac{1}{2} H_n(x)\right) \exp\left\{-\frac{x^2}{2\sigma_0^2}\right\} \\
\qquad = \frac{\sigma_0}{\sqrt{2}} \left(\sqrt{n} \psi_{n-1}(x) + \sqrt{n+1} \psi_{n+1}(x)\right).
\]

The coefficients \( x_{mn} \) are given by

\[
x_{mn} = \int_{-\infty}^{+\infty} \psi_m^*(x) x \psi_n(x) dx = \frac{\sigma_0}{\sqrt{2}} \left(\sqrt{n} \delta_{m(n-1)} + \sqrt{n+1} \delta_{m(n+1)}\right),
\]

and the matrix representation of the position operator is

\[
x = \frac{\sigma_0}{\sqrt{2}} \begin{pmatrix}
0 & 1 & 0 & 0 & \ldots \\
1 & 0 & \sqrt{2} & 0 & \ldots \\
0 & \sqrt{2} & 0 & \sqrt{3} & \ldots \\
0 & 0 & \sqrt{3} & 0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

For the momentum operator we obtain in a similar way the matrix representation

\[
p = \frac{\hbar}{\sqrt{2}\sigma_0} \begin{pmatrix}
0 & i & 0 & 0 & \ldots \\
-i & 0 & i\sqrt{2} & 0 & \ldots \\
0 & -i\sqrt{2} & 0 & i\sqrt{3} & \ldots \\
0 & 0 & -i\sqrt{3} & 0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

One easily verifies the commutation relation

\[ [p, x] = px - xp = \frac{\hbar}{i} \]

also for the infinite matrix representations of \( x \) and \( \hat{p} \). Both matrices for \( x \) and \( \hat{p} \) are Hermitean, i.e.,

\[ x_{mn}^* = x_{nm}, \quad p_{nm}^* = p_{mn}. \]
A.4 Time-Dependent Schrödinger Equation

The time dependence of wave functions is determined by the time-dependent Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} \psi(x,t) = H \psi(x,t) \ . \]

The eigenstates \( \varphi_n(x) \) of the Hamiltonian are the space-dependent factors in an ansatz

\[ \psi_n(x,t) = \exp \left\{ -\frac{i}{\hbar} E_n t \right\} \varphi_n(x) \ , \]

and the eigenvalues \( E_n \) determine the time dependence of the phase factor.

In the matrix representation of the harmonic oscillator the time-dependent Schrödinger equation simply reads

\[ i\hbar \frac{d}{dt} \psi(t) = H \psi(t) \ , \]

where \( \psi(t) \) is a vector in Hilbert space,

\[ \psi(t) = \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \\ \psi_2(t) \\ \vdots \end{pmatrix} . \]

Because of the linearity of the Schrödinger equation any linear combination

\[ \psi(x,t) = \sum_{n=0}^{\infty} a_n \psi_n(x,t) = \sum_{n=0}^{\infty} a_n \exp \left\{ -\frac{i}{\hbar} E_n t \right\} \varphi_n(x) \]

also solves the Schrödinger equation. In vectorial representation we have

\[ \psi(t) = \sum_{n=0}^{\infty} a_n \exp \left\{ -\frac{i}{\hbar} E_n t \right\} \varphi_n \ , \quad E_n = (n + \frac{1}{2})\hbar \omega \ . \]

The initial condition at \( t = 0 \) for the time-dependent Schrödinger equation is the initial wave function

\[ \psi(x,0) = \psi_i(x) = \sum_{n=0}^{\infty} \psi_{in} \varphi_n(x) \ . \]

In vector notation this is an initial state vector \( \psi_i \). Its decomposition into eigenvectors \( \varphi_n \),
\[
\begin{pmatrix}
\psi_{i0} \\
\psi_{i1} \\
\psi_{i2} \\
\vdots
\end{pmatrix} = \psi_i = \sum_{n=0}^{\infty} a_n \varphi_n = \begin{pmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots
\end{pmatrix},
\]
directly provides the identification of the expansion coefficients \(a_n\) with the components \(\psi_{in}\) of the initial vector \(\psi_i\),

\[a_n = \psi_{in}.\]

This way the time-dependent Schrödinger equation is solved by the expression

\[\psi(t) = \sum_{n=0}^{\infty} \psi_{in} \exp \left\{-\frac{i}{\hbar} E_n t \right\} \varphi_n,\]

for the initial condition

\[\psi(0) = \psi_i.\]

The time-dependent vector \(\psi_n(t)\) corresponding to \(\psi_n(x,t)\) is

\[\psi_n(t) = \exp \left\{-\frac{i}{\hbar} E_n t \right\} \varphi_n = \exp \left\{-\frac{i}{\hbar} H t \right\} \varphi_n,\]

where \(E_n\) is the energy eigenvalue corresponding to the eigenvector \(\varphi_n\), i.e., \(E_n = (n + \frac{1}{2})\hbar \omega\) for the harmonic oscillator. The last equality is meaningful if we define the exponential of a matrix by its Taylor series

\[\exp \left\{-\frac{i}{\hbar} H t \right\} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} H t \right)^n.\]

For the case of the diagonal matrix \(H\) the \(n\)th power is trivial,

\[H^n = \begin{pmatrix}
E_0^n & 0 & 0 & \cdots \\
0 & E_1^n & 0 & \cdots \\
0 & 0 & E_2^n & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix},\]

and the explicit matrix form is

\[
\exp \left\{-\frac{i}{\hbar} H t \right\} = \begin{pmatrix}
\exp \left\{-\frac{i}{\hbar} E_0 t \right\} & 0 & 0 & \cdots \\
0 & \exp \left\{-\frac{i}{\hbar} E_1 t \right\} & 0 & \cdots \\
0 & 0 & \exp \left\{-\frac{i}{\hbar} E_2 t \right\} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}.\]
Using the operator representation of
\[ \psi_n(x,t) = \exp \left\{ -\frac{i}{\hbar} E_n t \right\} \varphi_n = \exp \left\{ -\frac{i}{\hbar} H t \right\} \varphi_n \]
as derived above we may rewrite \( \psi(t) \) into the form
\[ \psi(t) = \sum_{n=0}^{\infty} \psi_n \exp \left\{ -\frac{i}{\hbar} E_n \right\} \varphi_n \]
\[ = \exp \left\{ -\frac{i}{\hbar} H t \right\} \sum_{n=0}^{\infty} \psi_n \varphi_n \]
\[ = \exp \left\{ -\frac{i}{\hbar} H t \right\} \psi(0) \]
\[ = U_H(t) \psi(0) . \]
The operator
\[ U_H(t) = \exp \left\{ -\frac{i}{\hbar} H t \right\} \]
is called the \textit{temporal-evolution operator}.

\section*{A.5 Probability Interpretation}

The eigenfunctions \( \varphi_n(x) \), equivalently the eigenvectors \( \varphi_n \), describe a state of the physical system with the energy eigenvalue \( E_n \). Thus, a precise measurement of the energy of this system in the state \( \varphi_n \) should be devised to produce as a result the value \( E_n \). In order to preserve the reproducibility of the measurement it should not change the eigenstate \( \varphi_n \) of the system during the measurement, i.e., immediately after the energy measurement the state of the system should still be \( \varphi_n \).

The question arises what result will be found in the same energy measurement carried out at a system in a state \( \varphi \) described by the wave function \( \varphi(x) \), or equivalently, by the vector \( \varphi \) being a superposition of eigenfunctions \( \varphi_n(x) \) or eigenvectors \( \varphi_n \),
\[ \varphi = \sum_{n=0}^{\infty} a_n \varphi_n , \]
with norm one, i.e.,
\[ \sum_{n=0}^{\infty} |a_n|^2 = 1 . \]
The single measurement of the energy will result in one of the energy eigenvalues which we call $E_m$. Reproducibility of the measurement then requires that the system is in the state $\varphi_m$ after the measurement.

The absolute square $|a_m|^2$ of the coefficients $a_m$ in the superposition of the $\varphi_m$ defining $\varphi$ is the probability with which the energy eigenvalue $E_m$ will be determined in the single measurement.

Let us assume that we prepare a large assembly of $N$ identical systems, all in the same state $\varphi_m$. If we carry out single measurements on these various identical systems we shall measure the energy eigenvalue $E_m$ with the abundance $|a_m|^2 N$.

Performing a weighted average over the results of all measurements yields the expectation value of the energy

$$\langle E \rangle = \frac{1}{N} \sum_{n=0}^{\infty} |a_n|^2 N E_n = \sum_{n=0}^{\infty} |a_n|^2 E_n .$$

Using the state-vector representation of $\varphi$,

$$\varphi = \left( \begin{array}{c} a_0 \\ a_1 \\ a_2 \\ \vdots \end{array} \right) ,$$

we find that the energy expectation value is simply

$$\varphi^+ H \varphi = (a_0^*, a_1^*, a_2^*, \ldots) \begin{pmatrix} E_0 & 0 & 0 & \ldots \\ 0 & E_1 & 0 & \ldots \\ 0 & 0 & E_2 & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$= \sum_{n=0}^{\infty} a_n^* E_n a_n = \langle E \rangle .$$

Equivalently, in wave-function formulation, we have

$$\int_{-\infty}^{+\infty} \varphi^*(x) H \varphi(x) \, dx = \int_{-\infty}^{+\infty} \varphi^*(x) \sum_{n=0}^{\infty} E_n a_n \varphi_n(x) \, dx$$

$$= \sum_{n=0}^{\infty} E_n a_n \int_{-\infty}^{+\infty} \varphi^*(x) \varphi_n(x) \, dx$$

$$= \sum_{n=0}^{\infty} E_n a_n a_n^* = \langle E \rangle .$$
B. Two-Level System

In Appendix A the equivalence of wave-function and matrix representation of quantum mechanics was shown. The simplest matrix structure is the one in two dimensions, i.e., in a space with two base states:

\[
\eta_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \eta_{-1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]

The linear space consists of all linear combinations

\[
\chi = \chi_1 \eta_1 + \chi_{-1} \eta_{-1} = \begin{pmatrix} \chi_1 \\ \chi_{-1} \end{pmatrix}
\]

of the base states with complex coefficients \(\chi_1\) and \(\chi_{-1}\). The two states \(\eta_1\) and \(\eta_{-1}\) form an orthonormal basis of this space, i.e.,

\[
\eta_1^+ \cdot \eta_1 = 1, \quad \eta_{-1}^+ \cdot \eta_{-1} = 1, \quad \eta_1^+ \cdot \eta_{-1} = \eta_{-1}^+ \cdot \eta_1 = 0.
\]

For the linear combination \(\chi\) to be normalized to one we have

\[
\chi^+ \cdot \chi = \chi_1^+ \chi_1 + \chi_{-1}^+ \chi_{-1} = |\chi_1|^2 + |\chi_{-1}|^2 = 1.
\]

This suggests a representation of the absolute values \(|\chi_r|, r = 1, -1\), of the complex coefficients by trigonometric functions:

\[
|\chi_1| = \cos \frac{\Theta}{2}, \quad |\chi_{-1}| = \sin \frac{\Theta}{2}.
\]

The use of the half-angle \(\Theta/2\) is a convention, the usefulness of which will become obvious in the sequel. The complex coefficients themselves are obtained by multiplication of the moduli \(|\chi_r|\) with arbitrary phase factors:

\[
\chi_1 = e^{-i\phi_1/2} \cos \frac{\Theta}{2}, \quad \chi_{-1} = e^{-i\phi_{-1}/2} \sin \frac{\Theta}{2}.
\]

Since a common phase factor is irrelevant the general form can be restricted to
\[ \chi_1 = e^{-i\Phi/2} \cos \frac{\Theta}{2}, \quad \chi_{-1} = e^{i\Phi/2} \sin \frac{\Theta}{2} \]

with
\[ \Phi = (\Phi_1 - \Phi_{-1})/2. \]

The general linear combination is therefore
\[ \chi(\Theta, \Phi) = e^{-i\Phi/2} \cos \frac{\Theta}{2} \eta_1 + e^{i\Phi/2} \sin \frac{\Theta}{2} \eta_{-1} = \left( e^{-i\Phi/2} \cos \frac{\Theta}{2}, e^{i\Phi/2} \sin \frac{\Theta}{2} \right). \]

The operators corresponding to physical quantities are Hermitean matrices
\[ A = \begin{pmatrix} A_{1,1} & A_{1,-1} \\ A_{-1,1} & A_{-1,-1} \end{pmatrix}. \]

The Hermitean conjugate of \( A \) is defined as
\[ A^+ = \begin{pmatrix} A^*_{1,1} & A^*_{1,-1} \\ A^*_{-1,1} & A^*_{-1,-1} \end{pmatrix}, \quad \text{i.e.,} \quad A^+_{rs} = A^*_{sr}. \]

The condition of Hermiticity,
\[ A^+ = A, \quad \text{i.e.,} \quad A^*_{sr} = A_{rs}, \]
requires
\[ A^*_{1,1} = A_{1,1}, \quad A^*_{1,-1} = A_{-1,1}, \quad A^*_{-1,1} = A_{1,-1}, \quad A^*_{-1,-1} = A_{-1,-1}. \]

Thus, the diagonal elements \( A_{1,1}, A_{-1,-1} \) are real quantities, the off-diagonal elements \( A_{1,-1}, A_{-1,1} \) are complex conjugates of each other. Hermiticity of the operator \( A \) ensures that the expectation value of \( A \) for a given general state is real,
\[ \chi^+ A \chi = \sum_{i,j=1,-1} \chi_i^* A_{ij} \chi_j \]
\[ = \chi_1^* A_{1,1} \chi_1 + \chi_1^* A_{1,-1} \chi_{-1} + \chi_{-1}^* A_{-1,-1} \chi_1 + \chi_{-1}^* A_{-1,1} \chi_{-1}. \]

All Hermitean matrices can be linearly combined as the superpositions
\[ A = a_0 \sigma_0 + a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3 \]
(with real coefficients \( a_0, \ldots, a_3 \)) of the unit matrix
\[ \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]
and the Pauli matrices
\[ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]
since the four matrices \( \sigma_0, \ldots, \sigma_3 \) are Hermitean. One directly verifies the relations
\[ \sigma_i^2 = \sigma_0, \quad i = 0, 1, 2, 3, \]
and
\[ \sigma_1 \sigma_2 = i \sigma_3, \quad \sigma_2 \sigma_3 = i \sigma_1, \quad \sigma_3 \sigma_1 = i \sigma_2. \]
These yield the commutation relations
\[ [\sigma_1, \sigma_2] = \sigma_1 \sigma_2 - \sigma_2 \sigma_1 = 2i \sigma_3 \]
and cyclic permutations.

The three Pauli matrices can be grouped into a vector in three dimensions,
\[ \sigma = (\sigma_1, \sigma_2, \sigma_3), \]
with the square
\[ \sigma^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 = 3 \sigma_0^2. \]
The base states \( \eta_1, \eta_{-1} \) are eigenstates of the Pauli matrix \( \sigma_3 \) and of the sum of their squares \( \sigma^2 \),
\[ \sigma_3 \eta_r = r \eta_r, \quad \sigma^2 \eta_r = 3 \sigma_0 \eta_r = 3 \eta_r, \quad r = 1, -1, \]
since \( \sigma_3 \) and \( \sigma_0 \) are diagonal matrices.

According to Section A the time-dependent Schrödinger equation reads
\[ i \hbar \frac{d}{dt} \xi(t) = H \xi(t), \]
where the Hamiltonian is a Hermitean \( 2 \times 2 \) matrix,
\[ H = \begin{pmatrix} H_{1,1} & H_{1,-1} \\ H_{-1,1} & H_{-1,-1} \end{pmatrix}, \]
with real diagonal matrix elements \( H_{1,1}, H_{-1,-1} \) and with off-diagonal elements \( H_{-1,1} = H_{1,-1}^* \). It can be represented by a superposition of the \( \sigma \) matrices,
\[ H = h_0 \sigma_0 + h_3 \sigma_3 + h_1 \sigma_1 + h_2 \sigma_2, \]
where
\[ h_0 = \frac{1}{2} (H_{1,1} + H_{-1,-1}), \quad h_3 = \frac{1}{2} (H_{1,1} - H_{-1,-1}), \]
and
\[ h_1 = \frac{1}{2}(H_{1,-1} + H_{-1,1}) = \text{Re} H_{1,-1} , \]
\[ h_2 = \frac{i}{2}(H_{1,-1} - H_{-1,1}) = -\text{Im} H_{1,-1} . \]

Introducing the \( h_i \) \((i = 0, 1, 2, 3)\) into the matrix \( H \) we obtain
\[
H = \begin{pmatrix}
    h_0 + h_3 & h_1 - ih_2 \\
    h_1 + ih_2 & h_0 - h_3
\end{pmatrix} .
\]

Introducing the factorization
\[
\xi_r(t) = \exp\left\{ -\frac{i}{\hbar} E_r t \right\} \chi_r , \quad r = 1, -1 ,
\]
into the time-dependent phase factor and the stationary state \( \chi_r \) we obtain the stationary Schrödinger equation
\[
H \chi_r = E_r \chi_r , \quad r = 1, -1 ,
\]
for the eigenstate \( \chi_r \) belonging to the energy eigenvalue \( E_r \). For the eigenvalues we find
\[
E_{\pm 1} = h_0 \pm |h| , \quad |h| = \sqrt{h_1^2 + h_2^2 + h_3^2} .
\]

Since there are only two eigenvalues our system is called a two-level system.

The eigenstates are
\[
\chi_{1} = \frac{1}{\sqrt{2|h|}} \begin{pmatrix}
    \sqrt{|h| + h_3} & e^{-i\phi/2} \\
    \sqrt{|h| - h_3} & e^{i\phi/2}
\end{pmatrix} ,
\]
\[
\chi_{-1} = \frac{1}{\sqrt{2|h|}} \begin{pmatrix}
    -\sqrt{|h| - h_3} & e^{-i\phi/2} \\
    \sqrt{|h| + h_3} & e^{i\phi/2}
\end{pmatrix} ,
\]
with the phase factor determined by
\[
e^{i2\phi} = \frac{h_1 + ih_2}{h_1 - ih_2} .
\]

Introducing the angle \( \Theta \) by
\[
\cos \frac{\Theta}{2} = \sqrt{\frac{|h| + h_3}{2|h|}} , \quad \sin \frac{\Theta}{2} = \sqrt{\frac{|h| - h_3}{2|h|}}
\]
we may write the eigenstates in the form
\[ \chi_1 = e^{-i\phi/2} \cos \Theta \eta_1 + e^{i\phi/2} \sin \Theta \eta_{-1}, \]
\[ \chi_{-1} = -e^{-i\phi/2} \sin \Theta \eta_1 + e^{i\phi/2} \cos \Theta \eta_{-1}. \]

They are normalized and orthogonal to each other.

The eigenstates \( \chi_1, \chi_{-1} \) of the two-level system exhibit a time dependence which is given by a phase factor only,

\[ \xi_r(t) = \exp \left\{ -\frac{i}{\hbar} E_r t \right\} \chi_r, \quad r = 1, -1. \]

If initially the system is not in an eigenstate the state oscillates. We assume that the initial state is

\[ \varphi(0) = \eta_{-1}. \]

Decomposition into the eigenstates yields

\[ \eta_{-1} = \zeta_1 \chi_1 + \zeta_{-1} \chi_{-1} \]

with

\[ \zeta_1 = \chi_1^\dagger \cdot \eta_{-1} = e^{-i\phi/2} \sin \Theta \]
\[ \zeta_{-1} = \chi_{-1}^\dagger \cdot \eta_{-1} = e^{-i\phi/2} \cos \Theta. \]

The time-dependent state is obtained as

\[ \varphi(t) = \zeta_1 \xi_1(t) + \zeta_{-1} \xi_{-1}(t) \]
\[ = e^{-i\phi/2} \sin \Theta e^{-i\omega_t t} \chi_1 + e^{i\phi/2} \cos \Theta e^{-i\omega_{-1} t} \chi_{-1} \]

with the angular frequencies

\[ \omega_r = E_r/\hbar, \quad r = 1, -1. \]

The probability to find the system (originally in the state \( \eta_{-1} \)) in the state \( \eta_1 \) is given by

\[ P_{1,-1} = \sin^2 \Theta \sin^2 \frac{\Theta}{\hbar} e^{-i\omega_{-1} |t|}, \]

and, of course, the probability to find it in the state \( \eta_{-1} \) is

\[ P_{-1,-1} = 1 - P_{1,-1}. \]
C. Analyzing Amplitude

C.1 Classical Considerations: Phase-Space Analysis

We consider a detector which is capable of measuring position and momentum of a particle simultaneously with certain accuracies. If the result of a measurement is the pair $x_D$, $p_D$ of values we may assume that the true values $x$, $p$ of the quantities to be measured are described by the uncorrelated bivariate Gaussian (cf. Section 3.5) probability density

$$
\rho_D(x, p, x_D, p_D) = \frac{1}{2\pi \sigma_{xD} \sigma_{pD}} \exp \left\{ -\frac{1}{2} \left[ \frac{(x-x_D)^2}{\sigma_{xD}^2} + \frac{(p-p_D)^2}{\sigma_{pD}^2} \right] \right\}.
$$

That is to say, the probability for the true values $x$, $p$ of the particle to be in the intervals between $x$ and $x + dx$ and between $p$ and $p + dp$ is

$$
dP = \rho_D(x, p)dx dp.
$$

The particle to be measured by the detector possesses position and momentum values $x$ and $p$. The particle may have been produced by a source which does not define exactly the values of $x$ and $p$ but according to a probability density

$$
\rho_S(x, p, x_S, p_S) = \frac{1}{2\pi \sigma_{xS} \sigma_{pS}} \exp \left\{ -\frac{1}{2} \left[ \frac{(x-x_S)^2}{\sigma_{xS}^2} + \frac{(p-p_S)^2}{\sigma_{pS}^2} \right] \right\}. 
$$

This is an uncorrelated bivariate Gaussian probability density with the expectation values $x_S$ and $p_S$ and the variances $\sigma_{xS}^2$ and $\sigma_{pS}^2$.

We now describe how much information can at best be obtained about the probability density $\rho_S(x, p)$ using the above detector. The probability for a particle prepared by the source to be detected within the intervals $(x_D, x_D + dx_D)$ and $(p_D, p_D + dp_D)$ is given by

$$
dP = W_{cl}(x_D, p_D, x_S, p_S) dx_D dp_D,
$$

with the probability density in phase space.
\[ w^{cl}(x_D, p_D, x_S, p_S) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho^{cl}_D(x, p, x_D, p_D) \rho^{cl}_S(x, p, x_S, p_S) \, dx \, dp \]
\[ = \frac{1}{2\pi \sigma_x \sigma_p} \exp \left\{ -\frac{1}{2} \left[ \frac{(x_D - x_S)^2}{\sigma_x^2} + \frac{(p_D - p_S)^2}{\sigma_p^2} \right] \right\} . \]

Here the variances \( \sigma_x^2 \) and \( \sigma_p^2 \) are obtained by summing up the variances of the detector and source distribution,
\[ \sigma_x^2 = \sigma_{xD}^2 + \sigma_{xS}^2 , \quad \sigma_p^2 = \sigma_{pD}^2 + \sigma_{pS}^2 . \]

The quantity \( w^{cl}(x_D, p_D, x_S, p_S) \) is the result of analyzing the phase-space probability density of the source \( \rho_S(x, p, x_S, p_S) \) with the help of the phase-space probability density \( \rho_D(x, p, x_D, p_D) \). The function \( w^{cl}(x_D, p_D, x_S, p_S) \) is itself a phase-space probability density and obtained through a process we shall call phase-space analysis.

This distribution can be measured in principle if the source consecutively produces a large number of particles which are observed in the detector. For a detector of arbitrarily high precision,
\[ \sigma_{xD} \to 0 , \quad \sigma_{pD} \to 0 , \]
the distribution \( w^{cl} \) approaches the source distribution \( \rho_S(x = x_D, p = p_D, x_S, p_S) \).

We have seen that with a detector of high precision and with a sufficiently high number of measurements the source distribution can be measured with arbitrary high accuracy. We now assume that the minimum-uncertainty relations,
\[ \sigma_{xD} \sigma_{pD} = \frac{\hbar}{2} , \quad \sigma_{xS} \sigma_{pS} = \frac{\hbar}{2} , \]
hold for the widths characterizing the detector and the source. Besides this restriction we stay within the framework of classical physics. Now it is no longer possible to measure the source distribution exactly.\(^1\) However, we may still measure the distribution in position alone or the distribution in momentum alone with arbitrary accuracy. To show this we construct the marginal distributions of \( w^{cl} \) in the variables \( x_D - x_S \), and \( p_D - p_S \), respectively,
\[ w^{cl}_x(x_D, x_S) = \frac{1}{\sqrt{2\pi \sigma_x}} \exp \left\{ -\frac{1}{2} \frac{(x_D - x_S)^2}{\sigma_x^2} \right\} \]
and
\[ ^1 \text{We could, however, compute the source distribution } \rho_S \text{ by unfolding it from } w^{cl}. \]
Fig. C.1. Phase-space distributions $\rho_S$ (top), $\rho_D$ (middle), and their product $\rho_S \rho_D$ (bottom) together with the marginal distributions of $\rho_S$ and $\rho_D$. The two columns differ only in the spatial mean $x_S$ of $\rho_S$. Units are used in which $\hbar = 1$.

\[
w_D = \int \rho_0(x,p) g_0(x,p) \, dp = 0.159
\]

\[
w_S = \int \rho_0(x,p) g_0(x,p) \, dx = 0.022
\]

The first distribution approaches the corresponding marginal position distribution of the source,

\[
\rho_S(x,x_S) = \int_{-\infty}^{+\infty} \rho_S(x,p,x_S,p_S) \, dp = \frac{1}{\sqrt{2\pi \sigma_{xS}^2}} \exp \left\{ -\frac{1}{2} \frac{(x - x_S)^2}{\sigma_{xS}^2} \right\}
\]

in the case of $\sigma_{x_D} \to 0$. However, because of the minimum uncertainty relations, $\sigma_{p_D}$ as well as $\sigma_p$ approach infinity. Therefore, the second distribution
Fig. C.2. The phase-space distribution $\rho_S$ (top), the distribution $\rho_D$ for a particular point $(x_D, p_D)$ of mean values (middle), and convolution of $\rho_S$ with $\rho_D$ for all possible mean values (bottom). Also shown are the marginal distributions. The two columns differ in the widths of $\rho_S$. Units $\bar{\hbar} = 1$ are used.

$w_{cl}^{\ast}$ becomes so wide – and actually approaches zero – that no information about the momentum distribution can be obtained from it.

Conversely, for $\sigma_{pD} \to 0$ the momentum distribution of the source can be measured accurately. However, then the information about the position distribution is lost.

We illustrate the concepts of this section in Figures C.1 and C.2. We begin with the discussion of the result of a single measurement, yielding the pair $x_D$, $p_D$ of measured values. In the two columns of Figure C.1 we show (from top to bottom) the probability density $\rho_S(x, p)$ characterizing the particle as pro-
duced by the source, the density $\rho_D(x, p)$ characterizing the detector for the case $x_D = 0, \ p_D = 0$, and the product function $\rho_S(x, p)\rho_D(x, p)$. The integral over the product function is the probability density $w^{cl}$. It is essentially different from zero only if there is a region, the overlap region, in which both $\rho_S$ and $\rho_D$ are different from zero. In the left-hand column of Figure C.1 $\rho_S$ and $\rho_D$ were chosen to be identical, so that $w^{cl}$ is large. In the right-hand column the overlap is smaller.

By very many repeated measurements, each yielding a different result $x_D, p_D$ we obtain the probability density $w^{cl}(x_D, p_D)$. In the two columns of Figure C.2 we show (from top to bottom) the probability density $\rho_S(x, p)$ characterizing the detector for the particular set measured values $x_D = 0, \ p_D = 0$, and the probability density $w^{cl}(x_D, p_D)$ for measuring the pair of values $x_D, p_D$. Also shown are the marginal distribution $\rho_{S_x}(x)$, $\rho_{D_x}(x)$, and $w^{cl}_x(x_D)$ in position, and $\rho_{S_p}(p)$, $\rho_{D_p}(p)$, and $w^{cl}_p(p_D)$ in momentum. Comparing in the left-hand column the diagram of $\rho_S$ with the diagram of $w^{cl}$ we see that the latter distribution is appreciably broader than the former in both variables. In the right-hand column, however, the spatial width of the detector distribution $\sigma_{x_D}$ is very small at the expense of the momentum width $\sigma_{p_D} = \hbar/(2\sigma_{x_D})$, which is very large. The distribution $w^{cl}$ is practically identical to $\rho_S$ what concerns its spatial variation. The width in momentum of $w^{cl}$ is, however, very much larger than that of $\rho_S$.

### C.2 Analyzing Amplitude: Free Particle

Quantum-mechanically we describe a particle by the minimum-uncertainty wave packet

$$\varphi_S(x) = \varphi_S(x, x_S, p_S) = \frac{1}{(2\pi)^{1/4}\sigma_{x_S}^{1/2}} \exp\left\{ - \frac{(x - x_S)^2}{4\sigma_{x_S}^2} + \frac{i}{\hbar} p_S(x - x_S) \right\}.$$  

We consider this wave packet as having been prepared by some physical apparatus, the source. The question now arises how the phase-space analysis of the particle as discussed in the last section can be described in quantum mechanics.

If, in a particle detector with position-measurement uncertainty $\sigma_{x_D}$ and momentum-measurement uncertainty $\sigma_{p_D} = \hbar/(2\sigma_{x_D})$, the values $x_D, \ p_D$ are measured, we want to interpret the result as in Section C.1. The same probability density

$$\rho_D(x, p, x_D, p_D) = \frac{1}{2\pi \sigma_{x_D} \sigma_{p_D}} \exp\left\{ - \frac{1}{2} \left[ \frac{(x - x_D)^2}{\sigma_{x_D}^2} + \frac{(p - p_D)^2}{\sigma_{p_D}^2} \right] \right\}.$$
describes the probability density of position \( x \) and momentum \( p \) of the particle. Quantum-mechanically this probability density is the phase-space distribution introduced by Eugene P. Wigner in 1932 of the wave packet

\[
\varphi_D(x, x_D, p_D) = \frac{1}{(2\pi \sigma_{x_D}^{1/2})^1} \exp \left\{ -\frac{(x - x_D)^2}{4\sigma_{x_D}^2} + \frac{i}{\hbar} p_D (x - x_D) \right\}.
\]

Therefore, \( \rho_D(x, p, x_D, p_D) \) is also called Wigner distribution of \( \varphi_D \) (cf. Appendix D).

Let us construct the analyzing amplitude

\[
a(x_D, p_D, x_S, p_S) = \frac{1}{\sqrt{2\pi \sigma_x \sigma_p}} \int_{-\infty}^{+\infty} \varphi_D^*(x, x_D, p_D) \varphi_S(x, x_S, p_S) \, dx
\]

representing the overlap between the particle’s wave function \( \varphi_S \) and the detecting wave function \( \varphi_D \). It turns out to be

\[
a(x_D, p_D, x_S, p_S) = \frac{1}{\sqrt{2\pi \sigma_x \sigma_p}} \exp \left\{ \frac{(x_D - x_S)^2}{4\sigma_x^2} - \frac{(p_D - p_S)^2}{4\sigma_p^2} - \frac{i}{\hbar} \sigma_{x_D} p_D + \sigma_{x_S} p_S \right\} ,
\]

where, like in Section C.1,

\[
\sigma_x^2 = \sigma_{x_D}^2 + \sigma_{x_S}^2 , \quad \sigma_p^2 = \sigma_{p_D}^2 + \sigma_{p_S}^2 .
\]

The absolute square of the analyzing amplitude

\[
|a|^2 = \frac{1}{2\pi \sigma_x \sigma_p} \exp \left\{ -\frac{1}{2} \left[ \frac{(x_D - x_S)^2}{\sigma_x^2} + \frac{(p_D - p_S)^2}{\sigma_p^2} \right] \right\} = w^{cl}(x_D, p_D, x_S, p_S)
\]

is identical to the probability density \( w^{cl}(x_D, p_D, x_S, p_S) \) of Section C.1.

We conclude that the probability amplitude analyzing the values \( x_D \) and \( p_D \) of position and momentum of a particle as a result of the interaction of a particle with a detector is given by

\[
a(x_D, p_D, x_S, p_S) = \frac{1}{\sqrt{\hbar}} \int_{-\infty}^{+\infty} \varphi_D^*(x, x_D, p_D) \varphi_S(x, x_S, p_S) \, dx
\]

Here, \( \varphi_S \) is the wave function of the particle and \( \varphi_D \) the analyzing wave function. The probability to observe a position in the interval between \( p_D \) and \( p_D + dp_D \) is

\[
dP = |a(x_D, p_D, x_S, p_S)|^2 \, dx_D \, dp_D .
\]
In analogy to the classical case we may now ask whether we can still recover the original quantum-mechanical spatial probability density

\[ \rho_S(x) = |\varphi_S(x)|^2 = \frac{1}{\sqrt{2\pi}\sigma_{xs}} \exp\left\{-\frac{1}{2}\frac{(x - x_S)^2}{\sigma_{xs}^2}\right\} \]

from \( |a|^2 \). Information about the position of the particle only is obtained by integrating \( |a|^2 \) over all values of \( p_D \), i.e., by forming the marginal distribution with respect to \( x_D \),

\[ |a|^2_x = \int_{-\infty}^{+\infty} |a|^2 \, dp_D = w_{xi}(x_D, x_S) . \]

The result is the same as in the classical case. Again in the limit \( \sigma_{xD} \to 0 \) we find that the function \( |a|^2_x \) approaches the quantum-mechanical probability density \( \rho_S(x) \) which is equal to the classical distribution \( \rho_{S,x}(x) \).

In Figures C.3 and C.4 we demonstrate the construction of the analyzing amplitude using particular numerical examples. Each column of three plots in the two figures is one example. At the top of the column the particle wave function is shown as two curves depicting \( \text{Re}\varphi_S(x) \) and \( \text{Im}\varphi_S(x) \) together with the numerical values of the parameters \( x_S, p_S, \sigma_{xs} \) which define \( \varphi(x) \). Likewise, the middle plot shows the detector wave function, given by \( \text{Re}\varphi_D(x) \) and \( \text{Im}\varphi_D(x) \). The bottom plot contains the real and imaginary parts of the product function

\[ \varphi_D^*(x)\varphi_S(x) , \]

which after integration and absolute squaring yields the probability density

\[ |a|^2 = \frac{1}{\hbar} \left| \int_{-\infty}^{+\infty} \varphi_D^*(x)\varphi_S(x) \, dx \right|^2 \]

of detection. Also given in the bottom plot is the numerical value of \( |a|^2 \). Four different situations are shown in the two figures. In each case the same detector function \( \varphi_D \) is used. Only the particle wave function \( \varphi_S \) changes from case to case.

(i) In the left-hand column of Figure C.3 \( \varphi_S \) and \( \varphi_D \) are identical. For that case we know that the overlap integral is explicitly real and that

\[ \int_{-\infty}^{+\infty} \varphi_S^*\varphi_S \, dx = 1, \]

so that \( |a|^2 = 1/\hbar = 1/2\pi \) in the units \( \hbar = 1 \) used.

(ii) In the right-hand column of Figure C.3 the particle wave packet is moved to a position expectation value \( x_S \neq x_D \), but we still have \( p_S = p_D, \sigma_{xs} = \sigma_{xD} \). By construction, the overlap function is different from zero in that \( x \) region where both \( \varphi_S \) and \( \varphi_D \) are sizably different from zero. As expected, the value of \( |a|^2 \) is considerably smaller than in case (i).
(i) In the left-hand column of Figure C.4 the position expectation values and the widths of particle and detector wave function are identical, \( x_S = x_D, \sigma_{xS} = \sigma_{xD} \), but the momentum expectation values differ, \( p_S \neq p_D \). As in case (i) the product function \( \varphi_D^* \varphi_S \) is different from zero in the region \( x \approx x_0 \) but due to the different momentum expectation values it oscillates. Therefore, the value of \( |a|^2 \) is much smaller than in case (i) since positive and negative regions of the product function nearly cancel when the integration is performed.
Fig. C.4. As Figure C.3 but for different functions \( \psi_S \). The two columns differ only in the value of \( \sigma_{xS} \).

(iv) In the right-hand column of Figure C.4 the particle wave packet has a larger width \( \sigma_{xS} > \sigma_{xD} \). All other parameters are as in case (iii). The product function is similar to that for case (iii) and is concentrated in the region \( x_D - \sigma_{xD} \leq x \leq x_D + \sigma_{xD} \) where both wave functions are appreciably different from zero. However, the amplitude of the product function is smaller than in case (iii) since the amplitude of \( \psi_S(x) \) is smaller in the overlap region. Therefore, the value of \( |a|^2 \) is also smaller.
C.3 Analyzing Amplitude: General Case

The lesson learned in the last section can be generalized to the analysis of an arbitrary normalized wave function $\varphi(x)$ describing a single particle in terms of an arbitrary complete or overcomplete set of normalized wave functions $\varphi(x)$ or $\varphi(x, q_1, \ldots, q_N)$. The functions $\varphi_n(x)$ can in particular be eigenfunctions of a Hermitean operator, e.g., the energy. Examples for a set of overcomplete functions $\varphi(x, q_1, \ldots, q_n)$ are

- free wave packets $\varphi_D(x, x_D, p_D)$ as in the last section,
- coherent states of the harmonic oscillator $\varphi(x, x_0, p_0)$ as we shall study in detail in the next section, and
- minimum-uncertainty states of a set of noncommuting operators like the operators $L_x, L_y, L_z$ of angular momentum or $S_x, S_y, S_z$ of spin as investigated in Sections 10.5 and 17.2.

The analyzing amplitude for the different cases is given by

$$a = \frac{1}{N_1} \int_{-\infty}^{+\infty} \varphi_n^*(x) \varphi(x) \, dx$$

or

$$a = \frac{1}{N_2} \int_{-\infty}^{+\infty} \varphi^*(x, q_1, \ldots, q_N) \varphi(x) \, dx$$

Of course, a mutual analysis of two sets of analyzing functions is also of interest, e.g.,

$$a = \frac{1}{N_3} \int_{-\infty}^{+\infty} \varphi_n^*(x) \varphi(x, q_1, \ldots, q_N) \, dx$$

The normalization constants have to be individually determined for every type of analyzing amplitude.

C.4 Analyzing Amplitude: Harmonic Oscillator

For the harmonic oscillator of frequency $\omega$ we have discussed in Sections 6.3 and 6.4 two sets of states in particular:

(i) The eigenstates $\varphi_n$ corresponding to the energy eigenvalues $E_n = (n + \frac{1}{2})\hbar\omega$,

$$\varphi_n(x) = (\sqrt{2\pi} 2^n n!\sigma_0)^{-1/2} H_n\left(\frac{x}{\sigma_0}\right) \exp\left\{-\frac{x^2}{2\sigma_0}\right\} ,$$
with the ground-state width

\[ \sigma_0 = \sqrt{2\sigma_x} \quad , \quad \sigma_x = \sqrt{\frac{\hbar}{2m\omega}} . \]

Plots of the \( \varphi_n \) are shown in Figure 6.5.

(ii) The coherent states,

\[ \psi(x, t, x_0, p_0) = \sum_{m=0}^{\infty} a_m(x_0, p_0) \varphi_m(x) \exp \left\{ -\frac{i}{\hbar} E_m t \right\} , \]

where the complex coefficients \( a_n \) are given by

\[ a_n(x_0, p_0) = \frac{z^n}{\sqrt{n!}} \exp \left\{ -\frac{1}{2} z^* z \right\} , \quad n = 0, 1, 2, \ldots . \]

The variable \( z \) is complex and a dimensionless linear combination of the initial expectation values \( x_0 \) of position and \( p_0 \) of momentum,

\[ z = \frac{x_0}{2\sigma_x} + i \frac{p_0}{2\sigma_p} , \quad \sigma_p = \frac{\hbar}{2\sigma_x} . \]

Plots of the coherent states \( \psi(x, t) \) are shown in Figure 6.6c.

The set of energy eigenfunctions \( \varphi_n(x) \) is complete, the set of coherent states is overcomplete. We can form four kinds of analyzing amplitudes.

**Eigenstate – Eigenstate Analyzing Amplitude**

We analyze the energy eigenfunctions using energy eigenfunctions as analyzing wave functions. Thus, we obtain as analyzing amplitude

\[ a_{mn} = \int_{-\infty}^{+\infty} \varphi_m(x) \varphi_n(x) \, dx = \delta_{mn} , \]

which yields as probability

\[ a_{mn}^2 = \delta_{mn} . \]

This result, based on the orthonormality of the eigenfunctions \( \varphi_n(x) \), is illustrated in Figure C.5 which shows the functions \( \varphi_m \varphi_n \). Whereas \( \varphi_m^2 \) is non-negative everywhere so that the integral over \( \varphi_m^2 \) cannot vanish it is qualitatively clear from the figure that the integral over \( \varphi_m \varphi_n \) vanishes for \( m \neq n \).

The analysis of an eigenstate \( \varphi_n(x) \) with all eigenstates \( \varphi_m(x) \) thus yields with probability \( a_{mn}^2 = 1 \) the answer that the original wave function was indeed \( \varphi_n \), and with probability \( a_{mn} = 0 \) the result that the original wave function was \( \varphi_m \) with \( m \neq n \). Such an analysis can also be considered as an energy determination which with certainty yields the energy eigenvalue \( E_n \).
C.4 Analyzing Amplitude: Harmonic Oscillator

Fig. C.5. Product $\phi_m(x)\phi_n(x)$ of the wave functions of the harmonic oscillator for $\hbar \omega = 1$. The long-dash curve indicates the potential energy $V(x)$, the short-dash lines show the energy eigenvalue $E_n$ of the functions $\phi_n$. These lines also serve as zero lines for the product functions.

Eigenstate – Coherent-State Analyzing Amplitude

The function to be analyzed is the time-dependent wave function $\psi(x,t,x_0,p_0)$ of the coherent state. The analyzing function is the energy eigenfunction $\phi_n(x)$. As analyzing amplitude we obtain

$$a(n,x_0,p_0) = \int_{-\infty}^{+\infty} \phi_n(x)\psi(x,t,x_0,p_0) \, dx$$

$$= \frac{z^n}{\sqrt{n!}} \exp \left\{ -\frac{1}{2} z^* z \right\} \exp \left\{ -\frac{i}{\hbar} E_n t \right\} .$$

The corresponding probability is given by

$$|a(n,x_0,p_0)|^2 = \frac{(|z|^2)^n}{n!} e^{-|z|^2} , \quad |z|^2 = \frac{x_0^2}{4\sigma_x^2} + \frac{p_0^2}{4\sigma_p^2} .$$

The probabilities $|a(n,x_0,p_0)|^2$ for fixed $x_0$, $p_0$ are distributed in the integer $n$ according to a Poisson distribution, cf. Appendix G. Its physical interpretation can be understood if we express $|z|^2$ in terms of the expectation value of the total energy of an oscillator with initial values $x_0$ and $p_0$,
\[ E_0 = \frac{p_0^2}{2m} + \frac{m}{2} \omega^2 x_0^2. \]

We find
\[ |z|^2 = \frac{E_0}{\hbar \omega} = n_0, \]
i.e., \(|z|^2\) equals the number \(n_0\) of energy quanta \(\hbar \omega\) making up the energy \(E_0\) of the classical oscillator. This number, of course, need not be an integer. For the absolute square of the analyzing amplitude we thus find
\[ |a_n(x_0, p_0)|^2 = \frac{n_0^n}{n!} e^{-n_0}. \]

It is the probability of a Poisson distribution for the number of energy quanta \(n\) found when analyzing a coherent wave function with the eigenfunctions \(\varphi_n\). It has the expectation value
\[ \langle n \rangle = n_0 \]
and the variance
\[ \text{var}(n) = n_0. \]

**Coherent-State – Eigenstate Analyzing Amplitude**

Analyzing the eigenstate wave functions \(\varphi_n(x)\) with the coherent state wave functions for \(t = 0\),
\[ \varphi_D(x, x_D, p_D) = \sum_{n=0}^{\infty} a_n(x_D, p_D)\varphi_n(x), \]
with the coefficients
\[ a_n(x_D, p_D) = \frac{z_D^n}{\sqrt{n!}} \exp \left\{ -\frac{1}{2} z_D^* z_D \right\}, \quad z_D = \frac{x_D}{2\sigma_x} + i \frac{p_D}{2\sigma_p}, \]
we find as the analyzing amplitude
\[ a(x_D, p_D, n) = \frac{1}{\sqrt{\hbar}} \int_{-\infty}^{+\infty} \varphi_D^*(x, x_D, p_D)\varphi_n(x) \, dx \]
\[ = \frac{1}{\sqrt{\hbar} \sqrt{n!}} \exp \left\{ -\frac{1}{2} z_D^* z_D \right\}, \]
and for its absolute square
\[ |a(x_D, p_D, n)|^2 \]
\[ = \frac{1}{2\pi(\sqrt{2\sigma_x})(\sqrt{2\sigma_p})} \frac{1}{n!} \left( \frac{x_D^2}{4\sigma_x^2} + \frac{p_D^2}{4\sigma_p^2} \right)^n \exp \left\{ -\left( \frac{x_D^2}{4\sigma_x^2} + \frac{p_D^2}{4\sigma_p^2} \right) \right\}. \]
For a given quantum number $n$ of the eigenstate, $|a|^2$ is a probability density in the $x_D, p_D$ phase space of the analyzing coherent state which is shown in Figure C.6 for a few values of $n$. It has the form of a ring wall with the maximum probability at

$$|z_D|^2 = \frac{x_D^2}{4\sigma_x^2} + \frac{p_D^2}{4\sigma_p^2} = n_D .$$

In terms of the energy

$$E_D = \frac{p_D^2}{2m} + \frac{m}{2} \omega^2 x_D^2$$

of a classical particle of mass $m$ with position $x_D$ and momentum $p_D$ in a harmonic oscillator of angular frequency $\omega$, we have

$$|z_D|^2 = \frac{x_D^2}{4\sigma_x^2} + \frac{p_D^2}{4\sigma_p^2} = n_D ,$$

where $n_D$ is the average number of energy quanta $\hbar \omega$ in the analyzing wave function $\varphi_D(x, x_D, p_D)$. We find
\[ |a(x_D, p_D, n)|^2 = \frac{1}{\hbar} e^{-n_D n_D^R/n!} . \]

For a given eigenstate \( \varphi_n(x) \) of the harmonic oscillator the probability density in the \( x_D, p_D \) phase space of coherent states depends only on the average number \( n_D \) of quanta in the analyzing coherent state.

The expectation value of \( n_D \) is given by
\[
\langle n_D \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} n_D |a(x_D, p_D, n)|^2 dx_D dp_D = n + 1 .
\]

Its variance has the same value:
\[
\text{var}(n_D) = n + 1 .
\]

**Coherent-State – Coherent-State Analyzing Amplitude**

Using as analyzing wave functions the coherent states \( \varphi_D(x, x_D, p_D) \), the analyzing amplitude for the time-dependent coherent states \( \psi(x, t, x_0, p_0) \) turns out to be

\[
a(x_D, p_D, x_0, p_0, t) = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \varphi_D^*(x, x_D, p_D) \psi(x, t, x_0, p_0) dx
= \frac{1}{\sqrt{h}} \exp \left\{ -\frac{1}{2} \left( z_D^* z_D + 2z_D^* z(t) + z^*(t) z(t) \right) \right\} \exp \left\{ -\frac{i}{2} \omega t \right\}
\]

with
\[
z(t) = z e^{-i\omega t} , \quad z = \frac{x_0}{2\sigma_x} + i \frac{p_0}{2\sigma_p} .
\]

The absolute square yields
\[
|a(x_D, p_D, x_0, p_0, t)|^2 = \frac{1}{2\pi (\sqrt{2}\sigma_x)(\sqrt{2}\sigma_p)} \exp \left\{ -\frac{1}{2} \left[ \frac{(x_D - x_0(t))^2}{2\sigma_x^2} + \frac{(p_D - p_0(t))^2}{2\sigma_p^2} \right] \right\}
\]

with
\[
x_0(t) = x_0 \cos \omega t + \frac{p_0}{m\omega} \sin \omega t , \quad p_0(t) = -m\omega x_0 \sin \omega t + p_0 \cos \omega t
\]

representing the expectation values of position and momentum of the coherent state \( \psi(x, t, x_0, p_0) \) at time \( t \). It is a bivariate Gaussian in the space of \( x_D \) and \( p_D \) centered about the classical positions \( x_0(t) \), \( p_0(t) \) of the oscillator. The
probability density $|a(x_D, p_D, x_0, p_0, t)|^2$ shows the same behavior as that of a classical particle. The expectation values of the position $x_D$ and of momentum $p_D$ are simply given by the classical values

$$\langle x_D \rangle = x_0(t), \quad \langle p_D \rangle = p_0(t).$$

The variances of $x_D$ and $p_D$ are

$$\text{var}(x_D) = 2\sigma_x^2, \quad \text{var}(p_D) = 2\sigma_p^2.$$  

This is twice the values of the ones of the coherent state itself, a consequence of the broadening caused by the analyzing wave packet $\varphi_D(x)$ having itself the variances $\sigma_x^2$ and $\sigma_p^2$.

The classical Gaussian phase-space probability density corresponding to $\psi(x, t, x_0, p_0)$ is of the same form as $|a(x_D, p_D, x_0, p_0, t)|^2$. It possesses, however, the widths $\sigma_x$ and $\sigma_p$, and has the explicit form

$$\rho^{\text{cl}}(x, p, x_0, p_0, t) = \frac{1}{2\pi\sigma_x\sigma_p} \exp\left\{-\frac{1}{2} \left[ \frac{(x - x_0(t))^2}{\sigma_x^2} + \frac{(p - p_0(t))^2}{\sigma_p^2} \right]\right\}.$$  

By the same token the classical phase-space density corresponding to the detecting wave packet is

$$\rho^{\text{cl}}_D(x, p, x_D, p_D) = \frac{1}{2\pi\sigma_x\sigma_p} \exp\left\{-\frac{1}{2} \left[ \frac{(x - x_D)^2}{\sigma_x^2} + \frac{(p - p_D)^2}{\sigma_p^2} \right]\right\}.$$  

The functions $\rho^{\text{cl}}$ and $\rho^{\text{cl}}_D$ are equal to the Wigner distributions (cf. Appendix D) of $\varphi$ and $\varphi_D$, respectively. The analyzing probability density $|a|^2$ can again be written as

$$|a(x_D, p_D, x_0, p_0, t)|^2 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho^{\text{cl}}_D(x, p, x_D, p_D) \rho^{\text{cl}}(x, p, x_0, p_0, t) \, dx_D \, dp_D,$$

which once more shows the reason for the broadening of $|a|^2$ relative to $\rho$. 

The quantum-mechanical analog to a classical phase-space probability density is a distribution introduced by Eugene P. Wigner in 1932. In the simple case of a one-dimensional system described by a wave function $\phi(x)$ the Wigner distribution is defined by

$$W(x, p) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \exp \left\{ \frac{i}{\hbar} p y \right\} \phi(x - \frac{y}{2}) \phi^*(x + \frac{y}{2}) \, dy .$$

For an uncorrelated Gaussian wave packet with the wave function

$$\phi(x, x_0, p_0) = \frac{1}{\sqrt{2 \pi} \sqrt{\sigma_x}} \exp \left\{ -\frac{(x - x_0)^2}{4\sigma_x^2} + \frac{i}{\hbar} p_0 (x - x_0) \right\}$$

it has the form of a bivariate normalized Gaussian:

$$W(x, p, x_0, p_0) = \frac{1}{2\pi \sigma_x \sigma_p} \exp \left\{ -\frac{1}{2} \left[ \frac{(x - x_0)^2}{\sigma_x^2} + \frac{(p - p_0)^2}{\sigma_p^2} \right] \right\} ,$$

where $\sigma_x$ and $\sigma_p$ fulfill the minimum-uncertainty relation

$$\sigma_x \sigma_p = \frac{\hbar}{2} .$$

The expression obtained for $W(x, p, x_0, p_0)$ coincides with the classical phase-space probability density for a single particle introduced in Section 3.6. The marginal distributions in $x$ or $p$ of the Wigner distribution are

$$W_p(x) = \int_{-\infty}^{+\infty} W(x, p) \, dp = \phi^*(x)\phi(x) = \rho(x)$$

and

$$W_x(p) = \int_{-\infty}^{+\infty} W(x, p) \, dx = \tilde{\phi}^*(p)\tilde{\phi}(p) = \rho_p(p) ,$$

where $\tilde{\phi}(p)$ is the Fourier transform.
\[
\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \exp \left\{ -\frac{i}{\hbar} px \right\} \varphi(x) \, dx
\]

of the wave function \( \varphi(x) \), i.e., \( \tilde{\phi}(p) \) is the wave function in momentum space.

For the case of the Gaussian wave packet we find for the marginal distributions

\[
W_p(x) = \frac{1}{\sqrt{2\pi \sigma_x}} \exp \left\{ -\frac{1}{2} \frac{(x - x_0)^2}{\sigma_x^2} \right\},
\]

\[
W_x(p) = \frac{1}{\sqrt{2\pi \sigma_p}} \exp \left\{ -\frac{1}{2} \frac{(p - p_0)^2}{\sigma_p^2} \right\}.
\]

An alternative representation for the Wigner distribution can be obtained by introducing the wave function in momentum space into the expression defining \( W(x, p) \) with the help of

\[
\varphi(x) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{+\infty} \exp \left\{ i\frac{p}{\hbar} x \right\} \tilde{\phi}(p) \, dp.
\]

We find

\[
W(x, p) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \exp \left\{ -\frac{i}{\hbar} xq \right\} \tilde{\phi} \left( p - \frac{q}{2} \right) \tilde{\phi}^* \left( p + \frac{q}{2} \right) \, dq.
\]

A note of caution should be added: For a general wave function \( \varphi(x) \) the Wigner distribution is not a positive function everywhere. Thus, in general it cannot be interpreted as a phase-space probability density. It is, however, a real function

\[
W^*(x, p) = W(x, p).
\]

As an example we indicate the Wigner distribution \( W(x, p, n) \) for the eigenfunction \( \varphi_n(x) \) of the harmonic oscillator,

\[
W(x, p, n) = \frac{(-1)^n}{\pi \hbar} L_n^0 \left( \frac{x^2}{\sigma_x^2} + \frac{p^2}{\sigma_p^2} \right) \exp \left\{ -\frac{1}{2} \left( \frac{x^2}{\sigma_x^2} + \frac{p^2}{\sigma_p^2} \right) \right\}.
\]

Here, the widths \( \sigma_x, \sigma_p \) are given by

\[
\sigma_x = \sqrt{\hbar/(2m\omega)} \quad , \quad \sigma_p = \hbar/(2\sigma_p),
\]

and \( L_n^0(x) \) is the Laguerre polynomial with upper index \( k = 0 \) as discussed in Section 13.4.

Figure D.1 shows the Wigner distributions for the lowest four eigenstates of the harmonic oscillator \( n = 0, 1, 2, 3 \) plotted over the plane of the scaled variables \( x/\sigma_x, \ p/\sigma_p \). Accordingly, the plots are rotationally symmetric about the \( z \) axis of the coordinate frame. The nonpositive regions of \( W(x, p, n) \) can be clearly seen. The corresponding plots for the absolute square of the analyzing amplitude are shown in Figure C.6.
The relation to the analyzing amplitude can easily be inferred from the following observation. For an arbitrary analyzing wave function $\varphi_D(x)$ we form the Wigner distribution

$$W_D(x, p) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \exp \left\{ \frac{i}{\hbar} py' \right\} \varphi_D(x - \frac{y'}{2}) \varphi_D^*(x + \frac{y'}{2}) \, dy' .$$

Then, the integral over $x$ and $p$ of the product of $W_D$ and $W$ yields

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} W_D(x, p) W(x, p) \, dx \, dp = \frac{1}{\hbar} \left| \int_{-\infty}^{+\infty} \varphi_D^*(x) \varphi(x) \, dx \right|^2 = |a|^2 .$$

This is to say, analyzing the Wigner distribution $W(x, p)$ of a wave function $\varphi(x)$ with the Wigner distribution $W_D(x, p)$ of an (arbitrary) analyzing wave function $\varphi_D(x)$ yields exactly the absolute square of the analyzing amplitude

$$a = \frac{1}{\sqrt{\hbar}} \int_{-\infty}^{+\infty} \varphi_D^*(x) \varphi(x) \, dx$$

introduced in Appendix C.
The temporal evolution of a Wigner distribution

\[ W(x, p, t) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} p y} \psi^\ast(x + \frac{y}{2}, t) \psi(x - \frac{y}{2}, t) \, dy \]

corresponding to a time-dependent solution \( \psi(x, t) \) of the Schrödinger equation with the Hamiltonian \( H = p^2/2m + V(x) \), \( p = (\hbar/i) d/dx \), is governed by the Wigner–Moyal equation. It is the quantum-mechanical analog of the Liouville equation for a classical phase-space distribution. For potentials \( V(x) \) which are constant, linear, or quadratic in the coordinate \( x \) or linear combinations of these powers the two equations of Wigner and Moyal, and of Liouville are identical. For these types quantum-mechanical and classical phase-space distributions that coincide at one instant \( t \) in time, say the initial one, coincide at all the times.
E. Gamma Function

The gamma function $\Gamma(z)$ introduced by Leonhard Euler is a generalization of the factorial function for integers $n$,

$$n! = 1 \cdot 2 \cdot 3 \cdots n \quad , \quad 0! = 1! = 1 \quad ,$$

to noninteger and eventually complex numbers $z$. It is defined by Euler’s integral

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t} \, dt \quad , \quad \text{Re}(z) > 0 \quad .$$

By partial integration of

$$\int_0^\infty t^z e^{-t} \, dt = \Gamma(1+z)$$

we find the recurrence formula

$$\Gamma(1+z) = -t^z e^{-t}\big|_0^\infty + z \int_0^\infty t^{z-1}e^{-t} \, dt = z\Gamma(z)$$

valid for complex $z$.

From Euler’s integral we obtain

$$\Gamma(1) = 1$$

and, thus, with the help of the recurrence relation for non-negative integer $n$,

$$\Gamma(1+n) = n! \quad .$$

Euler’s integral can also be computed in closed form for $z = 1/2$,

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \quad ,$$

so that – again through the recurrence relation – it is easy to find the gamma function for positive half-integer arguments.
For nonpositive integer arguments the gamma function has poles as can be read off the reflection formula
\[ \Gamma(1 - z) = \frac{\pi}{\Gamma(z) \sin(\pi z)} = \frac{\pi z}{\Gamma(1 + z) \sin(\pi z)} . \]

In Figure E.1 we show graphs of the real and the imaginary part of \( \Gamma(z) \) as surfaces over the complex \( z \) plane. The most striking features are the poles for nonpositive real integer values of \( z \). For real arguments \( z = x \) the gamma function is real, i.e., \( \text{Im}(\Gamma(x)) = 0 \). In Figure E.2 we show \( \Gamma(x) \) and \( 1/\Gamma(x) \). The latter function is simpler since it has no poles. The gamma function for purely imaginary arguments \( z = iy \), \( y \) real, is shown in Figure E.3.

For complex argument \( z = x + iy \) an explicit decomposition into real and imaginary part can be given,
\[ \Gamma(x + iy) = (\cos \theta + i \sin \theta) |\Gamma(x)| \prod_{j=0}^{\infty} \frac{|j + x|}{\sqrt{y^2 + (j + x)^2}} , \]
where the angle \( \theta \) is determined by
\[ \theta = y \psi(x) + \sum_{j=0}^{\infty} \left[ \frac{y}{j + x} - \arctan \frac{y}{j + x} \right] . \]
Here \( \psi(x) \) is the digamma function
\[ \psi(x) = \frac{d}{dx} (\ln \Gamma(x)) = \frac{\Gamma'(x)}{\Gamma(x)} . \]

For integer \( n \) the following formula follows from the recurrence formula:
\[ \Gamma(n + z) = \Gamma(1 + (n - 1 + z)) = (n - 1 + z)(n - 2 + z) \cdots (1 + z)z \Gamma(z) . \]

For purely imaginary \( z = iy \) we find
\[ \Gamma(n + iy) = (n - 1 + iy)(n - 2 + iy) \cdots (1 + iy)iy \Gamma(iy) . \]

The gamma function of a purely imaginary argument can be obtained by specialization of the argument \( x + iy \) to \( x = 0 \) in \( \Gamma(x + iy) \) to yield
\[ \Gamma(iy) = (\sin \theta - i \cos \theta) \sqrt{\frac{\pi}{y \sinh y}} , \]
with
\[ \theta = -\gamma y + \sum_{j=1}^{\infty} \left[ \frac{y}{j} - \arctan \frac{y}{j} \right] , \]
where Euler’s constant \( \gamma \) is given by
\[ \gamma = -\psi(1) = \lim_{n \to \infty} \left( \sum_{k=1}^{n-1} \frac{1}{k} - \ln n \right) = 0.5772156649 \ldots . \]
Fig.E.1. Real part (top) and imaginary part (bottom) of $\Gamma(z)$ over the complex $z$ plane.
Fig. E.2. The functions $\Gamma(x)$ and $1/\Gamma(x)$ for real arguments $x$. 
Fig. E.3. Real and imaginary parts of the gamma function for purely imaginary arguments.
F. Bessel Functions and Airy Functions

Bessel’s differential equation

\[ x^2 \frac{d^2 Z_\nu(x)}{dx^2} + x \frac{dZ_\nu(x)}{dx} + (x^2 - \nu^2)Z_\nu(x) = 0 \]

is solved by the Bessel functions of the first kind \( J_\nu(x) \), of the second kind (also called Neumann functions) \( N_\nu(x) \), and of the third kind (also called Hankel functions) \( H^{(1)}_\nu(x) \) and \( H^{(2)}_\nu(x) \) which are complex linear combinations of the former two. The Bessel functions of the first kind are

\[ J_\nu(x) = \left( \frac{x}{2} \right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(\nu+k+1)} \left( \frac{x^2}{4} \right)^k \]

where \( \Gamma(z) \) is Euler’s gamma function.

The Bessel functions of the second kind are

\[ N_\nu(x) = \frac{1}{\sin \nu \pi} [J_\nu(x) \cos \nu \pi - J_{-\nu}(x)] \]

For integer \( \nu = n \) one has

\[ J_{-n}(x) = (-1)^n J_n(x) \]

The modified Bessel functions are defined as

\[ I_\nu(x) = \left( \frac{x}{2} \right)^\nu \sum_{k=0}^{\infty} \frac{1}{k!\Gamma(\nu+k+1)} \left( \frac{x^2}{4} \right)^k \]

The Hankel functions are defined by

\[ H^{(1)}_\nu(x) = J_\nu(x) + iN_\nu(x) \]

\[ H^{(2)}_\nu(x) = J_\nu(x) - iN_\nu(x) \]

The following relations hold for the connections of the functions just discussed and the spherical Bessel, Neumann, and Hankel functions, cf. Section 10.8. The spherical Bessel functions of the first kind are
The spherical Bessel functions of the second kind (also called spherical Neumann functions) are given by
\[ n_\ell(x) = -\sqrt{\frac{\pi}{2x}} N_{\ell+1/2}(x) = (-1)^\ell j_{-\ell-1}(x) , \]
and the spherical Bessel functions of the third kind (also called spherical Hankel functions of the first and second kind) are
\[ h_\ell^{(+)}(x) = n_\ell(x) + ij_\ell(x) = i[j_\ell(x) - in_\ell(x)] = i\sqrt{\frac{\pi}{2x}} H_{\ell+1/2}^{(1)}(x) , \]
\[ h_\ell^{(-)}(x) = n_\ell(x) - ij_\ell(x) = -i[j_\ell(x) + in_\ell(x)] = -i\sqrt{\frac{\pi}{2x}} H_{\ell+1/2}^{(2)}(x) . \]

In Figures F.1 and F.2 we show the functions \( J_\nu(x) \) and \( I_\nu(x) \) for \( \nu = -1, -2/3, -1/3, \ldots, 11/3 \). The features of these functions are simple to describe for \( \nu \geq 0 \). The functions \( J_\nu(x) \) oscillate around zero with an amplitude that decreases with increasing \( x \), whereas the functions \( I_\nu(x) \) increase monotonically with \( x \). At \( x = 0 \) we find \( J_\nu(0) = I_\nu(0) = 0 \) for \( \nu > 0 \). Only for \( \nu = 0 \) we have \( J_0(0) = I_0(0) = 1 \). For \( \nu > 1 \) there is a region near \( x = 0 \) in which the functions essentially vanish. The size of this region increases with increasing index \( \nu \). For negative values of the index \( \nu \) the functions may become very large near \( x = 0 \).

Closely related to the Bessel functions are the Airy functions \( \text{Ai}(x) \) and \( \text{Bi}(x) \). They are solutions of the differential equation
\[ \left( \frac{d^2}{dx^2} - x \right) f(x) = 0 \]
and are given by
\[
\text{Ai}(x) = \begin{cases} 
\frac{1}{3} \sqrt{x} \left\{ I_{-1/3} \left( \frac{2}{3} x^{3/2} \right) \right. & - I_{1/3} \left( \frac{2}{3} x^{3/2} \right) \right\} , & \text{for} \ x > 0 \\
\frac{1}{3} \sqrt{x} \left\{ J_{-1/3} \left( \frac{2}{3} |x|^{3/2} \right) \right. & + J_{1/3} \left( \frac{2}{3} |x|^{3/2} \right) \right\} , & \text{for} \ x < 0
\end{cases},
\]
and
\[
\text{Bi}(x) = \begin{cases} 
\sqrt{\frac{x}{3}} \left\{ I_{-1/3} \left( \frac{2}{3} x^{3/2} \right) \right. & + I_{1/3} \left( \frac{2}{3} x^{3/2} \right) \right\} , & \text{for} \ x > 0 \\
\sqrt{\frac{x}{3}} \left\{ J_{-1/3} \left( \frac{2}{3} |x|^{3/2} \right) \right. & - J_{1/3} \left( \frac{2}{3} |x|^{3/2} \right) \right\} , & \text{for} \ x < 0
\end{cases}.
\]

Graphs of these functions are shown in Figure F.3. Both functions oscillate for \( x < 0 \). The wavelength of the oscillation decreases with decreasing \( x \). For \( x > 0 \) the function \( \text{Ai}(x) \) drops fast to zero whereas \( \text{Bi}(x) \) diverges.
Fig. F.1. Bessel functions $J_\nu(x)$. 

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Fig. E.2. Modified Bessel functions $I_\nu(x)$. 
Fig. F.3. Airy functions \( \text{Ai}(x) \) and \( \text{Bi}(x) \).
In Section 3.3 we first introduced the probability density $\rho(x)$, which is normalized to one,

$$\int_{-\infty}^{+\infty} \rho(x) \, dx = 1$$

We also introduced the concepts of the expectation value of $x$,

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x) \, dx$$

and of the variance of $x$,

$$\text{var}(x) = \sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle$$

We now replace the continuous variable $x$ by the discrete variable $k$ which can assume only certain discrete values, e.g., $k = 0, 1, 2, \ldots$. In a statistical process the variable $k$ is assumed with the probability $P(k)$. The total probability is normalized to one,

$$\sum_k P(k) = 1$$

where the summation is performed over all possible values of $k$.

The average value, mean value, or expectation value of $k$ is

$$\langle k \rangle = \sum_k k P(k)$$

and the variance of $k$ is

$$\text{var}(k) = \sigma_k^2 = \langle (k - \langle k \rangle)^2 \rangle = \sum_k (k - \langle k \rangle)^2 P(k)$$

The simplest case is that of an alternative. The variable only takes the values

$$\kappa = 0, 1$$

The process yields with probability $p = P(1)$ the result $\kappa = 1$ and with probability $P(0) = 1 - p$ the result $\kappa = 0$. Therefore, the expectation value of $\kappa$ is

$$\langle \kappa \rangle = 0 \cdot (1 - p) + 1 \cdot p = p$$
We now consider a process which is a sequence of $n$ independent alternatives each yielding the result $\kappa_i = 0, 1$, $i = 1, 2, \ldots, n$. We characterize the result of the process by the variable

$$k = \sum_{i=1}^{n} \kappa_i,$$

which has the range

$$k = 0, 1, \ldots, n.$$

A given process yields the result $k$ if $\kappa_i = 1$ for $k$ of the $n$ alternatives and $\kappa_i = 0$ for $(n - k)$ alternatives. The probability for the sequence

$$\kappa_1 = \kappa_2 = \cdots = \kappa_k = 1, \quad \kappa_{k+1} = \cdots = \kappa_n = 0$$

is $p^k (1 - p)^{n-k}$. But this is only one particular sequence leading to the result $k$. In total there are

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

such sequences where

$$n! = 1 \cdot 2 \cdot 3 \cdot \ldots \cdot n, \quad 0! = 1! = 1.$$

Therefore, the probability that our process yields the result $k$ is

$$P(k) = \binom{n}{k} p^k (1 - p)^{n-k}.$$

This is the binomial probability distribution. The expectation value can be computed by introducing $P(k)$ into the definition of $\langle k \rangle$ or, even simpler, from

$$\langle k \rangle = \sum_{i=1}^{n} \langle \kappa_i \rangle = np.$$

In Figure G.1 we show the probabilities $P(k)$ for various values of $n$ but for a fixed value of the product $\lambda = np$. The distribution changes drastically for small values of $n$ but seems to approach a limiting distribution for very large $n$. Indeed, we can write

$$P(k) = \frac{n!}{k!(n-k)!} \left(\frac{\lambda}{n}\right)^k \frac{(1 - \frac{\lambda}{n})^n}{(1 - \frac{\lambda}{n})^k}.$$
Fig. G.1. Binomial distributions for various values of $n$ but fixed product $np = 3$.

\[
\begin{align*}
\frac{\lambda^k}{k!} \left( 1 - \frac{\lambda}{n} \right)^n \frac{n(n-1) \cdots (n-k+1)}{n^k (1 - \frac{\lambda}{n})^k} \\
&= \frac{\lambda^k}{k!} \left( 1 - \frac{\lambda}{n} \right)^n \left( \frac{1}{n} \right)^{k-1} \left( 1 - \frac{\lambda}{n} \right) \left( 1 - \frac{2}{n} \right) \cdots \left( 1 - \frac{k-1}{n} \right) \\
&= \frac{\lambda^k}{k!} \left( 1 - \frac{\lambda}{n} \right)^n \left( 1 - \frac{1}{n} \right)^{k-1} \left( 1 - \frac{2}{n} \right) \cdots \left( 1 - \frac{k-1}{n} \right) 
\end{align*}
\]

In the limit $n \to \infty$ every term in brackets in the last factor approaches one, and since

\[
\lim_{n \to \infty} \left( 1 - \frac{\lambda}{n} \right)^n = e^{-\lambda}
\]

we have

\[
P(k) = \frac{\lambda^k}{k!} e^{-\lambda}
\]

This is the Poisson probability distribution. It is shown for various values of the parameter $\lambda$ in Figure G.2. The expectation value of $k$ is

\[
\langle k \rangle = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} e^{-\lambda} = \sum_{k=1}^{\infty} \frac{\lambda^k}{k!} e^{-\lambda} = \sum_{k=1}^{\infty} \frac{\lambda^k (k-1)!}{(k-1)!} e^{-\lambda} = \lambda \sum_{j=0}^{\infty} \frac{\lambda^j}{j!} e^{-\lambda} = \lambda.
\]
In a similar way one finds
\[ \langle k^2 \rangle = \lambda (\lambda + 1) \]
and therefore, also the variance of \( k \) is equal to \( \lambda \),
\[
\text{var}(k) = \langle (k - \langle k \rangle)^2 \rangle = \langle k^2 - 2k \langle k \rangle + \langle k \rangle^2 \rangle \\
= \langle k^2 \rangle - 2\langle k \rangle^2 + \langle k \rangle^2 = \langle k^2 \rangle - \langle k \rangle^2 \\
= \lambda (\lambda + 1) - \lambda^2 = \lambda.
\]
The Poisson distribution is markedly asymmetric for small values of \( \lambda \). For large \( \lambda \), however, it becomes symmetric about its mean value \( \lambda \) and in that case its bell shape resembles that of the Gaussian distribution.
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<tr>
<td>$f(p)$</td>
<td>spectral function with respect to momentum</td>
</tr>
<tr>
<td>$f(\vartheta)$</td>
<td>scattering amplitude</td>
</tr>
<tr>
<td>$f_\ell$</td>
<td>partial scattering amplitude</td>
</tr>
<tr>
<td>$f_{\ell m}(\Theta, \Phi)$</td>
<td>directional distribution</td>
</tr>
<tr>
<td>$g$</td>
<td>gyromagnetic factor</td>
</tr>
<tr>
<td>$h$</td>
<td>Planck’s constant</td>
</tr>
<tr>
<td>$h = h/(2\pi)$</td>
<td>$P_\ell^m$</td>
</tr>
<tr>
<td>$h_\ell^{(+)}(\rho)$</td>
<td>spherical Hankel function of the first kind</td>
</tr>
<tr>
<td>$h_\ell^{(-)}(\rho)$</td>
<td>spherical Hankel function of the second kind</td>
</tr>
<tr>
<td>$\hat{r}$</td>
<td>position vector</td>
</tr>
</tbody>
</table>
\( R(r), R_{\ell}(k,r) \)  radial wave function    \( \eta_{\ell}(r) \)  scattered partial wave
\( R_{n\ell} \)  radial eigenfunction    \( \vartheta, \Theta \)  polar angle
\( s \)  spin quantum number    \( \vartheta \)  scattering angle
\( S = (S_1, S_2, S_3) \)  spin-vector operator    \( \lambda \)  wavelength
\( S_\ell \)  scattering-matrix element    \( \mu_0 \)  vacuum permeability
t    time    \( \mu \)  reduced mass
\( T \)  oscillation period    \( \mu \)  magnetic moment
\( T \)  transmission coefficient    \( \rho \)  probability density
\( T \)  kinetic energy    \( \rho^{\text{cl}} \)  classical phase-space probability density
\( T_T, T_R \)  transition-matrix elements
\( U \)  voltage    \( \sigma_0 \)  width of ground state of harmonic oscillator
\( v_0 \)  group velocity    \( \sigma_1, \sigma_2, \sigma_3 \)  Pauli matrices
\( v_p \)  phase velocity    \( \sigma_k \)  width in wave number
\( V \)  potential (energy)    \( \sigma_\ell \)  partial cross section
\( V_{\ell}^{\text{eff}} \)  effective potential    \( \sigma_p \)  width in momentum
\( w \)  average energy density    \( \sigma_x \)  width in position
\( W \)  Wigner distribution    \( \sigma_{\text{tot}} \)  total cross section
\( W_{\ell}, W_{\ell m} \)  coefficients in the angular decomposition of a wave packet    \( \varphi(x) \)  stationary wave function
\( x \)  position    \( \varphi_p(r) \)  stationary harmonic wave function
\( \langle x \rangle \)  position expectation value    \( \varphi \)  state vector of stationary state
\( Y_{\ell m} \)  spherical harmonic    \( \phi, \Phi \)  azimuthal angle
\( Z \)  atomic number    \( \chi \)  magnetic susceptibility
\( \alpha \)  fine-structure constant    \( \chi \)  general spin state
\( \delta_\ell \)  scattering phase shift    \( \psi(x,t) \)  time-dependent wave function
\( \Delta k \)  wave-number uncertainty    \( \psi_p(r,t) \)  harmonic wave function
\( \Delta p \)  momentum uncertainty    \( \psi \)  state vector
\( \Delta x \)  position uncertainty    \( \omega \)  angular frequency
\( \varepsilon_0 \)  vacuum permittivity    \( \Omega \)  solid angle
\( \eta_1, \eta_{-1} \)  spin \( \frac{1}{2} \) base states    \( \nabla \)  nabla (or del) operator
\( \eta_{k}(r) \)  scattered wave    \( \nabla^2 \)  Laplace operator
Basic Equations

de Broglie wave
\[ \psi_p(r, t) = \frac{1}{(2\pi \hbar)^{3/2}} \exp \left( -\frac{i}{\hbar} E t \right) \exp \left( \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right) \]

time-dependent Schrödinger equation
\[ \frac{i\hbar}{\partial t} \psi(r, t) = -\frac{\hbar^2}{2M} \nabla^2 + V(r) \psi(r, t) \]

stationary Schrödinger equation
\[ \left[ -\frac{\hbar^2}{2M} \nabla^2 + V(r) \right] \varphi_E(r) = E \varphi_E(r) \]

momentum operators
\[ \hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = \frac{\hbar}{i} \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = \frac{\hbar}{i} \nabla \]

angular-momentum operators
\[ \hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}} = \frac{\hbar}{i} \mathbf{r} \times \nabla \]

radial Schrödinger equation for spherically symmetric potential
\[ -\frac{\hbar^2}{2M} \left[ \frac{1}{r} \frac{d^2}{dr^2} r - \frac{\ell(\ell + 1)}{r^2} - \frac{2M}{\hbar^2} V(r) \right] R_\ell(k, r) = E R_\ell(k, r) \]

stationary scattering wave
\[ \varphi_k^{(+)}(r) \frac{kr \gg 1}{1} e^{ikr} + f(\vartheta) \frac{e^{ikr}}{r} \]

scattering amplitude
\[ f(\vartheta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell(k) P_\ell(\cos \vartheta) \]

differential, partial, and total cross sections
\[ \frac{d\sigma}{d\Omega} = \left| f(\vartheta) \right|^2, \quad \sigma_\ell = \frac{4\pi}{k^2} (2\ell + 1) \left| f_\ell(k) \right|^2, \quad \sigma_{\text{tot}} = \sum_{\ell=0}^{\infty} \sigma_\ell \]
Physical Constants

Planck’s constant  
\[ h = 4.136 \cdot 10^{-15} \text{ eVs} = 6.626 \cdot 10^{-34} \text{ Js} \]
\[ \bar{h} = \frac{h}{2\pi} = 6.582 \cdot 10^{-16} \text{ eVs} = 1.055 \cdot 10^{-34} \text{ Js} \]

speed of light  
\[ c = 2.998 \cdot 10^8 \text{ m s}^{-1} \]

elementary charge  
\[ e = 1.602 \cdot 10^{-19} \text{ C} \]

fine-structure constant  
\[ \alpha = \frac{e^2}{4\pi \varepsilon_0 \bar{h} c} = \frac{1}{137.036} \]

electron mass  
\[ m_e = 0.5110 \text{ MeV}/c^2 = 9.110 \cdot 10^{-31} \text{ kg} \]

proton mass  
\[ m_p = 938.3 \text{ MeV}/c^2 = 1.673 \cdot 10^{-27} \text{ kg} \]

neutron mass  
\[ m_n = 939.6 \text{ MeV}/c^2 = 1.675 \cdot 10^{-27} \text{ kg} \]

Conversion Factors

mass  
1 kg = 5.609 \cdot 10^{35} \text{ eV}/c^2,  
1 eV/c^2 = 1.783 \cdot 10^{-36} \text{ kg} 

energy  
1 J = 6.241 \cdot 10^{18} \text{ eV},  
1 eV = 1.602 \cdot 10^{-19} \text{ J} 

momentum  
1 kg \text{ m s}^{-1} = 1.871 \cdot 10^{27} \text{ eV}/c,  
1 eV/c = 5.345 \cdot 10^{-28} \text{ kg m s}^{-1}